



Institute for Advanced Computational Science

Robert J. Harrison, Director
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Agenda

Thursday, September 7

Time	Event	Speaker	Location
08:00-08:30 am	Coffee & Danish		IACS Seminar Room
08:30-08:45 am	Opening remarks	Provost Michael Bernstein	IACS Seminar Room
08:45-10:15 am	Review & Future Plans	Director Robert Harrison	IACS Seminar Room
10:15-10:30 am	Break		IACS Seminar Room
10:30-11:30 am	Faculty Presentations		IACS Seminar Room
11:30-12:45 pm	Sit-down Lunch w/ IACS Graduate Students		IACS Seminar Room
12:45-02:00 pm	Poster Session		IACS Seminar Room & Lobby
02:00-04:00 pm	Meetings w/ individual faculty		Faculty Offices
04:00-05:30 pm	Closed-Door Preliminary discussion for Committee and comments/questions for IACS Leadership Team		IACS Seminar Room
07:00 pm	Dinner, Fifth Season		

Agenda

Friday, September 8

Time	Event	Speaker	Location
08:00-08:30 am	Coffee & Danish		IACS Seminar Room
08:30-10:15 am	Student Presentations		IACS Seminar Room
10:15-10:30 am	Break		Faculty Offices
10:30-12:10 pm	Faculty Presentations		IACS Seminar Room
12:10-01:00 pm	Lunch with closed-door discussions		
01:00-01:30 pm	Close-out session	Board, Leadership team, Provost, Vice Provost	IACS Seminar Room
01:30 pm	Report writing	Board members only	IACS Seminar Room

Advisory Board Charge

- Review institute's plans, activities, and accomplishments of faculty and staff
- Make observations and recommendations directed toward ensuring the greatest success and impact of IACS
- Comment on format/content of AB meeting
- Provide feedback in a report that will be shared with the university leadership and the institute director, faculty and staff

Review Board Charge

- Review the activities and accomplishments of the institute and its faculty and staff over the past 5 years
- Make observations and recommendations directed toward ensuring the greatest success and impact of IACS
- Provide feedback in a report to the Provost that will be shared with the university leadership and the institute director, faculty, and staff

What is IACS?



- A multidisciplinary institute with a focus on computational and data science
- \$20M endowment to support 3 endowed chairs and operations (~\$13M)
- 13 core faculty, 35+ affiliate faculty, 100+ students with plans to grow to 16+ core and 150+ students
- Newly renovated space
 - ~6000 sq. ft., 17 faculty offices, 45 students
- Vision and mission to excel, lead and serve
- Education and research without walls

BNL Connections

- Strong coordination at multiple levels between SBU/IACS and BNL
 - BNL operated by BSA (consortium of SBU & Battelle)
 - Alliance in joint initiative in computation and data
 - Commitment to 10-20 joint hires with SBU over next 5-10 years with focus on computation and data
 - History of large joint projects with many joint appointments and fluid movement between institutions
 - RJH 50-50 appointment, at BNL founded and directed Center for Data Driven Discovery; is now chief computational scientist
 - BC 75-25 appointment, at BNL she is the Director for Computer Science & Mathematics

NYCCS

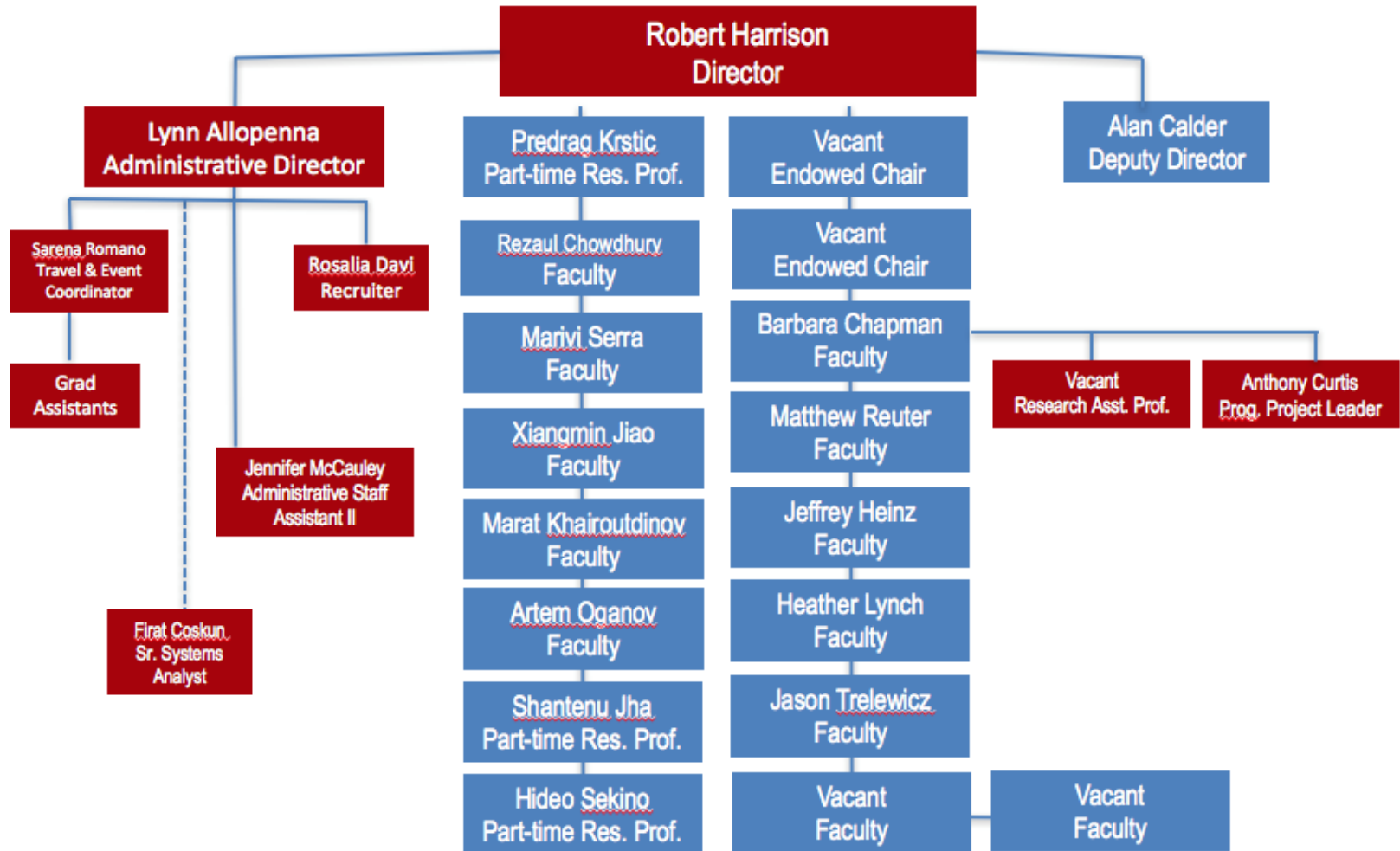
<http://www.bnl.gov/nyccs>



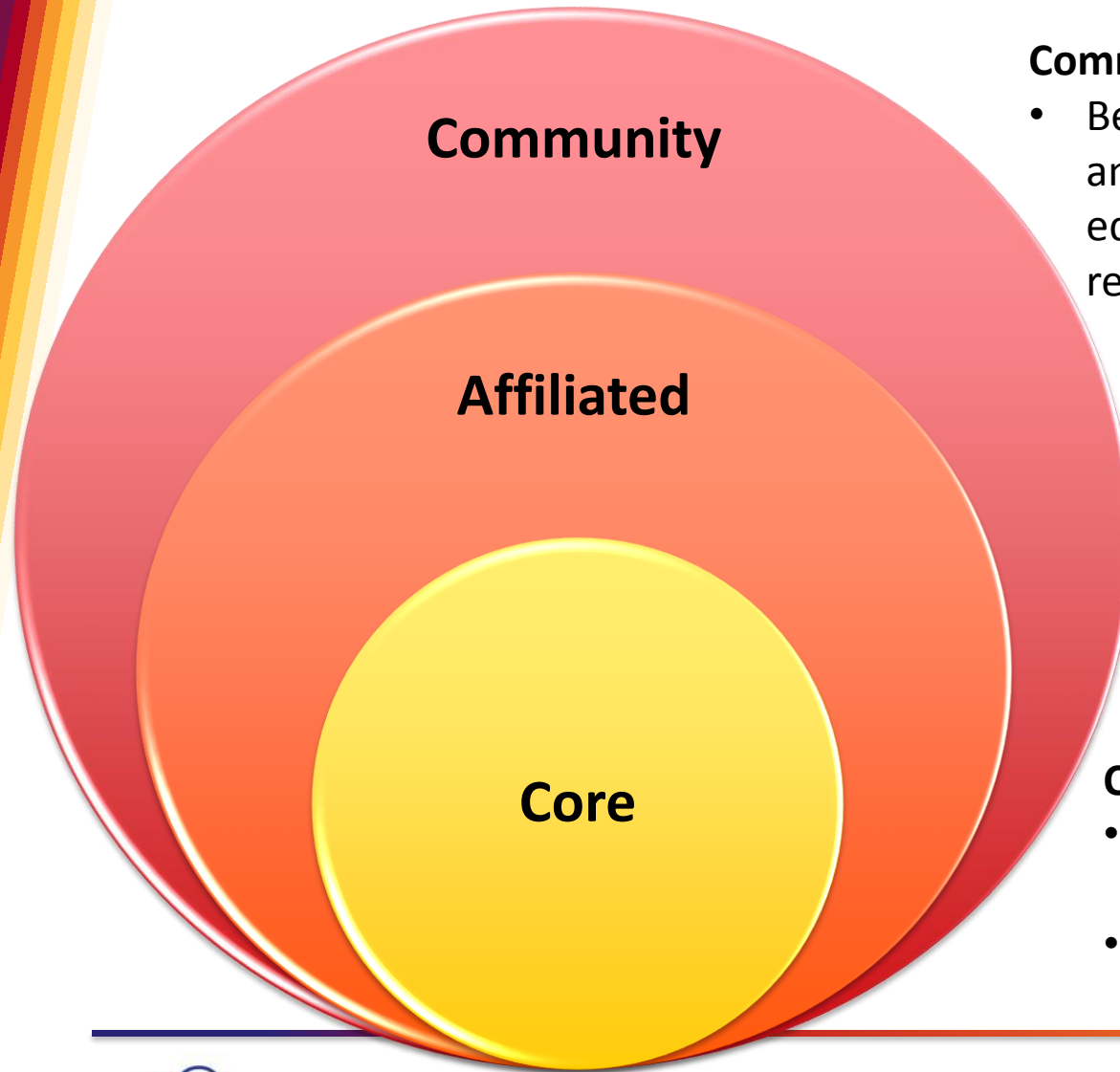
- The New York Center for Computational Sciences (NYCCS)
 - Umbrella HPC activity spanning BNL and SBU
 - The BNL high-performance computer center
 - Primary resource is now a ~700 TFLOP IBM BG Q
- At conception with funding by NY State
 - At SBU home to original faculty cluster hire in HPC
 - At BNL home to NY Blue, large IBM Blue Gen
 - To assist New York State industry in the utilization of
 - HPC to gain a competitive edge in product development and data management that translates into job creation, cost savings and job retention.



Currently hosts ~400 scientific and industrial users with ~130 projects over the last three years. Industrial partners include GE Energy Research, IBM, LIPA, NYISO, and Finanalytica



IACS Faculty and Community



Community

- Benefiting from our institutional and intellectual leadership, education and training, shared resources, and online materials

Affiliated faculty & students

- Collaborators and strategic partners
- Have full access to IACS resources and student awards/fellowships

Core faculty and students

- Faculty have 50% appointment in IACS with MOU
- Fundamentals and applications of computational science

IACS Core Faculty - I

- Alan Calder (astro. phys.)
Deputy Director



- Barbara Chapman (comp.sci.)

- Rezaul Chowdhury (comp. sci.)



- Marivi Fernández-Serra (cond. matt.)



IACS Core Faculty - II

- Robert J. Harrison (chemistry)
Director



- Jeffrey Heinz
(linguistics)



- Xiangmin Jiao (app. math.)



IACS Core Faculty - III

- Marat Khairoutdinov (atmos. Sci.)



