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

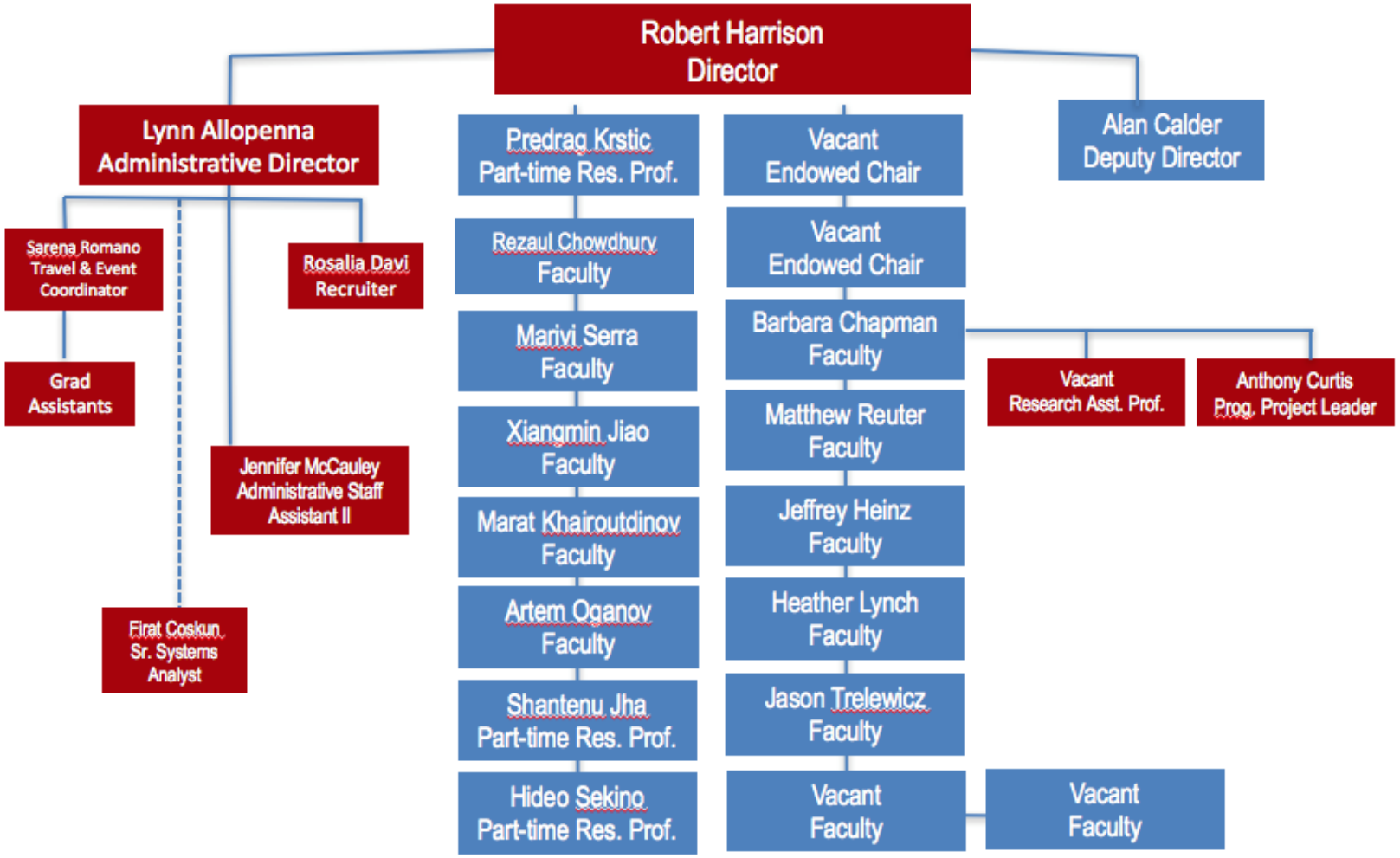
- The New York Center for Computational Sciences (NYCCS)
  - Umbrella HPC activity spanning BNL and SBU
  - The BNL high-performance computer center
  - Primary resource is now a ~700 TFLOP IBM BG Q
- At conception with funding by NY State
  - At SBU home to original faculty cluster hire in HPC
  - At 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

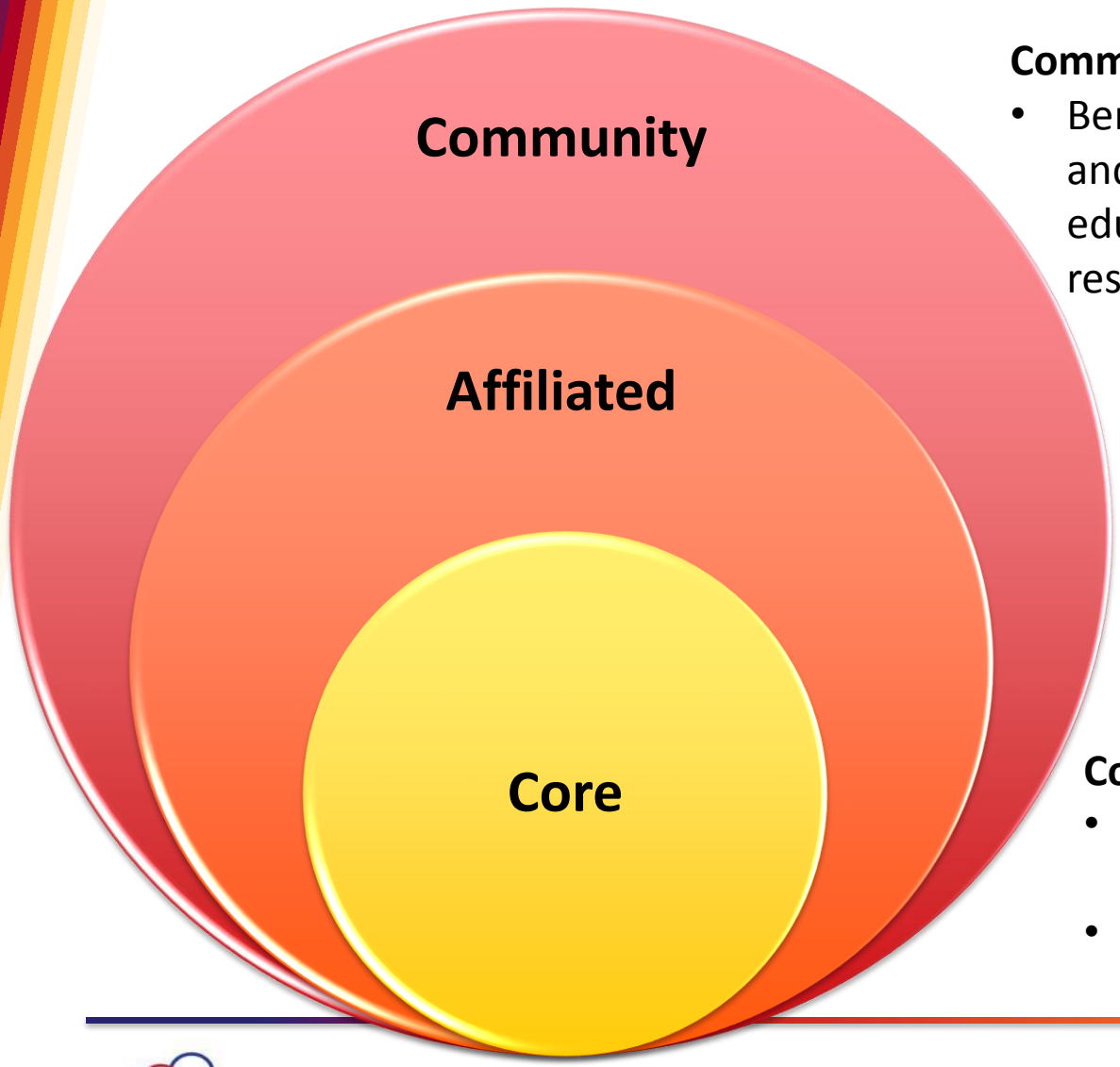
Stony Brook University

Institute for Advanced Computational Science
Organization Chart

iACS INSTITUTE FOR ADVANCED COMPUTATIONAL SCIENCE



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)