- Predrag Krstić
(IACS)



- Heather Lynch (Ecology & Evolution)



IACS Core Faculty - IV

- Artem Oganov (materials)



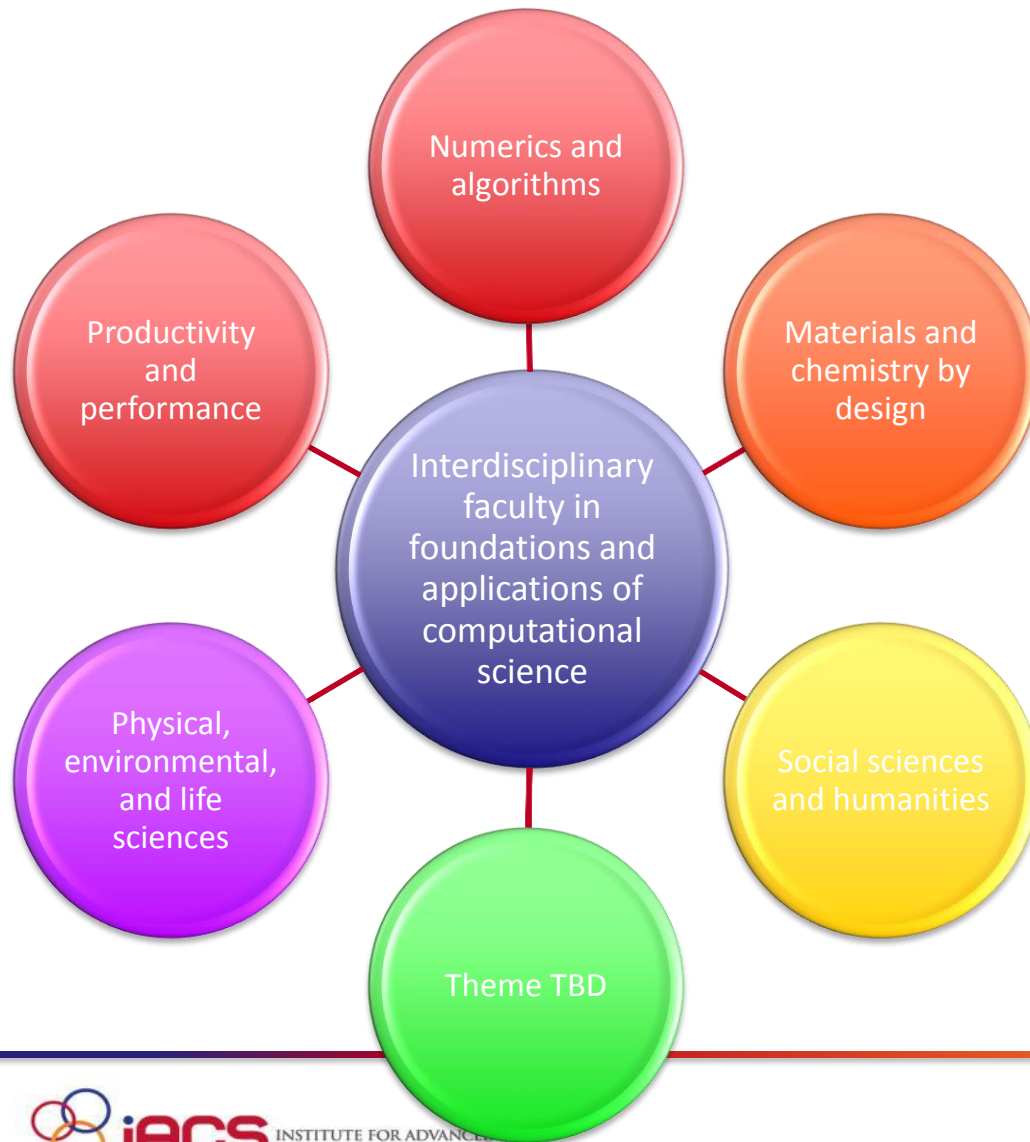
- Matt Reuter (math/chem. phys.)



- Jason Trelewicz (materials)



IACS Research Themes



Numerics and algorithms:

Jiao, Chowdhury, Harrison, (all)

Materials and chemistry by design:

Fernández-Serra, Oganov, Krstić, Harrison, Reuter, Trelewicz

Social sciences and humanities:

Heinz, van de Rijt (and affiliates)

Physical, env. and life sciences:

Calder, Fernández-Serra, Reuter, Khairoutdinov, Oganov, Krstić, Lynch, Trelewicz

Productivity and performance:

Chapman, Chowdhury, Harrison (all)

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 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;
- Grow our research programs and facilities, and establish regional, national and international partnerships with industry, government laboratories and academia.

Goals and Objectives

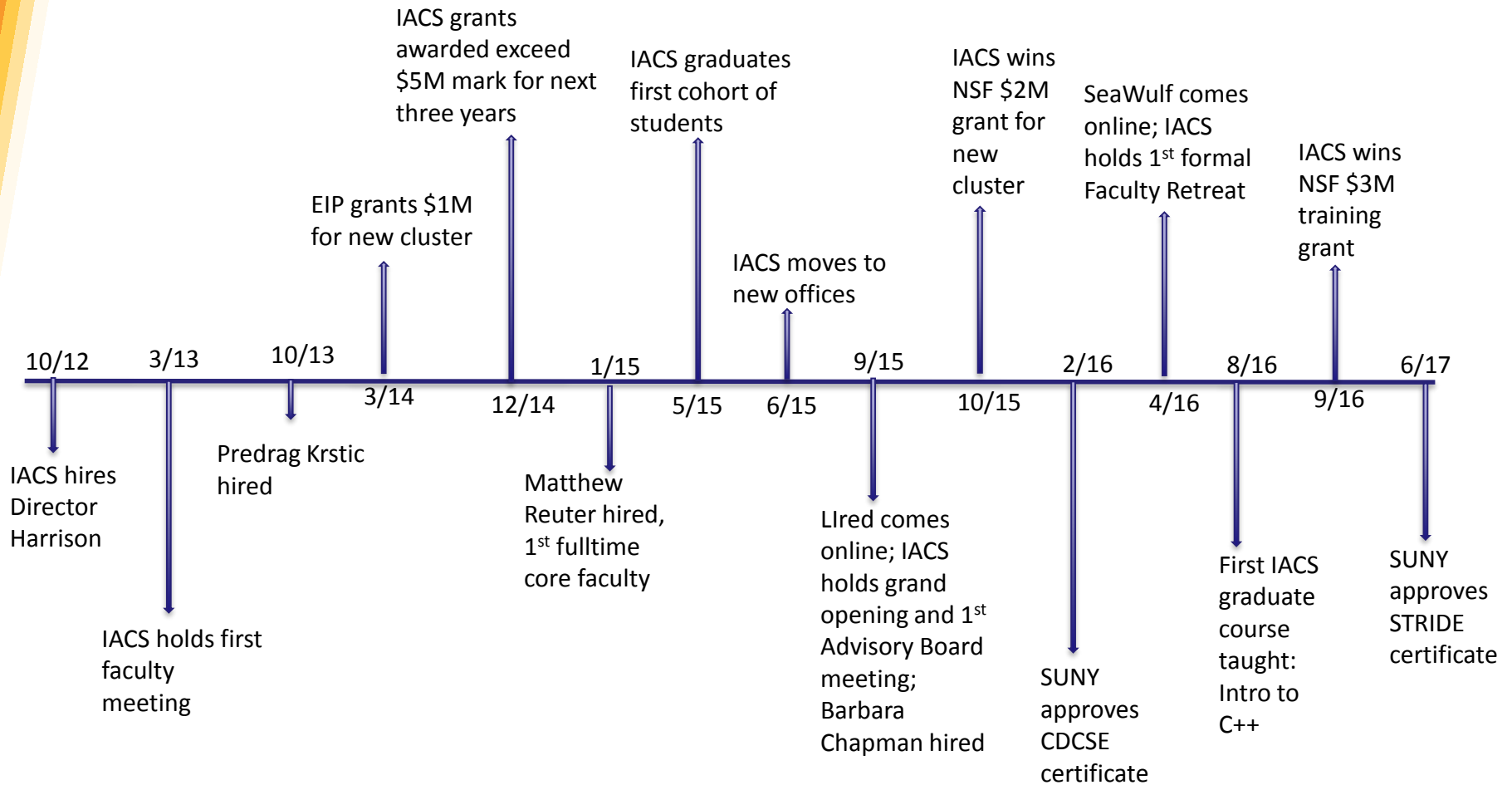
- Establish internationally recognized research and education programs in data and computing
- Grow IACS research funding and funding across SBU
- Provide leadership and benefit across SBU, SUNY and our local community
- Provide economic impact to the region and NYS

Key Performance Indicators

- Number and size of collaborative and interdisciplinary proposals and grants
- Total amount of external funding
- Where our graduates are getting jobs and their assessment of success and IACS
- Number and economic impact of projects with industry
- Utilization of our computer clusters (# users, % utilization, etc.)
- Number and impact of research papers published, patents, etc.
- Increase in caliber and diversity of graduate applicants
- (Recruiting at all levels, but especially the endowed chairs)

Five Years in Review

IACS Timeline



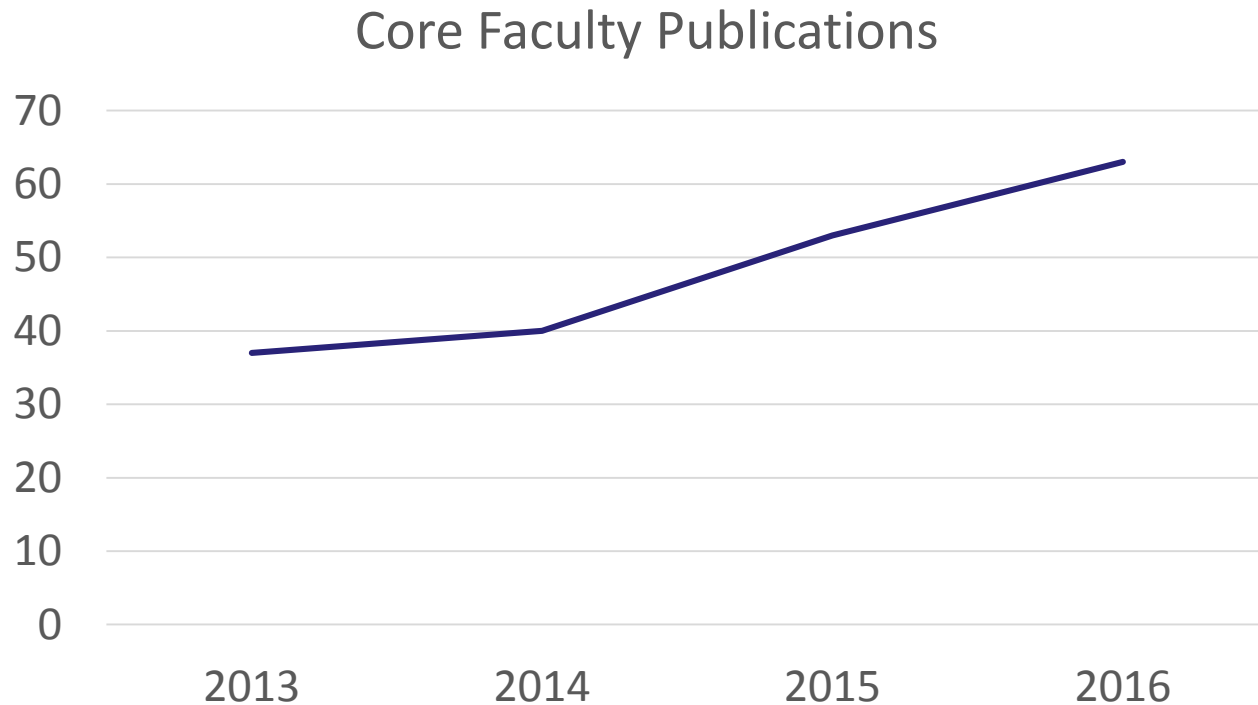
IACS Space Before and after



KPI: IACS Core Faculty Publications

	Calder	Chapman	Chowdhury	Serra	Harrison	Jiao	MK	Krstic	Oganov	Reuter	Total
2013	4		4	4	7		2	5	10		37
2014	2		3	3	3	1		5	24		40
2015	5	2	5	5	1	2	4	4	23	3	54
2016	7	1	6	9	2	4	1	6	25	2	63
2017	2		3	4				6	13	2	30