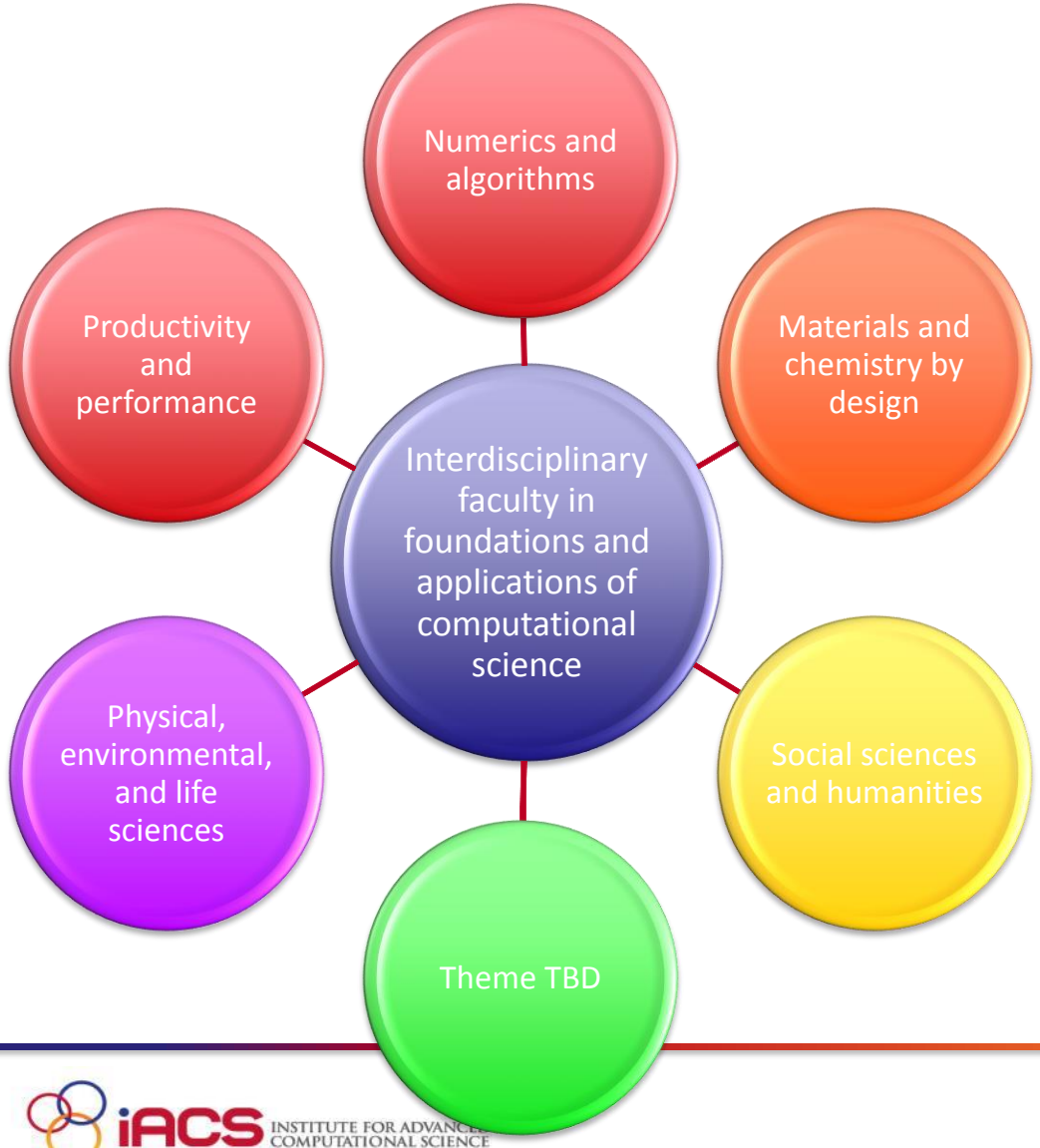
IACS Core Faculty - IV

- 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

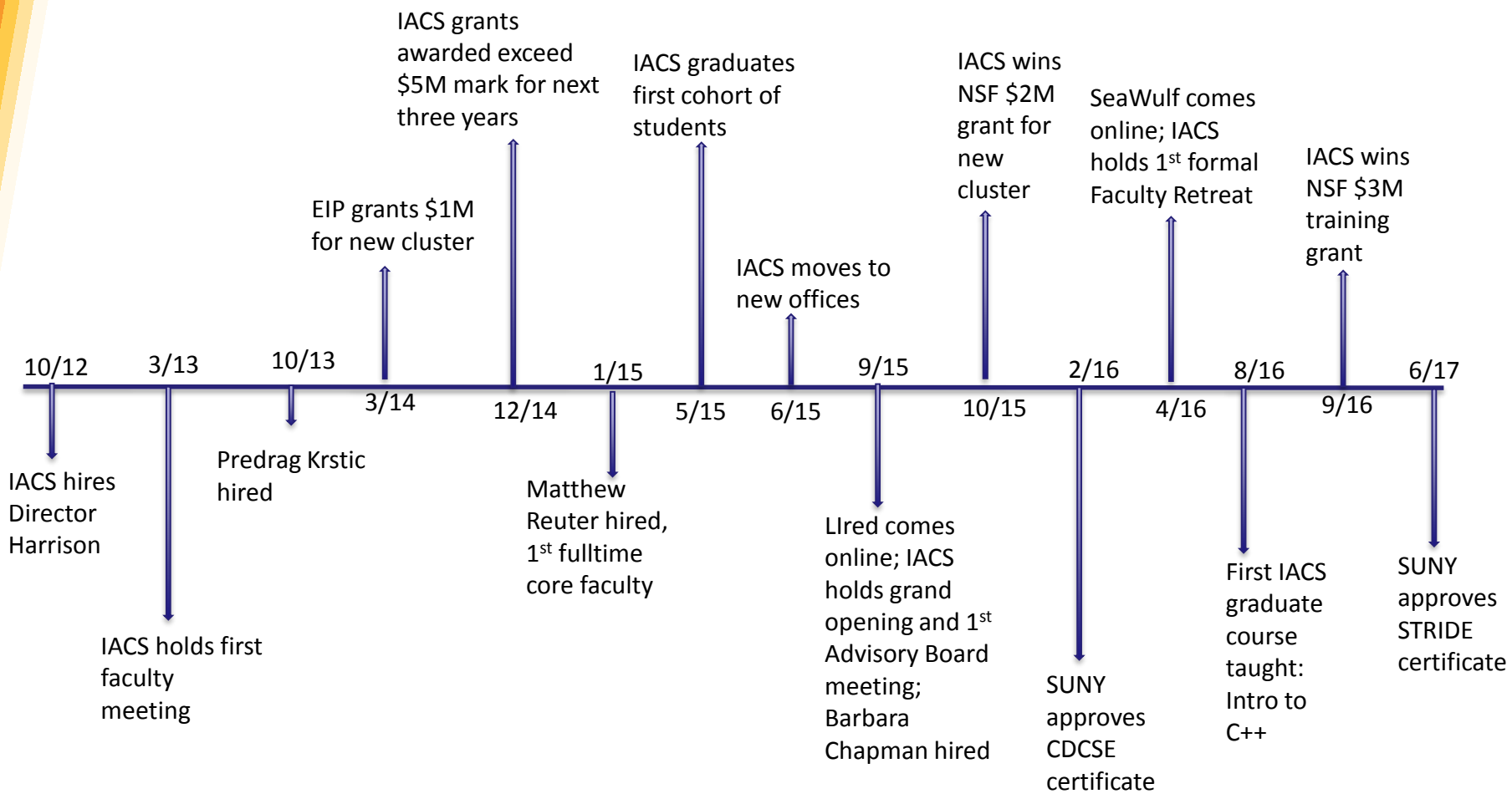
- Establish internationally recognized research and education programs in data and computing
- Grow IACS research funding and funding across SBU
- Provide leadership and benefit across SBU, SUNY and our local community
- Provide economic impact to the region and NYS

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)

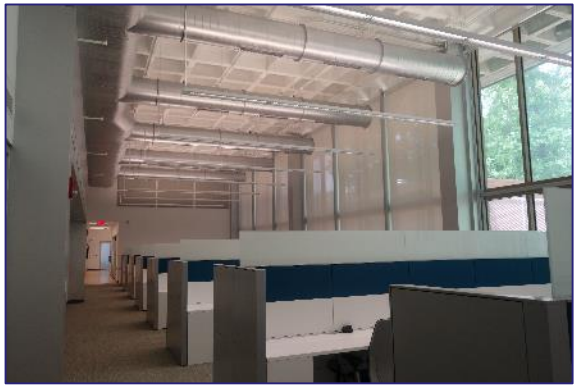
Five Years in Review

IACS Timeline



IACS Space
Before and after

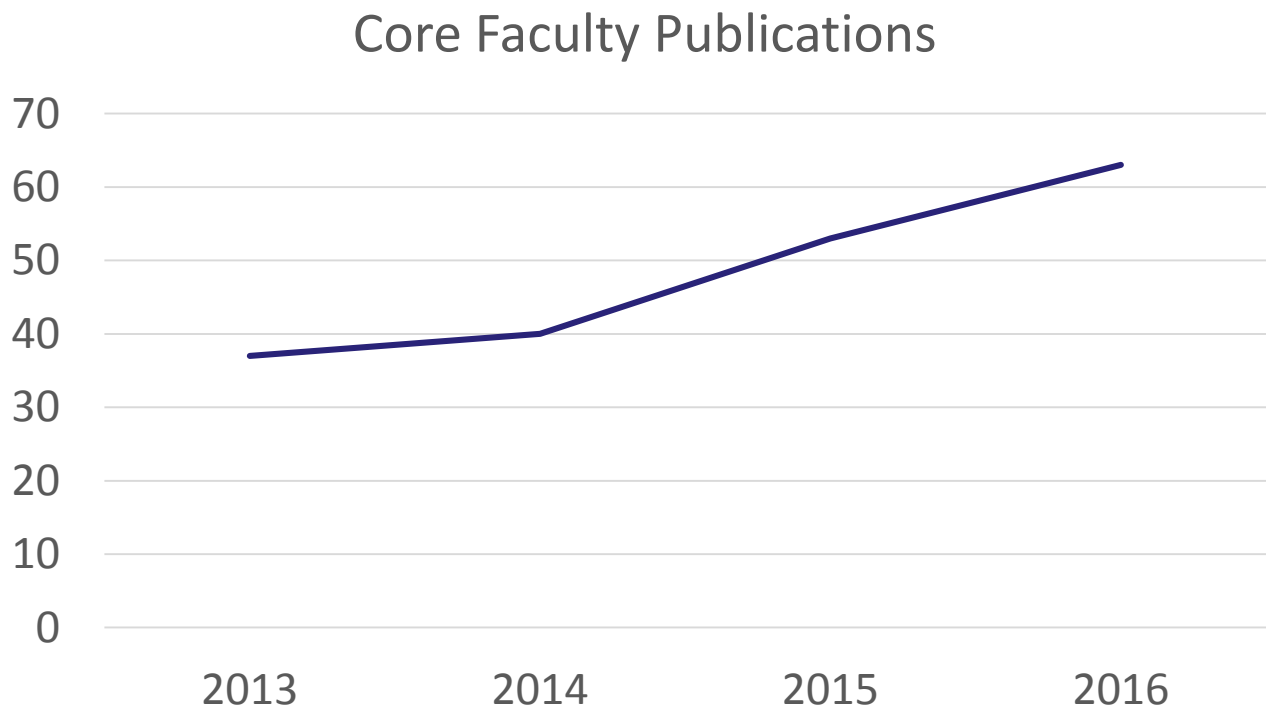


KPI: IACS Core Faculty Publications

	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

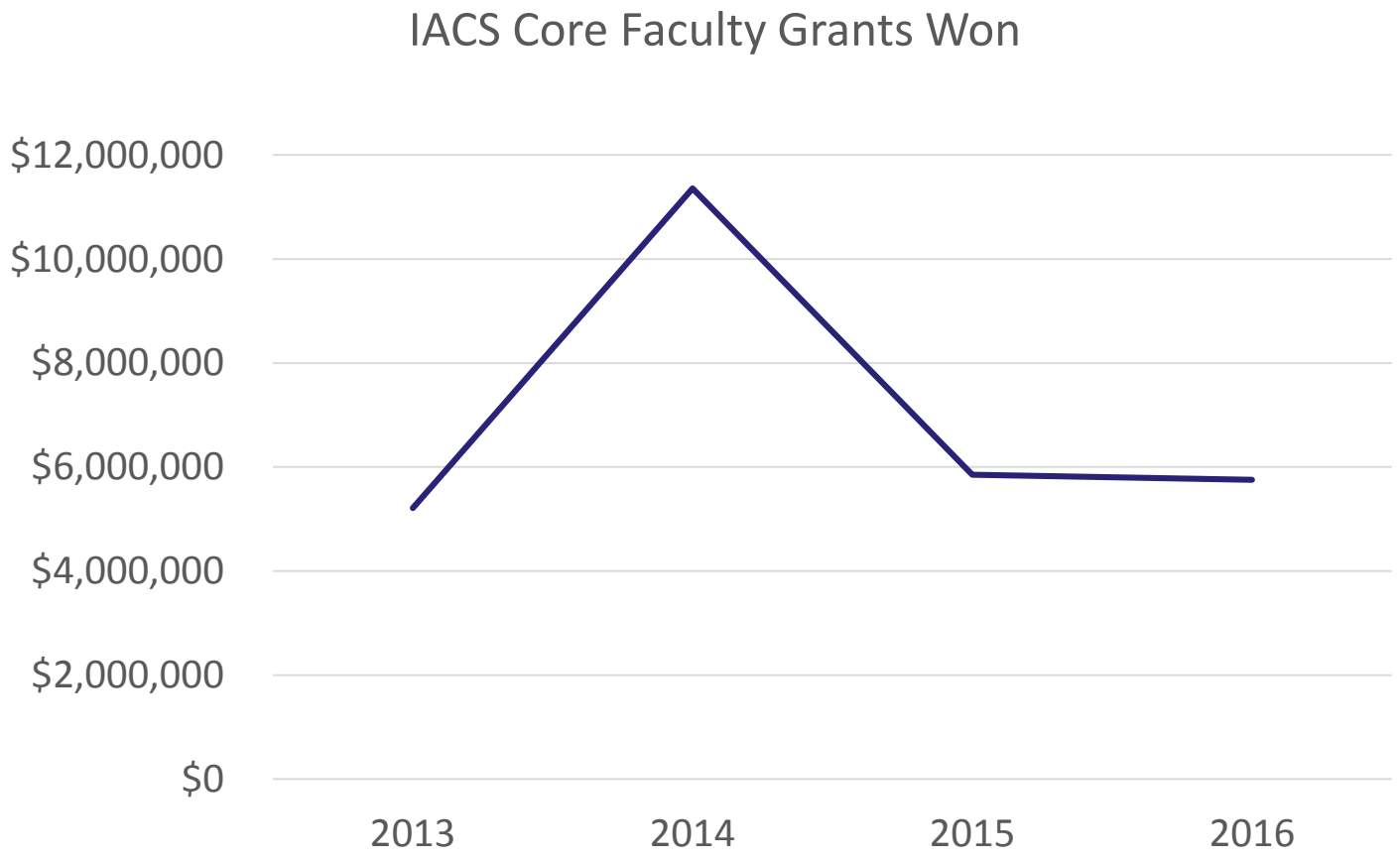
IACS Core Faculty Publications



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



KPI: Multidisciplinary Grants & Publications

	Interdisciplinary Grants			Interdisciplinary 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

	2010-11			2011-12			2012-13			2013-14		
Department	**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.																		
Napply	3	91	214	4	84	229	4	61	184	4	68	211	4	66	194	3	58	176
Enroll%	67%	13%	18%	0%	14%	15%	0%	20%	15%	0%	20%	10%	25%	15%	18%	0%	10%	14%
N	3	19	50	0	14	47	1	19	42	0	7	30	1	13	47	0	6	24
Grad%	0%	16%	12%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
Ret+Grad%	0%	74%	64%	0%	64%	70%	100%	95%	86%	0%	86%	97%	0%	0%	0%	100%	100%	100%
Comp. Sci.																		