IACS Core Faculty Publications

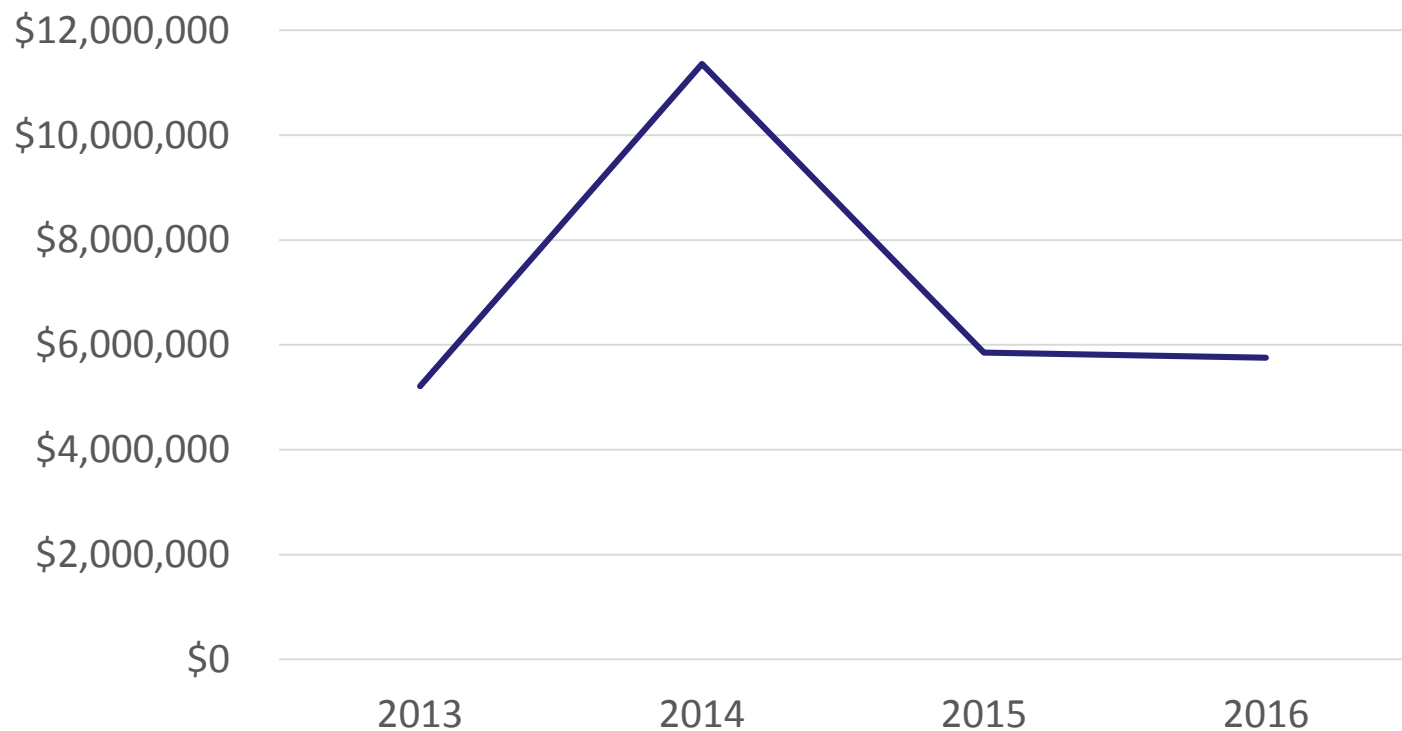


KPI: IACS Core Faculty Grants

	# grants submitted	\$ amount	# grants won	\$ amount
2013	40	\$14,431,375	18	\$5,210,366
2014	49	\$61,639,560	18	\$11,359,809
2015	31	\$22,190,383	13	\$5,849,564
2016	24	\$16,408,120	11	\$5,757,086
2017	22	\$20,021,706	8	\$2,242,539

IACS Core Faculty Grants

IACS Core Faculty Grants Won



KPI: Multidisciplinary Grants & Publications

	Interdisciplinary			Interdisciplinary	
	Grants			Publications	
2013	6		2013	3	
2014	7		2014	4	
2015	5		2015	5	
2016	4		2016	4	
2017	2		2017	2	
	24			18	

KPI: Recruiting

- Research Professor Predrag Krstic, IACS
- Assistant Professor Matthew Reuter, Applied Math & Statistics
- Professor Barbara Chapman, Applied Math & Statistics
- Professor Jeffrey Heinz, Linguistics
- Programming Project Leader Anthony Curtis
- Senior Systems Administrator Firat Coskun
- Senior Systems Administrator Eric Rosenberg
- Diversity Outreach Coordinator Rosalia Davi
- Travel and Event Coordinator Sarena Romano
- STRIDE Program Coordinator Jennifer McCauley

KPI: Recruiting

- Recruiting efforts continue for two endowed chairs; one is AMS, one in CS
 - Nine interviewed, two chair offers made, one hire at full professor level
- Recruiting efforts continue for junior positions and joint hires
 - 12 interviewed w/ CS, pharma, one offer, 3 informal offers, no hires
- Recruiting efforts continue for interdepartmental joint hires (including with BNL)
 - Three hired: Mat Sci, Linguistics, Ecology & Evolution

KPI: Alumni

- Assistant Professor of Mathematics, St. Peter's University, NJ
- Postdoctoral Associate, University of Maryland
- Founder & CEO, Learning is Beautiful
- Postdoctoral Associate, Michigan State University
- Solutions Architect, NVIDIA
- Research Scientist, Google
- HPC Software Architect, Intel Corporation
- Technical Staff, Vmware
- Senior R&D Engineer, Synopsys Inc.
- Software Development Engineer, Amazon.com Inc.

KPI: Diversity

SBU as a whole

- Graduate students
 - Female 55.8%
 - Hispanic: 9.6%
 - African American: 7.9%
 - Asian: 13.7%
 - White: 45.1%
- Faculty
 - Female 30.2%
 - Hispanic: 3.9%
 - African American: 2.6%
 - Asian: 13.7%
 - White: 69%

IACS

- Graduate students (core 2016)
 - Female: 30%
 - Hispanic/Latino: 6.8%
 - African American: 3.4%
 - Asian: 13.7%
 - White: 75.8%
- Faculty (core 2017)
 - Female: 23.1%
 - Hispanic: 0%
 - African American: 0%
 - Asian: 15.4%
 - White: 84.6%

STRIDE participating programs diversity and graduation stats

Years to doctoral degree for selected discipline for students graduating in the given year

Department	2010-11			2011-12			2012-13			2013-14		
	Minority	Women	Total	Minority	Women	Total	Minority	Women	Total	Minority	Women	Total
App. Math.	5.1 (2)	4.3 (8)	5.2 (20)	6.3 (1)	3.4 (8)	4.7 (23)	* (0)	4.8 (8)	5.0 (25)	* (0)	5.1 (7)	4.3 (26)
Comp. Sci.	* (0)	6.1 (3)	7.0 (13)	* (0)	4.0 (1)	5.0 (7)	6.0 (1)	6.3 (1)	5.6 (18)	* (0)	5.7 (2)	5.6 (15)
Ecol & Evol.	* (0)	6.3 (4)	6.6 (5)	* (0)	6.3 (1)	5.8 (4)	7.0 (2)	6.2 (6)	6.4 (11)	* (0)	6.3 (1)	6.3 (3)
Sociology	7.0 (1)	8.9 (2)	7.3 (7)	* (0)	7.1 (3)	8.1 (4)	* (0)	* (0)	6.8 (2)	* (0)	8.5 (4)	9.1 (6)
SoMAS	* (0)	6.1 (7)	5.9 (12)	8.3 (1)	7.1 (6)	6.6 (9)	* (0)	7.4 (8)	7.1 (12)	* (0)	6.0 (4)	6.0 (7)

Each cell contains years to graduation with number graduating in parenthesis.

Recruitment, graduation and retention rates for doctoral degree

	Fall of entry																	
	2010			2011			2012			2013			2014			2015		
	6th year			5th year			4th year			3rd year			2nd year			1st year		
	U	F	T	U	F	T	U	F	T	U	F	T	U	F	T	U	F	T
Appl. Math.																		
<i>N</i> apply	3	91	214	4	84	229	4	61	184	4	68	211	4	66	194	3	58	176
<i>Enroll%</i>	67%	13%	18%	0%	14%	15%	0%	20%	15%	0%	20%	10%	25%	15%	18%	0%	10%	14%
<i>N</i>	3	19	50	0	14	47	1	19	42	0	7	30	1	13	47	0	6	24
<i>Grad%</i>	0%	16%	12%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
<i>Ret+Grad%</i>	0%	74%	64%	0%	64%	70%	100%	95%	86%	0%	86%	97%	0%	0%	0%	100%	100%	100%
Comp. Sci.																		
<i>N</i> apply	1	68	365	1	78	364	0	71	308	2	57	289	3	55	261	3	85	313
<i>Enroll%</i>	100%	6%	8%	0%	3%	8%	0%	10%	7%	0%	7%	11%	33%	18%	20%	0%	12%	13%
<i>N</i>	1	7	39	0	2	29	0	8	21	1	5	37	2	10	54	0	10	41
<i>Grad%</i>	0%	0%	3%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
<i>Ret+Grad%</i>	0%	86%	70%	0%	100%	66%	0%	38%	57%	100%	80%	95%	100%	100%	100%	100%	100%	100%
Ecol/Evol																		
<i>N</i> apply	4	27	53	3	27	54	3	38	66	3	25	46	5	22	44	5	15	34
<i>Enroll%</i>	25%	7%	6%	33%	15%	17%	33%	13%	15%	0%	32%	26%	20%	18%	18%	0%	0%	15%
<i>N</i>	1	2	3	0	3	8	0	5	8	0	5	9	1	4	8	0	0	5
<i>Grad%</i>	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
<i>Ret+Grad%</i>	0%	100%	67%	0%	67%	63%	100%	100%	100%	100%	100%	100%	100%	100%	100%	100%	100%	100%
SoMAS																		
<i>N</i> apply	2	36	72	2	48	72	1	50	96	0	44	84	2	42	78	3	41	69
<i>Enroll%</i>	0%	17%	17%	0%	27%	25%	0%	14%	15%	0%	23%	21%	50%	19%	18%	33%	10%	16%
<i>N</i>	1	8	15	0	14	19	0	9	17	3	11	19	2	10	17	1	4	11
<i>Grad%</i>	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
<i>Ret+Grad%</i>	0%	100%	93%	0%	57%	58%	0%	89%	94%	33%	73%	79%	100%	100%	100%	100%	100%	100%

U – underrepresented minority

F – Female

T – Total

*N*apply – number of applications

N – number of Ph.D. students enrolled that year from any source

Enrollment rate computed as fraction of applicants of the same category that are enrolled at any point in the future

IACS Computer Resources



- Handy – startup funds
 - 40 dual-socket Sandybridge nodes, 2 NVIDIA K20 GPUs, 2 Intel KNC, 250 TB disk
- LI-red – \$1M grant from regional economic development council
 - 100 dual-socket Haswell nodes, 250 TB disk
 - 1 quad-socket Haswell node with 3 TB memory
 - 1 IBM Power8 node
- Two Intel KNL development systems
- Sea-wulf – \$1.4M NSF MRI + \$300 NYSTAR + \$300 SBU internal including \$67K from IACS
 - 160+ dual-socket Haswell nodes, 1PB disk, 32 NVIDIA K80 GPUs
- Seed institutional approach to computing – more later

KPI: Cluster Usage

Total Users = 515

CLASSES TAUGHT USING CLUSTERS (188 additional, temporary users)

BIO 303 Advanced Human Genetics (32)
BS 3910 Introduction to Bioinformatics (taught at SUNY Old Westbury) (3)
CSE 590 Topics in Computer Science (6)
CSE 628 Natural Language Processing (60)
EST 508 Project in Global Operations Management (16)
AMS 530 Principals in Parallel Computing (17)
AMS 536 Molecular Modeling of Biological Molecules (4)
AMS 562 Introduction to Scientific Programming in C++ (20)
AMS 598 Big Data Analysis (20)
AMS 487 Data + Computing + Discovery REU (10)

KPI: Cluster Usage

On-campus users

Applied Mathematics & Statistics; Biochemistry & Cell Biology; Biomedical Engineering; Biomedical Informatics; Cancer Center; Chemistry; Civil Engineering; Computer Science; Ecology & Evolution; Economics; Geosciences, Institute for Advanced Computational Science; Institute for Theoretical Physics; Laufer Center for Physical and Quantitative Biology; Linguistics; Materials Science; Mechanical Engineering; Medicine; Neurobiology & Behavior; Neurology; Pharmacology; Physics; Political Science; Psychology; Radiation Oncology; Sociology; School of Marine & Atmospheric Sciences; and Technology & Society.

External users

University of Texas, SUNY Old Westbury, Oak Ridge National Laboratory, University of Tennessee Knoxville, Brookhaven National Laboratory, University of California Berkeley, St. John's University, The Ohio State University, Virginia Tech, Arctic University of Norway, Michigan State University, Los Alamos National Laboratory, University of Colorado Boulder, Comenius University in Bratislava, Texas Tech University, Humboldt-University Berlin, University in Tromsø, Toyohashi University of Technology, University of Alabama, University of Minnesota, University of Arkansas, Cornell University, and Universidad Metropolitana.



Institute for Discovery and Innovation in Medicine & Engineering (I-DIME)



An economic engine and resource for the entire state with special focus on LI-region industries and institutions

Co-locate industry staff, and staff/faculty from SBU, BNL, CSHL and other LI research institutions
Access for both private industry and public research

70,000 gross sq. ft. building, SBU R&D Park
150 new and 30 retained jobs
\$200M over 5 years, including external funding
resulting in a 2:1 match

Design: \$7M
Construction: \$48M
Core computer infrastructure: \$12M
Power Upgrades: \$8M

Self-sustaining rental income average more than \$5M over five years of operation
Cutting-edge research into brain chips, next-generation drug development, new frontiers in precision-directed cancer treatment

CDCSE Certificate

Graduate Certificate in Data and Computing for Scientists and Engineers (CDCSE)

Purpose:

CDCSE will prepare students for successful research careers that develop, interpret or apply advanced computational and data-centric techniques in their field of study. CDCSE will provide essential skills and foundational knowledge in programming, data-science and modern computer science and applied mathematics, and will enable them to communicate effectively across this intrinsically multidisciplinary field.