Napply	1	68	365	1	78	364	0	71	308	2	57	289	3	55	261	3	85	313
Enroll%	100%	6%	8%	0%	3%	8%	0%	10%	7%	0%	7%	11%	33%	18%	20%	0%	12%	13%
N	1	7	39	0	2	29	0	8	21	1	5	37	2	10	54	0	10	41
Grad%	0%	0%	3%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
Ret+Grad%	0%	86%	70%	0%	100%	66%	0%	38%	57%	100%	80%	95%	100%	100%	100%	100%	100%	100%
Ecol/Evol																		
Napply	4	27	53	3	27	54	3	38	66	3	25	46	5	22	44	5	15	34
Enroll%	25%	7%	6%	33%	15%	17%	33%	13%	15%	0%	32%	26%	20%	18%	18%	0%	0%	15%
N	1	2	3	0	3	8	0	5	8	0	5	9	1	4	8	0	0	5
Grad%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
Ret+Grad%	0%	100%	67%	0%	67%	63%	100%	100%	100%	100%	100%	100%	100%	100%	100%	100%	100%	100%
SoMAS																		
Napply	2	36	72	2	48	72	1	50	96	0	44	84	2	42	78	3	41	69
Enroll%	0%	17%	17%	0%	27%	25%	0%	14%	15%	0%	23%	21%	50%	19%	18%	33%	10%	16%
N	1	8	15	0	14	19	0	9	17	3	11	19	2	10	17	1	4	11
Grad%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
Ret+Grad%	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