Status:

Application in State Education Department awaiting final approval.
First class fully registered at 20 maximum enrollment in fall 2016

CDCSE Certificate

17 credits in four years

95-course catalog:

✧ 3 core courses

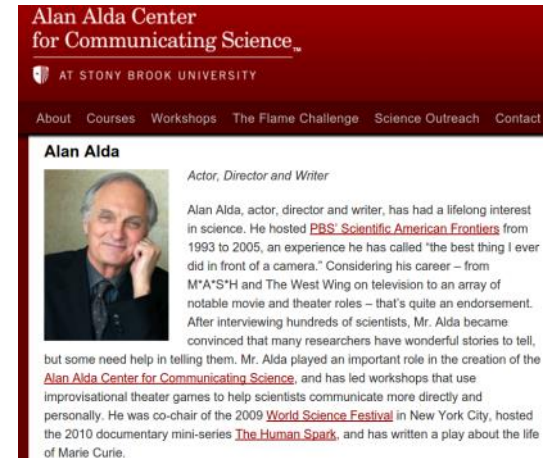
JRN 501 Distilling Your Message

JRN 503 Improvisation for Scientists


AMS 561 Intro to Computational Science

✧ 32 on-ramp, introductory courses

✧ 60 general courses



STRIDE



STRIDE

Stony Brook University and the Institute for Advanced Computational Science invite students to take part in STRIDE: Science Training and Research to Inform DEcisions.

Within all sectors of industry and government, effective decision making depends on the ability of scientists to interpret data and communicate results in a way that supports the decision-making process. Learn how to communicate your research to the policy makers; understand the perspectives of stakeholders; and translate scientific uncertainty into action.

Science Training and Research to Inform DEcisions

Science Training & Research to Inform DEcisions (STRIDE)

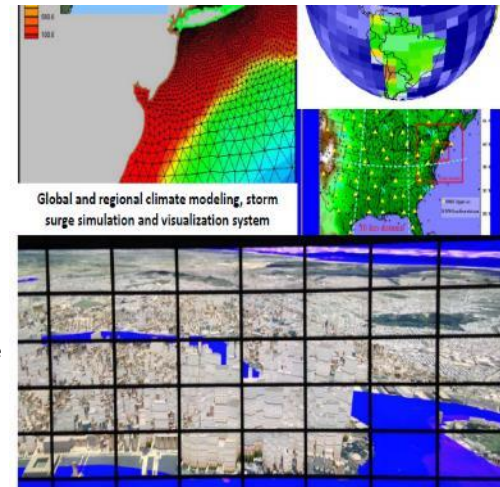
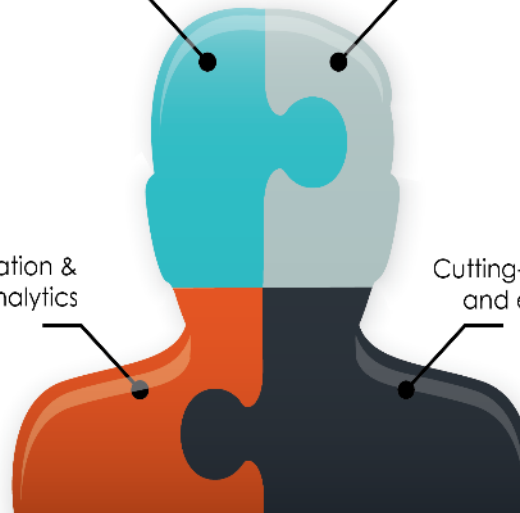


Understanding decision
maker requirements

Science communication

Visualization &
Data analytics

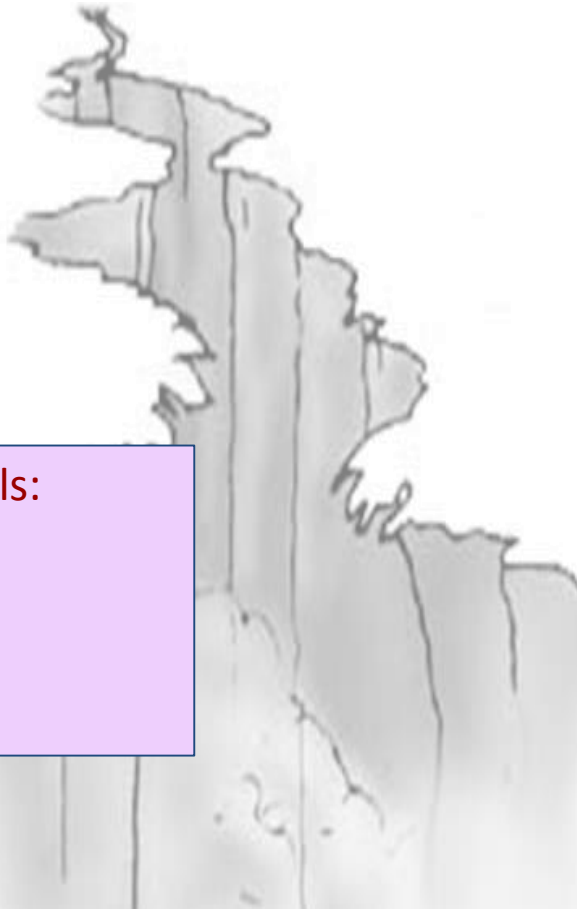
Cutting-edge science
and engineering



Vertically-integrated graduate training:

- Connects scientific and computational research to decision support
- Prepares students for high-impact careers across the spectrum of academic, industrial, government, and non-profit settings
- Connects science to real-world applications

Science Training & Research to Inform DEcisions (STRIDE)

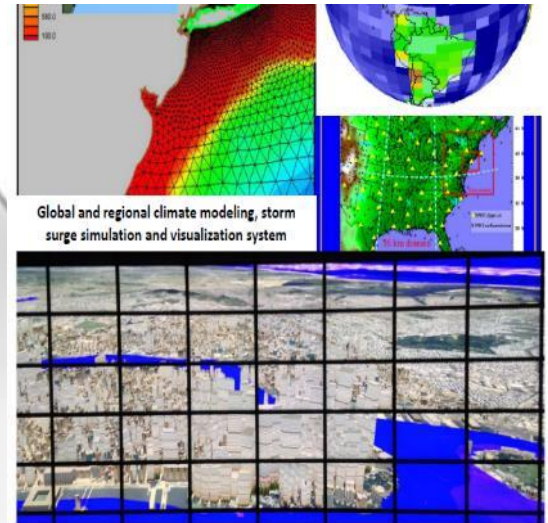


“data-focused” skills:

- modeling
- statistics
- computation
- visualization

“people- and policy-focused” skills:

- negotiation
- stakeholder engagement
- expert elicitation
- energy/environmental policy



Decision-making often requires a rapid response ➤ Need experts that straddle the traditional divide between data-science and policy

Research Themes



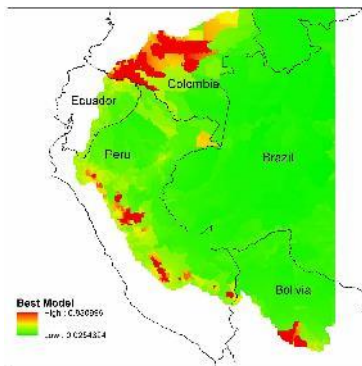
Climate Change and Coastal Resilience



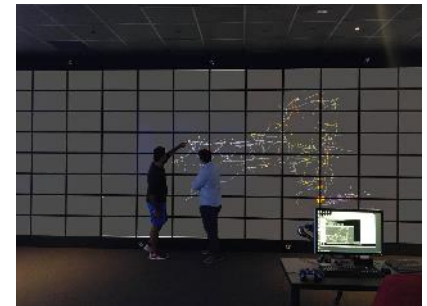
Marine Resource Management



Tracking and Targeting Illegal Deforestation



Powering the Smart Grid Through Data Infrastructure



STRIDE Advanced Graduate Certificate



Course Title	Credits	Course Title	Credits
JRN 503: Improvisation for Scientists	1	Policy or applied science elective	3
Statistics course	3	JRN 511: Scientific Communication for Decision Makers	1
MAR 534: Scientific Decision	1	CSE 564: Visualization	3
JRN 501: Distilling Your Message	1	Seminar electives, Environment or Energy	2
Total required credits: 15			

- To be eligible for the certificate program students
 - must be enrolled in a participating graduate program
 - must receive permission from the Graduate Program Director in home departments & STRIDE Graduate Certificate Director
- No prerequisite courses or minimum GPA required for students to enroll
- Certificate can be completed in two years, but students can take up to four years if needed; Program can be started in any year of a student's career as long as they complete all requirements of the certificate
- State approval of the certificate may take 1-2 years – students can start taking courses in advance (up to 12 credits)
- CS and AMS students are required to take one of their electives in a domain science

New Graduate Courses

- The following new interdisciplinary courses have been developed to support the certificates (with more to come):
- PHY 504: Computational Methods in Physics and Astrophysics – Taught Spring 2017 (12 Physics; 4 Geoscience; 2 Chemistry; 1 Materials Science; 3 Non-matriculated; Total 22)
- AMS 561: Intro to Computational Science – Taught Spring 2017(13 Applied Math; 2 Biology; 1 Cognitive Science; 2 Electrical Engineering; 5 Integrative Neuroscience; 3 Linguistics; 3 Marine and Atmospheric Science; 1 Molecular & Cellular Biology; 2 Psychology; 1 Sociology; 2 Tech & Society; Total 35)
- AMS 562: Intro to Scientific Programming in C++ – Taught Fall 2016(13 Applied Math; 2 Mechanical Engineering; 1 Political Science; 1 Biology; 2 Non-matriculated; Total 19)
- JRN 511: Scientific Communication to Decision Makers (not yet taught)
- MAR 534: Scientific Decision Support (not yet taught)

Past Year's Highlights

New IACS Core Faculty



Jeffrey Heinz
Linguistics



Heather Lynch
Ecology & Evolution



Jason Trelewicz
Materials Science

New IACS Affiliate Faculty



Francis Alexander
CSI @ BNL



Meifeng Lin
CSI @ BNL



Janet Nye
SOMAS



Christine
O'Connell
Journalism



Liliana Davalos
Ecology & Evolution

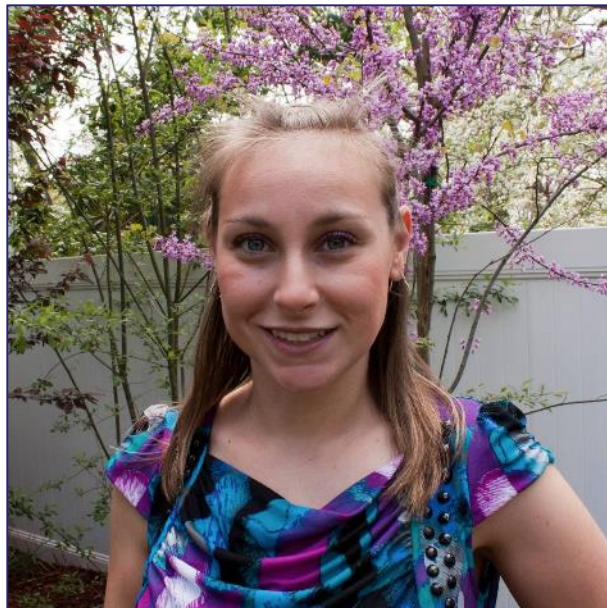


Robert Rizzo
AMS



Carlos Simmerling
Laufer Center

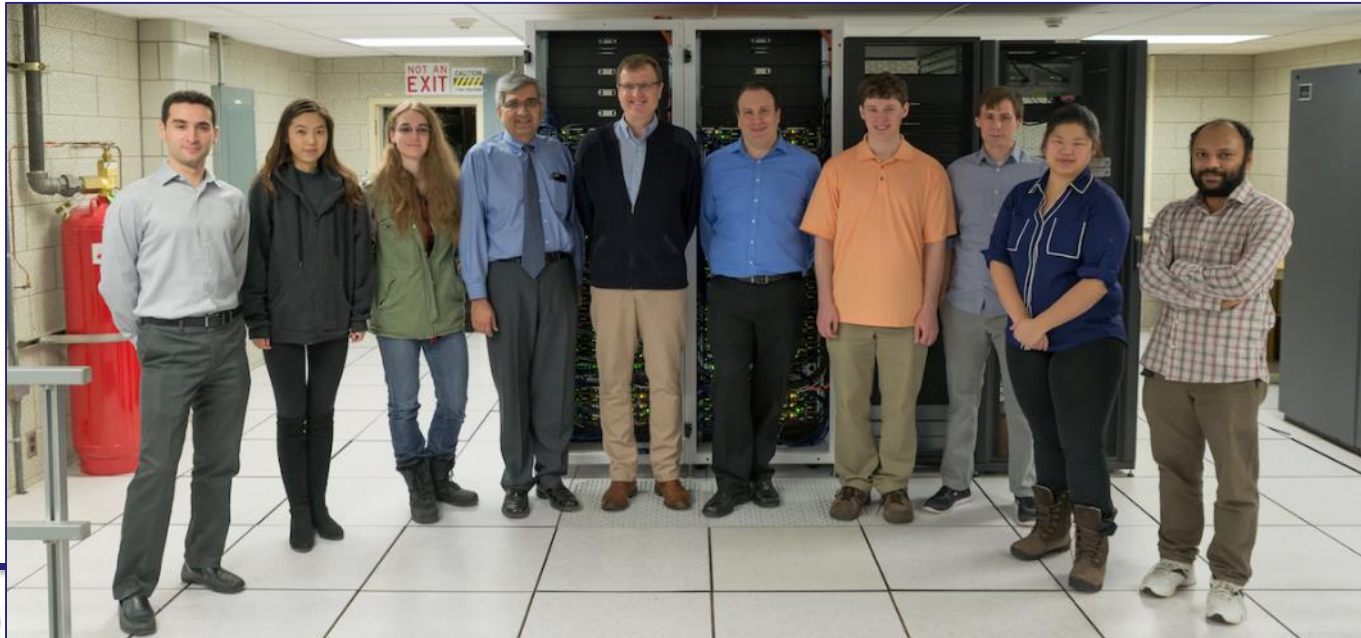
New staff



Jennifer McCauley
Administrative Staff Assistant II
STRIDE Program Coordinator

Research Computing Staff

Jointly funded by DoIT (Chief Information Officer) and IACS. To bootstrap research computing CIO is also supporting multiple graduate students to personalize service to HPC users across campus



Faculty Seminar Series

Speakers:

Valerio Pascucci
Dima Kozakov
Fadi Abdeljwad
Michael Zingale
Victoria Stodden
Christine O'Connell
Maria Klawe
Massimiliano Stengel
Shantenu Jha
Brenda Rubenstein
Kathleen Knobe
Carl Safina
Martin McCullagh
Ji Yin Cao
Joel Creswell
Kathryn Fullam
Elaine DeMasi
Bill Fagan
James Demmel

IMPLEMENTING REPRODUCIBLE COMPUTATIONALLY-ENABLED RESEARCH

VICTORIA STODDEN
UNIVERSITY OF ILLINOIS-URBANA-CHAMPAIGN



Imagine an entire research record for all major computations about the function, form,

HOW TO MAKE COMPACT WAVE FUNCTIONS ON THE CHEAP: STOCHASTIC VARIATIONAL ALGORITHMS FOR QUANTUM PHYSICS AND CHEMISTRY

BRENDA RUBENSTEIN
BROWN UNIVERSITY



Most modern computing platforms have necessary electronic structure codes that are variational. Quantum chemistry codes must have methods to handle the many-body problem.

DEVELOPING ACCURATE IMPLICIT SOLVENT MODELS FOR THE SIMULATION OF HYDROPHOBIC AGGREGATION

MARTIN MCCULLAGH
COLORADO STATE UNIVERSITY



Hydrophobic aggregation is a ubiquitous process in chemistry and biology that leads to important phenomena such as protein folding and assembly. Given an accurate Hamiltonian of a system that encompasses these phenomena, computational sampling techniques can be utilized to determine properties such as structure of the native state and folding kinetics. The standard Hamiltonian used to sample these systems contains the degrees of freedom of all solute and solvent particles and is referred to explicit solvent all-atom molecular dynamics. Unfortunately, protein folding and assembly happens at time and length scales that are unapproachable using this conventional technique. One way to overcome this limitation is to build the physics of the solvent into the Hamiltonian of the system. In this talk, I will explore the currently available versions of this technique, referred to as implicit solvation, and present a new approach that accurately captures hydrophobic aggregation. Our model, named IS-SPA, is specifically designed to capture the discrimination thermodynamics and kinetic aggregation of hydrophobic solutes in water. We further develop the IS-SPA sampling method to accurately capture the dynamics and thermodynamics of hydrophobic aggregation in large-scale processes such as hydrophobic coagulation.

Martin received his BS in Math and Chemistry from Emory University in Atlanta. Working under George C. Schatz at Northwestern University, Martin earned his PhD in Computational Chemical Chemistry, modeling how light transmission with DNA conjugation enables their photovoltaic devices. Moving on to an IBM postdoctoral fellowship at the University of Chicago with Gregory A. Voth, Martin worked on modeling energy landscapes in proteins using metadynamics techniques. He joined the faculty in the Chemistry Department at Colorado State University in 2014 where he has been working on modeling and assembly and energy transduction in bioelectronic systems.

FRI., APRIL 28TH
IACS BUILDING
SEMINAR RM | 2:30 PM

**INSTITUTE FOR ADVANCED
COMPUTATIONAL SCIENCE**

PH: 631-632-4629
FX: 631-632-4125

<http://www.iacs.stonybrook.edu>
iacs@stonybrook.edu



16 seminars held in CY 2015
24 seminars held in CY 2016
19 seminars planned for CY 2017

Student Seminar Series

New Student Seminar Series started in fall 2016, organized by the IACS Student Association

Students are offered a 'trial run' in front of their peers two days before presenting

13 student presentations given in fall 2016 - spring 2017

IACS STUDENT SEMINAR SERIES

AUTONOMOUS SATELLITE-BASED SURVEYS OF ANTARCTIC SEALS USING MULTI-SCALE CONVOLUTIONAL NEURAL NETWORKS

ABSTRACT
As animals pass in and out the frozen continent of Antarctica in the late spring, observers provide a wealth of data on the movement of the seals. Over 100 seals change up to 100 miles in a day, and the data they collect is complex, often noisy, and often incomplete. In this paper, we present a multi-scale convolutional neural network (CNN) that can automatically detect and track seals in satellite imagery. The network is trained on a large dataset of satellite imagery, and is able to detect seals in a variety of environments. The network is trained on a large dataset of satellite imagery, and is able to detect seals in a variety of environments. The network is trained on a large dataset of satellite imagery, and is able to detect seals in a variety of environments.

IACS STUDENT SEMINAR SERIES

UNCERTAINTY QUANTIFICATION AND SENSITIVITY ANALYSIS FOR INERTIAL CONFINEMENT FUSION SIMULATIONS

ABSTRACT
During the inertial confinement fusion (ICF) simulations, the results are used to study the physics of the fusion process. In this paper, we present a multi-scale convolutional neural network (CNN) that can automatically detect and track seals in satellite imagery. The network is trained on a large dataset of satellite imagery, and is able to detect seals in a variety of environments. The network is trained on a large dataset of satellite imagery, and is able to detect seals in a variety of environments.

IACS STUDENT SEMINAR SERIES

INTERCONNECT TOPOLOGY DISCOVERY BY COMPUTATIONAL CLUSTER EMULATION

WEDNESDAY, MAY 3RD 1:15-2:15 PM

INSTITUTE FOR ADVANCED COMPUTATIONAL SCIENCE
IACS Seminar Room
IACS BUILDING

PH: 631-632-4629 • FX: 631-632-4125
<http://www.iacs.tycho.brook.edu> • iacs@tycho.brook.edu

ABSTRACT
As animals pass in and out the frozen continent of Antarctica in the late spring, observers provide a wealth of data on the movement of the seals. Over 100 seals change up to 100 miles in a day, and the data they collect is complex, often noisy, and often incomplete. In this paper, we present a multi-scale convolutional neural network (CNN) that can automatically detect and track seals in satellite imagery. The network is trained on a large dataset of satellite imagery, and is able to detect seals in a variety of environments. The network is trained on a large dataset of satellite imagery, and is able to detect seals in a variety of environments.

BIOGRAPHY
William S. Brown is a Ph.D. student in the Applied Mathematics and Statistics Department at the University of Maryland, College Park. He is currently working on his thesis, which is titled "Uncertainty Quantification and Sensitivity Analysis for Inertial Confinement Fusion Simulations". He is also a member of the IACS Student Association.

ABSTRACT
Computers are getting smaller and smaller, while the number of transistors on a chip is increasing exponentially. However, the need for more powerful machines is also increasing. The performance of computing systems is being significantly improved by increasing the number of processors in a system. In this paper, we present a multi-scale convolutional neural network (CNN) that can automatically detect and track seals in satellite imagery. The network is trained on a large dataset of satellite imagery, and is able to detect seals in a variety of environments. The network is trained on a large dataset of satellite imagery, and is able to detect seals in a variety of environments.

ABSTRACT
The interconnect topology of computational clusters is not only a key factor in the performance of the cluster, but also a key factor in the design of the cluster. In this paper, we present a multi-scale convolutional neural network (CNN) that can automatically detect and track seals in satellite imagery. The network is trained on a large dataset of satellite imagery, and is able to detect seals in a variety of environments. The network is trained on a large dataset of satellite imagery, and is able to detect seals in a variety of environments.

LUKASZ ORLOWSKI
Lukasz Orłowski is a Ph.D. student in the Applied Mathematics and Statistics Department at the University of Maryland, College Park. He is currently working on his thesis, which is titled "Uncertainty Quantification and Sensitivity Analysis for Inertial Confinement Fusion Simulations". He is also a member of the IACS Student Association.

IACS Researcher Awards



Five awarded in 2016, total value \$75,570

Six awarded in 2017, total value \$80,780

IACS Awards 2017

Junior Researchers

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

Alena Aksenova (LIN) – *Subregular Toolkit Implemented in Python*

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

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

Bento Gonçalves (E&E) – *Autonomous pan-Antarctic Pack-ice Seal Census using Remote Sensing and Deep Learning*

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

IACS Travel & Writing Awards

ARE YOU PUBLISHING YOUR FIRST PAPER?

All IACS students are eligible for the
IACS Young Writer's Award,
a one-time prize of

\$500

to celebrate your first paper that is
accepted in a peer-reviewed publication.

See website for details.

Writing

6 awarded in CY 2015

11 awarded in CY 2016

6 awarded in CY 2017 (so far)

Travel

7 awarded in 14/15

4 awarded in 15/16

8 awarded in 16/17



Workshops, Tutorials, Courses

PHY 546: Python for Scientific Computing
Instructor: Michael Zingale, michael.zingale@stonybrook.edu
Mondays, 3:00-3:53pm
1 credit, Students need to bring laptops to class

Python for Scientific Computing

a weekly graduate seminar on techniques for scientific programming
Instructor: Michael Zingale (michael.zingale@stonybrook.edu)

Python has seen a rapid growth in the scientific community, particularly in the areas of prototyping, analysis, and visualization. This seminar will focus on the use of Python in scientific computing.

- Flipped classroom
- We'll be outside

PHY 504: Computational Methods in Physics and Astrophysics

Instructor: Alan Calder (alan.calder@stonybrook.edu), 3 Credits
Time: Monday, Wednesday, Friday 9:00 to 9:53 AM
Location: Math SNC Site. Students will use the computers provided.

An introduction to procedural and object-oriented programming in a high-level language such as C++ or

This new graduate introduction to programming course is being offered in the

meant to be an
for students with no
science. Students will
experience to begin
or take advanced
that assume

is a physics course, the
will be appropriate for
backgrounds.

Stony Brook University | Institute for Advanced Computational Science

Home About Directory Events Research Resources Opportunities

EVENTS

Seminars
Workshops
Events

EVENT CALENDAR

Calendar link

GPU Programming Workshop

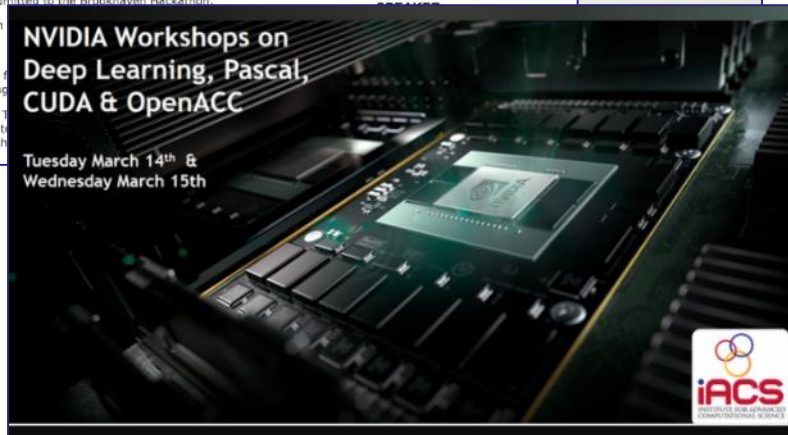
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The overwhelming interest in the GPU Hackathon hosted at Brookhaven National Laboratory (www.bnl.gov/gpuhackathon) makes it clear that there is a strong demand for hands-on training for GPU programming. We will partner with NVIDIA and in particular its PGI compiler team to organize a 3-day hands-on GPU programming workshop/mini-Hackathon for teams that were not admitted to the Brookhaven Hackathon.

Registration

NVIDIA Workshops on Deep Learning, Pascal, CUDA & OpenACC

Tuesday March 14th & Wednesday March 15th



ACS COMPUTES! HS SUMMER CAMP

THIS HANDS-ON CAMP INTRODUCES STUDENTS TO THE PROGRAMMING SKILLS AND SOFTWARE/COMPUTER TECHNOLOGIES THAT DRIVE ADVANCES IN SCIENCE, INDUSTRY, BUSINESS AND SOCIETY.

LEARN MORE

ATTENTION ALL MIDDLE SCHOOL AND HIGH SCHOOL STUDENTS:

n a c i o
North American Computational Linguistics Olympiad

WHY?

Try deciphering an ancient script or deducing the logical patterns of Swahili, Hawaiian, or Finite State Transducers!

Compete for a chance to attend the international competition and compete against students from all over the world!

NO EXPERIENCE NECESSARY! PARTICIPATION IS FREE!



What?
2017 North American Computational Linguistics Olympiad

When?
Thursday, January 26, 2017 from 10am-1pm

Where?
Stony Brook University
FACS Seminar Room

To register:
Visit www.nacloweb.org and select Stony Brook University as your host site

FOR MORE INFORMATION:
Visit our website: www.nacloweb.org or www.nacloweb.org

Optional Practice Session: Thursday, January 15, 2017 from 1:00-2:00pm
Stony Brook University's iACS Seminar Room

IACS Research Day 2017

Philip McDowall, IACS Jr. Researcher Award winner
Automating the Penguin Census Pipeline

Associate Professor Heather Lynch

The Nascent Merger Between Remote Sensing and Computer Vision and its Impact on the Future of Spatial Ecology

Zeyang Ye, Jr. Researcher Award Winner

Performance of Applications of Parallel Markov Chain Monte Carlo Methods

Assistant Professor Rezaul Chowdhury

Computer-aided Design of Robust Performance-portable Algorithms and Implementations

Adrian Soto-Cambres, Jr. Researcher Award Winner

Can Machine Learning Settle the Debate of the Dual Microscopic Character of Water?

Aditi Ghai, Jr. Researcher Award Winner

Towards Adaptive Hybrid Multigrid Method for PDE Based Systems

Associate Professor Marivi Fernandez-Serra

Understanding Water/Solid Functional Interfaces for Photocatalysis and Electrochemical Applications



Conferences and workshops



NY Scientific Data Summit, August 7-9, 2017
New York University



Polar Data Science + HPC, July 31-August 4, 2017
IACS @ SBU



Data + Computing = Discovery, June 12-August 4, 2017
IACS @ SBU



Algorithms and Us, May 4-5, 2017
IACS @ SBU

Conferences and workshops



October 17-19, 2017 SUNY Global Center

Topical areas:

- Longitudinal Multi-modal data in predictive oncology
- Multiscale data in predictive oncology
- Clinical and commercial applications
- Computational frontiers - HPC, sensors, edge computing
- In partnership with SBU medical school, NIH program offices
- Strategic for branding and positioning of SBU/IACS/med.school

Grant Highlights

TEAMS (Calder) Pending

- US Department of Energy, SciDAC
- \$616,000 to SBU of a total \$7.25M grant
- Partners include ORNL, LBNL, ANL, LANL, UCB, UCSD, Princeton, MSU, NDU, UTK, UW, NDU.

NWChem-Ex (Harrison)

- ✧ US Department of Energy, ASCR
- ✧ \$1.355M@BNL, 10/16-9/20 (\$20M overall)
- ✧ Partners include BNL, ANL, LBNL, and ORNL along with Virginia Tech

Future Plans

Goals and Objectives

1. Establish internationally recognized research and education programs in data and computing
2. Grow IACS research funding and funding across SBU
3. Provide leadership and benefit across SBU, SUNY and our local community
4. Provide economic impact to the region and NYS

1. Establish Internationally Recognized Research and Education Programs in Data and Computing

- Grow our faculty in partnership with SBU departments, colleges, schools and BNL
- Establish educational programs with broad benefit
- Develop and support opportunities for undergraduate/graduate research
- Actively recruit students in all departments seeking excellence and diversity with an emphasis on data and computing

Planned faculty hires - I

- Striving for balance between applications and fundamentals of data/computational science
- Currently have 12 existing tenure-track faculty and 2 research professors
 - 3 in fundamentals (2 CS, 1 AMS)
 - 9 in applications
 - chem., chem.phys., 3 mat. sci., astro., atm. sci., ling., ecology
- Also navigating potentially slowed hiring schedule
 - SUNY 2020 not funded, campus budget deficit

Planned faculty hires - II

- Still have strong support from Provost and Deans (CAS, CEAS, SoMAS)
- Aligning with campus-wide initiatives (e.g., AI)
- Pursuing joint hires across campus and w. BNL
 - Expands number of faculty (1 line becomes 2 joint) and reduces immediate budget commitment
 - Respond nimbly to opportunities from others
 - Expands our impact and connections across campus
- Converted Lynch and Trelewicz to joint core faculty
 - Ramps us faster and recognizes their huge commitment
 - Future joint hires planned with their departments

Planned faculty hires - III

- 4+ positions in foundations of computation
 - Search (still) in progress; now expected summer 2018
 - Startup grant from Empire Innovation Program
 - Positions advertised simultaneously
 - 2 senior or up to 4 junior endowed chairs in AMS+CS
 - 2+ junior faculty in CS+AMS coordinated
 - Overall search committee (plus dept. committees)
 - Harrison (IACS), Glimm (AMS), Skiena (CS), Chowdhury (IACS/CS), Samaras (CS), Jiao (IACS/AMS), Samulyak (AMS), Sexton (IBM), Curley (Intel)

2. Establish educational programs with broad benefit

- Graduate Certificate in Data and Computation for Scientists & Engineers
- NSF NRT-DESE: Science Training and Research to Inform Decisions (STRIDE) and associated certificate (CSTRIDE)
- Initiated campus-wide discussions about undergraduate education in data/comp.sci. including visiting speakers (e.g., Shiflet, Gordon)
 - Limited traction so far – many stakeholders on campus
 - First, must make a success of the graduate training

Grow student excellence, diversity and success

- Jointly funding a full-time recruiter with the Center for Inclusive Education (CIE)
 - National and regional approaches; data analysis pending
- Co-funding and sponsoring CIE and Women in Science and Engineering (WISE) events
- Collaborating with faculty and engaging students from The College of New Rochelle and across SUNY
- Student awards
- Expanded training, tutorials, workshops
- Developed industrial, national lab and international internships

Grow IACS Research Funding and Funding Across SBU

- Identify, promote and organize around high-impact themes and products
- Provide administrative support for all aspects of proposal submissions
- Incentivize large, especially interdisciplinary, projects
- Enhance faculty research productivity
- Establish new revenue streams
- Coordinate across SBU, SUNY and NYS to develop and realize very large opportunities

Grow Funding

- Incentivize large, especially multidisciplinary projects
 - Proposed is 1 semester teaching waiver if developing \$2+M proposal; another semester if awarded (consistent with C/S department policy)
- IACS admins available to help with all phases of proposal submissions; graphics design and grant writer subcontracts
- Develop new funding streams
 - Structural issues now resolved
- Huge proposals/projects in flight
 - Data Analytics for Transforming Academics across SUNY (DATA SUNY): A Collaboration of University Centers (\$13+M)
 - Institute for Discovery and Innovations in Medicine & Engineering (I-DIME, \$75M)

3. Provide Leadership and Benefit Across SBU, SUNY and our Local Community

- Establish regional, national and international partnerships
- Effectively communicate and coordinate with all our stakeholders
- Lead development of an institutional approach to Research Computing
- Share our resources, events and activities
- Build community presence, impact and visibility
- Prepare students for leadership in their future careers

Leadership and Benefit

- Effective communication and coordination across campus and with medical school (regular meetings, MOUs)
- Grow research computing on campus and across SUNY
- Annually run: IACS Computes! HS Summer camp; Master Teachers Python workshop; Python 4-week module for PJHS, Mt. Sinai HS
- Tutorial and workshops every semester with pre-registration available for CIE students and survey driven topics
- University-wide and system-wide proposals

IACS committed from outset to an institutional approach to computing

- Seeded next generation SBU-wide cluster with our startup funds
 - Compute cluster (batch+web gateway+cloud)
 - Substantial fast shared storage for collaboration and data-intensive science
 - Located in DoIT-managed facility
- Help drive necessary campus network upgrade

Research Computing on Campus

- IACS playing lead role in establishing this in partnership with CIO, DoIT, VPR, Provost, etc.
 - Hiring our sys. admin. staff into DoIT
 - Bootstrapping staff hiring
 - Coskun, 100% IACS first year, 50% DoIT thereafter
 - Rosenberg, ditto
 - Weekly research computing call
 - Leading proposals for external funding for SBU-wide resources (I-DIME, LI-red, DATA-SUNY, NSF MRI SeaWulf)
 - Leading planning on other resources (research data backup and archive; sustainable approaches; peers)
 - Developed plans with CIO Dr. Melissa Woo for support of graduate students, oversee activities and expenditures
 - Tasks forces for research computing and data

4. Provide Economic Benefit to the Regions and NYS

- Ensure the success and growth of the HPC^{NY} state-funded industry-engagement consortium; seek the success of I-DIME
- Work with Research Computing to operate LI-red and SeaWulf to ensure benefit to industry and tracking ROI
- Engage with regional and state technology centers and economic development agencies
- Support and encourage faculty-led startups

Economic impact

- IACS faculty are instrumental in the success of High-Performance Computing Consortium (HPC^{NY}) with 6+ local industrial partners
- 33+% of LI-red and 15+% of new MRI cluster SeaWulf available for use across SUNY and for New York State industry
- Support faculty involvement in startups and technology transfer
- Proposed Institute for Discovery and Innovation in Medicine & Engineering (I-DIME) includes large space for incubator and START-UP NY

What should we be ...

- Doing better or differently?
- Doing that we are not doing now?
- Not doing that we are doing now?

And

- How do we compare to institutes we aspire to have as peers?
- How would you adjust the format/content of this meeting?

Additional Material



HPC^{NY} @ Stony Brook

Overview and Success Story

STONY BROOK UNIVERSITY

Institute for Advanced Computational Science






What is HPC^{NY}

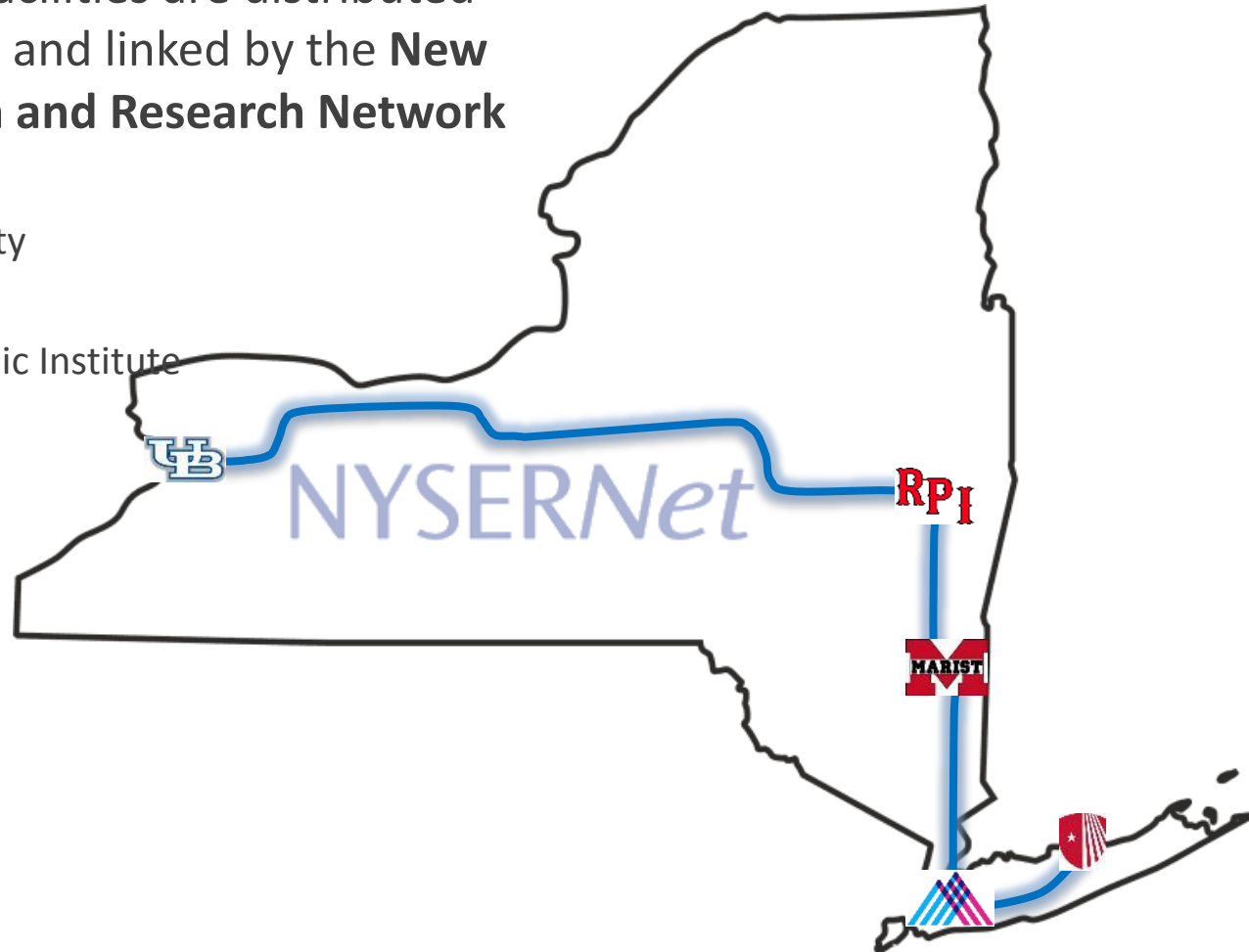
- HPC^{NY} is New York State's **High Performance Computing Consortium**.
- A network of university computing centers who partner with industries throughout the state to help foster business growth and process improvement.
- An HPC^{NY} partnership can help companies **create jobs, save costs, accelerate R&D, and obtain funding**.
- HPC^{NY} provides access to computational resources and world class expertise in **modeling, visualization, and analytics**.
- **Funded by ESD/NYSTAR**



The HPC^{NY} Consortium

- HPC² expertise and facilities are distributed throughout the state and linked by the **New York State Education and Research Network (NYSERNet)**:

-  — Stony Brook University
-  — University at Buffalo
-  — Rensselaer Polytechnic Institute
-  — Marist College
-  — Mount Sinai

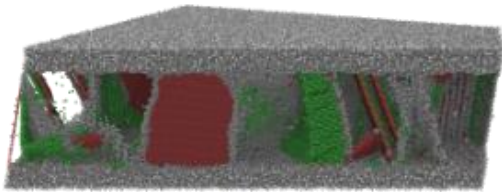


Powered by ESD/NYSTAR

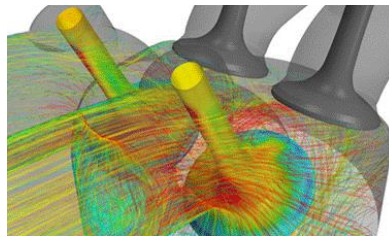


The SBU HPC^{NY} team

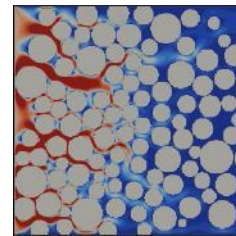
- A team of SBU faculty and staff with expertise in computational science, engineering, scientific programming, data analysis and database design, animation and visualization, and marketing.
 - Faculty include mechanical, chemical, and materials engineers, computational chemists, and computer scientists from across SBU campus including IACS core faculty.
- Research interests include:
 - Molecular modeling, computational chemistry, and crystallography
 - Materials design at the nanoscale for energy applications
 - Finite element modeling, computational fluid dynamics, thermal analysis, and coupled thermomechanical behavior in product design
 - Big data analytics, and source-to-source translation



Molecular Modeling



Fluid Dynamics

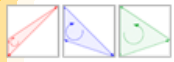


Thermal Analysis



Data Analytics

HPC^{NY} Industrial Partners



ThermoLift, Inc.

Computational Modeling of the Thermomechanical Properties of the Regenerator in a Thermally Driven Heat Pump



Partial Reformation of Mixed Fuels for Combustion in Heavy-duty Engines – A Modeling Study



Motiff Technologies: Supercomputing Audio



Modeling of Hybrid Batteries for Grid Storage

Theoretik

Enabling Stable Nanocrystalline Tungsten Alloys as Plasma Facing Materials for Fusion Reactors

Paralab Computing

Source-to-Source Translator for High-Performance Computing with R Language

Measuring Economic Impact

In Long Island, the impact of HPC^{NY} has been substantial.

Significant economic impacts have been produced over this phase of the project alone that include:

- **\$5.2M in federal and private funding,**
- **\$1.1M in cost savings, and**
- **15 jobs being created and/or retained at the participating Long Island companies.**

The program has attracted several new high-tech companies to the region and these companies are poised to be major players in their respective areas and bring significant numbers of high-tech jobs to the region.

Success Story: Innoveering

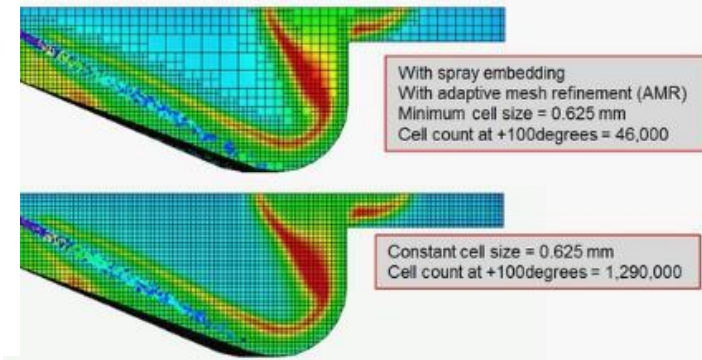
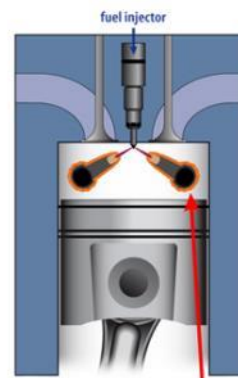
innoveering

innovative engineering solutions

- Exploring a partial fuel reformation technique to improve combustion efficiency and reduce CO and UHC emissions in heavy-duty diesel engines.
- HPC^{NY} team is investigating the reforming effects on natural gas combustion using new fuels with a focus on Syngas ($H_2 + CO$).
 - Computational fluid dynamics (CFD) simulations using ConvergeCFD for chemical kinetics and EnSight for visualization.



Direct fuel injection, Mixing-controlled burn, NO_x and soot emissions



Core Faculty

Alan C. Calder



Associate
Professor

- Department of Physics and Astronomy
- Deputy Director of the Institute for Advanced Computational Science
- Research is in the field of nuclear astrophysics, involving simulating explosive astrophysical phenomena
- Prior research appointments at the National Center for Supercomputing Applications and the University of Chicago, Center for Astrophysical Thermonuclear Flashes
- Received 2-year INCITE award of 50M Supercomputing Hours for Modeling Astrophysical Explosions

Barbara Chapman



Professor

- Applied Mathematics & Statistics Department, Computer Science Department
- Joint appointment with BNL
- Research involves parallel programming languages and compiler technology
- Developed OpenUH, state-of-the-art open source compiler for parallel programs
- Active participation in OpenMP, OpenACC and OpenSHMEM standards efforts
- Over 200 professional publications
- Service on national and international advisory committees, multiple editorial boards

Rezaul Alam Chowdhury



Assistant
Professor

- Computer Science Department
- Leads the Theoretical and Experimental Algorithmics (TEA) Group
- Research interests include high-performing resource-oblivious algorithms and data structures, parallel algorithms, structural bioinformatics, computer-generated algorithms and computer-aided algorithm design
- Worked at the Center for Computational Visualization, Institute for Computational Engineering & Sciences at UT Austin, and then the Structural Bioinformatics Group at BU and the SuperTech Research Group at MIT prior to joining SBU
- Research is supported by NSF grants including one CAREER grant

Marivi Fernández-Serra



Associate
Professor

- Department of Physics and Astronomy
- Research is in the field of computational condensed matter physics: fundamental properties of liquid water using quantum mechanical simulations
- Awarded a DOE Early Career award in 2010 to study to develop methods to simulate liquids under non equilibrium conditions.

Robert J. Harrison



Professor and
Director

- Director, IACS
- Joint appointment with BNL where he is Director of the Computational Science Center
- Distinguished expert in high-performance computing
- Previous director of the Joint Institute of Computational Science, Professor of Chemistry and Corporate Fellow
- Long career in high-performance computing and extensive service on national advisory committees

Jeffrey Heinz



Professor

- Department of Linguistics
- Research lies at the intersection of theoretical and mathematical linguistics, theoretical computer science, and computational learning theory, with specializations in phonology, linguistic typology, and grammatical inference
- The Linguistic Society of America recognized Heinz with its 2017 Early Career Award

Xiangmin Jiao



Associate
Professor

- Applied Mathematics & Statistics Department
- Research interests are in high-performance geometric and numerical computing in science and engineering
- Work focuses on developing efficient and robust algorithms and high-performance software implementations for applied computational and differential geometry, generalized finite difference and finite element methods, multigrid and iterative methods for sparse linear systems, and multiphysics coupling with applications in computational fluid dynamics and structural mechanics, biomedical engineering, climate modeling, etc.

Marat Khairoutdinov



Associate
Professor

- School Of Marine and Atmospheric Sciences
- Research is to better understand the role of clouds in the Earth climate system through high-resolution cloud modeling
- Developed one of the first Large-Eddy Simulation (LES) models
- Redesigned LES model, renamed System for Atmospheric Modeling or SAM, and has been used for research at Colorado State, PNNL, UWashington, Harvard, UMiami, UBritish Columbia, UOklahoma, NOAA, NASA Langley, UHawaii, UWisconsin, Scripps Institution of Oceanography, MIT, Yale, NYU and Columbia University

Predrag Krstić



Research
Professor

- IACS
- Founder & owner of TheoretiK consulting, carrying contracts with PPPL & Arizona State U.
- Adjunct Prof. in Physics & Astronomy at UTK
- Elected fellow of American Physical Society
- Consultant of International Atomic Energy Agency
- Previously senior scientist in ORNL
- Research covers a wide range of topics in theoretical and computational atomic, molecular and photonic physics; interactions of plasma with material surfaces; plasma physics and nuclear fusion; chemistry; molecular electronics and bionanotechnology, with more than 200 publications

Heather Lynch



Associate
Professor

- Ecology & Evolution Department
- 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
- 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

Artem R. Oganov



Professor

- Geosciences Department
- Research, interdisciplinary by nature, marries theoretical crystallography, condensed matter physics, theoretical chemistry, materials science, computational mathematics, and Earth sciences
- Research develops and applies novel computational methods, with the aim of predicting and understanding the behavior of materials (fundamentally interesting or technologically useful materials, planet-forming or synthetic materials, etc. etc.)

Matthew Reuter



Assistant
Professor

- Applied Mathematics & Statistics Department
- Research interests in electrical response properties of nanoscale systems, mathematical physics and applications of linear algebra in physics
- Lead author of 21 peer-reviewed journal articles
- Previously worked at Northwestern University and Oak Ridge National Laboratory
- Awards: Department of Energy Computational Science Graduate Fellow, Wigner Fellow at Oak Ridge National Laboratory

Jason R. Trelewicz

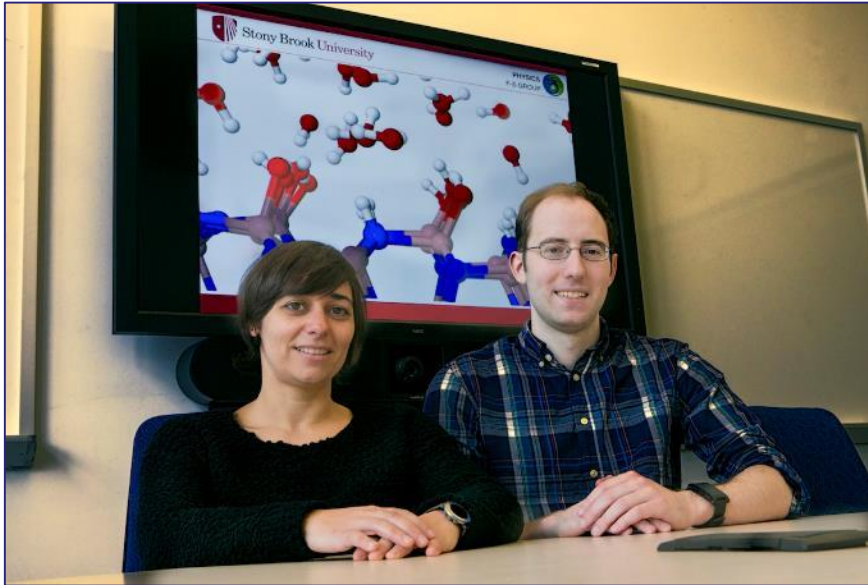


Assistant
Professor

- Materials Science & Chemical Engineering Department
- Research group, the Engineered Metallic Nanostructures Laboratory, focuses on the design, synthesis, stability, and physical behavior of interface engineered alloys through coupled simulations and experiments
- Prior to joining Stony Brook University, he spent four years in industry as a Principal Investigator at MesoScribe Technologies, Inc.
- Recipient of the 2017 DOE Early Career Award, 2016 NSF CAREER Award, and 2015 TMS Young Leader Professional Development Award

Past Highlights

IACS Core Faculty Publications



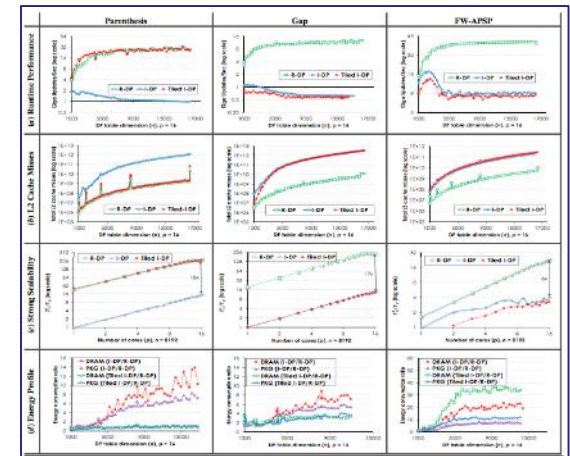
Marivi Fernandez Serra

Nature Communications

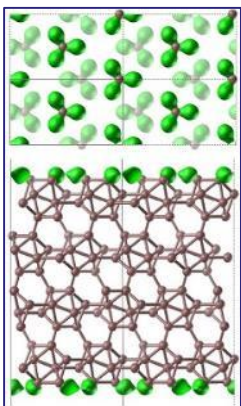
The Hydrogen-bond Network of Water Supports Propagating Optical Phonon-like Modes

Rezaul Chowdhury, PPoPP 2016

AUTOGEN: Automatic Discovery of Cache-Oblivious Parallel Recursive Algorithms for Solving Dynamic Programs



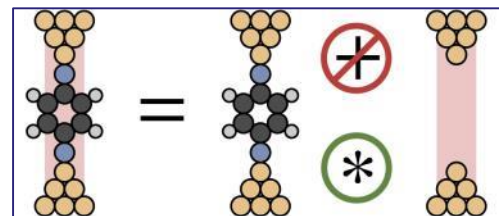
IACS Core Faculty Publications



Artem Oganov, *Phys. Rev. Lett.*
*Unexpected Reconstruction of the α -Boron (111)
Surface*

Matthew Reuter, *ACS Nano*

*Quantitative Interpretations of Break Junction
Conductance Histograms in Molecular Electron Transport*



Grant Highlights

The Molecular Science Software Institute (MolSSI)

- ✧ National Science Foundation
- ✧ \$19.4M w/ \$589K for SBU, Awarded, RJH co-PI
- ✧ Virginia Tech, Iowa State, Rice, Rutgers, Stanford, U of CA-Berkeley, U of Southern California

NRT-DESE Science Training and Research to Inform DEcisions (STRIDE)

- ✧ National Science Foundation (NRT)
- ✧ \$2.9M, Awarded, RJH PI
- ✧ IACS, AMS, C/S, Journalism, Biomedical Informatics, SoMAS, Ecology and Evolution

Grant Highlights

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

[View](#) [Edit](#)

Greg Filiano
Monday, March 14, 2016

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



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

Trelewicz, Chowdhury win NSF CAREER Awards

Rezaul Chowdhury Receives NSF CAREER Award for Parallel Algorithms Research

[View](#) [Edit](#)

Tuesday, April 19, 2016



Used with permission from the Department of Computer Science.

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

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

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

Grant Highlights

Major Research Instrumentation (MRI)

- ✧ National Science Foundation
- ✧ \$1.4M w/ \$300K match from NYSTAR
- ✧ \$300K internal match
- ✧ Awarded 10/1/15

Data-enabled Research & Education for Advanced Multidisciplinary Science (DREAMS)

- ✧ National Science Foundation (NRT)
- ✧ \$3M, pending
- ✧ IACS, C/S, AMS, Biomedical Informatics, SoMAS, Ecology and Evolution, Sociology

Grant Highlights

**Stony Brook Researchers
Receive Two-Year INCITE Award of
50 Million Supercomputing Hours for
Modeling Astrophysical Explosions**



IACS Director R.J. Harrison awarded \$15M compute hours from DOE

Tuesday, November 18, 2014
IACS Staff



IACS Director Robert Harrison was awarded 15,000,000 processor hours, from the Department of Energy's INCITE Leadership Computing program, on Argonne National Laboratory's IBM Blue Gene/Q for his proposal entitled Dynamic and Adaptive Parallel Programming for Exascale Research. Along with Harrison, the Co-Investigators are George Fann, Oak Ridge National Laboratory; Laura Ratcliff, Argonne National Laboratory; Saday Sadayappan, The Ohio State University; and Edward Valeev, Virginia Tech.

Research Summary

Many challenges await along the path from petascale to exascale and beyond for hardware architectures, as well as for system software

IACS Student Association

What do Matchmaking, Patents and Science Have in Common?



Research Events

- IACS Student Seminar Series
- Brown-Bag Lunch Sessions

Professional Development

- Scientific Communication Workshop
- Patents Workshop

Social Events

- Student-Faculty Dinners
- Group Outings to NYC

Social Networking

A poster for the IACS Student Association Kickoff Event. It features a blue background with a white diamond shape on the left containing the text 'NEED TO TAKE A BREAK FROM THE GRADUATE SCHOOL ROUTINE?'. The right side has white text on a blue background.

NEED TO TAKE A BREAK FROM THE GRADUATE SCHOOL ROUTINE?

IACS STUDENT ASSOCIATION Kickoff Event

THURSDAY, DECEMBER 3
6:00PM TO 8:00PM

THE BENCH BAR & GRILL
APPETIZERS AND DRINKS WILL BE PROVIDED

Come have a drink with your IACS peers. While you're there, meet the members of the new IACS Student Association.

See website for details.

iACS
INSTITUTE FOR ADVANCED COMPUTATIONAL SCIENCE

A poster for the IACS Student Association Movie Night. It features a blue background with a white rectangle in the center containing the event details. The title 'MOVIE NIGHT' is in large, glowing letters. The bottom right shows a bucket of popcorn and movie tickets.

THE IACS STUDENT ASSOCIATION PRESENTS

MOVIE NIGHT

**THURSDAY, JAN. 21
7:00PM TO 8:45PM**

LOOKING FOR SOMETHING TO DO DURING THE HOLIDAY BREAK? COME HANG OUT WITH YOUR IACS PEERS AND WATCH THE PHD MOVIE, A COMEDIC TAKE ON GRADUATE STUDENT LIFE.

RSVP REQUIRED

iACS
INSTITUTE FOR ADVANCED COMPUTATIONAL SCIENCE

ADMIT ONE

PIZZA, SNACKS, AND BEVERAGES WILL BE PROVIDED

A poster for the IACS Student Association Spring Break Warm Up. It features a dark background with a large, stylized yellow text 'Spring Break Warm Up'. On the left is a martini glass with a smiley face. The bottom has white text on a dark background.

THE IACS STUDENT ASSOCIATION PRESENTS

Spring Break Warm Up

MARCH 10TH, 5:30 - 8:30

THE ARDEN
(201 MAIN STREET, PORT JEFFERSON, NY 11777)

WHO SAYS SPRING BREAK BEGINS ON MONDAY? JOIN THE IACS STUDENT ASSOCIATION FOR HAPPY HOUR AT THE ARDEN AND GET A HEAD START ON SPRING BREAK!

IF YOU NEED TRANSPORTATION TO THE LOCATION, PLEASE RSVP BY MARCH 1ST. SEE WEBSITE FOR DETAILS.

iACS
INSTITUTE FOR ADVANCED COMPUTATIONAL SCIENCE

A poster for the IACS Student Association Dining for Success Etiquette Dinner. It features a white background with a black suit and white gloves holding a silver tray. The title 'DINING FOR SUCCESS' is in large, bold letters, and 'Etiquette Dinner' is in a script font. The date and time are in bold. The bottom has small text and the IACS logo.

DINING FOR SUCCESS
Etiquette Dinner

THURSDAY NOV. 19, 6PM-8PM

Join us for a three-course meal while learning how to navigate a formal place setting, a waiter's advance and make casual dinner-time conversation.

This is the perfect event to help you prepare for attending professional dining events and formal affairs.

See website for details.

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Drawing Diversity to Academia



iACS
INSTITUTE FOR ADVANCED
COMPUTATIONAL SCIENCE

**DRAWING DIVERSITY
TO ACADEMIA**

MONDAY, APRIL 18, 2016
1:30 PM - 3:15 PM
WANG CENTER THEATER

FOLLOWED BY A COFFEE SOCIAL FOR PARTICIPANTS

PANELISTS

DENNIS ASSANIS: PROVOST'S OFFICE, SBU

NOEL BLACKBURN: UNIVERSITY RELATIONS, BNL

FRANCES BRISBANE: HEALTH SCIENCES WORKFORCE DIVERSITY, SUNY

CARLOS MEDINA: DIVERSITY, EQUITY AND INCLUSION, SUNY

CHARLES ROBBINS: UNDERGRADUATE COLLEGES, SBU

TONI SPERZEL: CENTER FOR INCLUSIVE EDUCATION, SBU

CHARLES TABER: GRADUATE SCHOOL, SBU

RICHARD TAPIA: CENTER FOR EXCELLENCE AND EQUITY IN EDUCATION, RICE UNIVERSITY

IACS, along with the Center for Inclusive Education (CIE), sponsored Drawing Diversity to Academia, a panel session designed to discuss opportunities, best practices and novel ideas for increasing the participation and success of underrepresented minorities in STEM fields.



Workshops and Tutorials



**Master Teacher
Python Workshop**

Two Saturdays
September 10th and 17th, 2016
Participants learn to program and create lesson plans

[Learn More](#)

iACS INSTITUTE FOR ADVANCED COMPUTATIONAL SCIENCE



DATA CARPENTRY

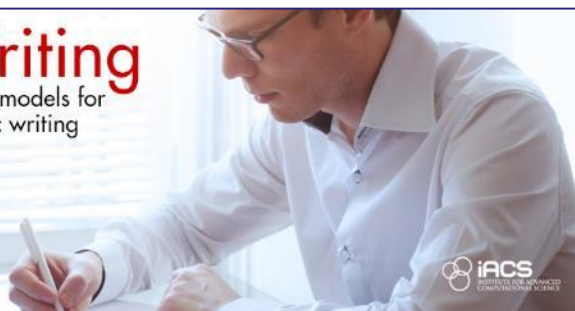
MAKING DATA SCIENCE MORE EFFICIENT

Science Writing

1-week workshop to develop models for
structure and style in scientific writing

August 22-26

[Learn More](#)



iACS INSTITUTE FOR ADVANCED COMPUTATIONAL SCIENCE

XSEDE | USER PORTAL

Extreme Science and Engineering
Discovery Environment

XSEDE Summer Boot Camp

June 14 - 17
SBU Institute for Advanced Computational Science

This four-day event will run from June 14 - 17 and will include MPI, OpenMP, OpenACC and accelerators and will be held at Stony Brook's Institute for Advanced Computational Science.



**IACS COMPUTES!
HS SUMMER CAMP**
JULY 11 - 20, 2016

THIS HANDS-ON CAMP INTRODUCES
STUDENTS TO THE PROGRAMMING SKILLS
AND SOFTWARE/COMPUTER TECHNOLOGIES
THAT DRIVE ADVANCES IN SCIENCE,
INDUSTRY, BUSINESS AND SOCIETY.

[LEARN MORE](#)



TUE, MAY 24 AT 8:30 AM, STONY BROOK, NY

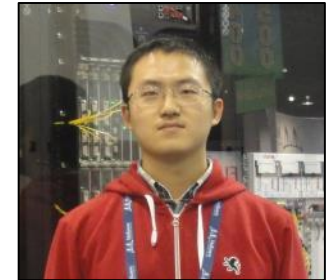
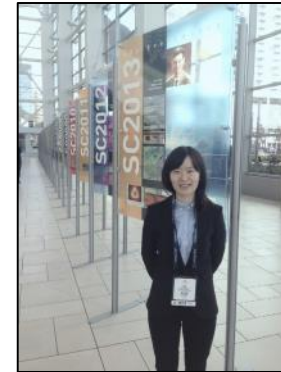
**2-Day OpenACC GPU Hands-on
Programming Workshop at
Stony Brook University**

By: NVIDIA

IACS Travel Grants to SC1X

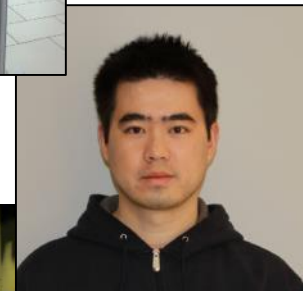
SuperComputing13

Gao Chao; Na Zhang;
Yufei Ren



SuperComputing14

Li Zhang; Jesmin Tithi



SuperComputing15

Na Zhang