Napply – 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 Bratislavia, Texas Tech University, Humboldt-University Berlin, University in Tromso, 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:

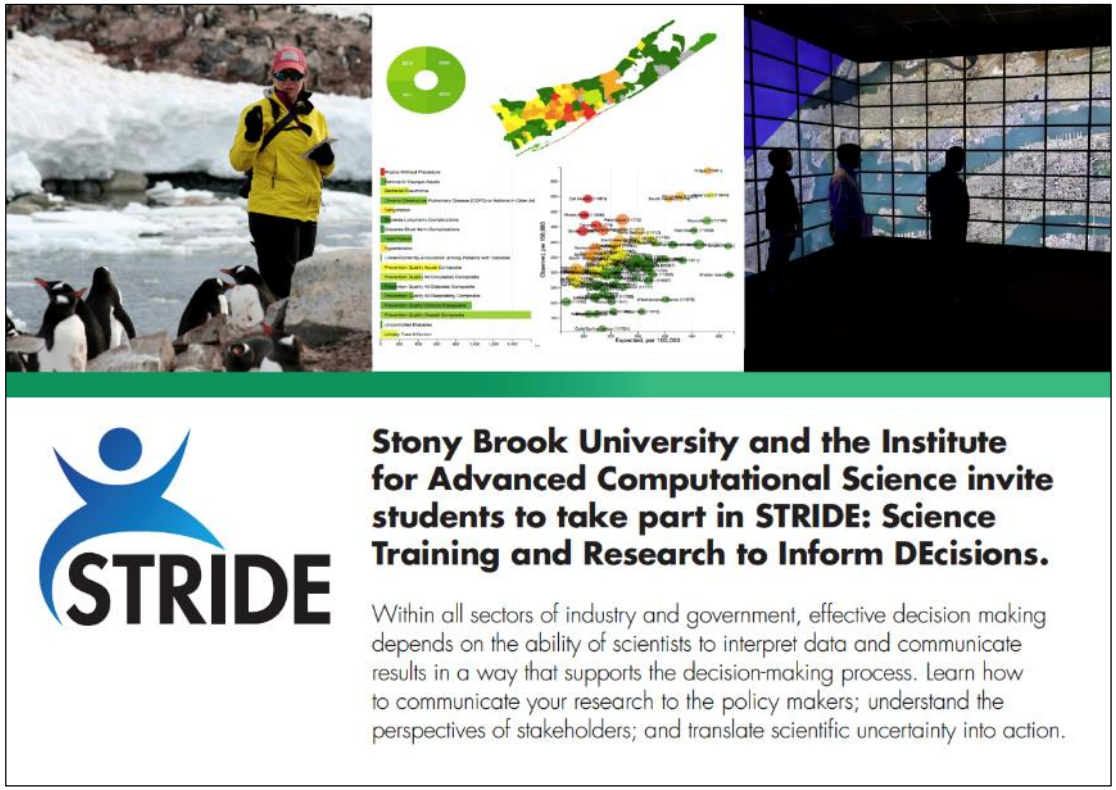
✧ 3 core courses

JRN 501 Distilling Your Message
JRN 503 Improvisation for Scientists
AMS 561 Intro to Computational Science

✧ 32 on-ramp, introductory courses

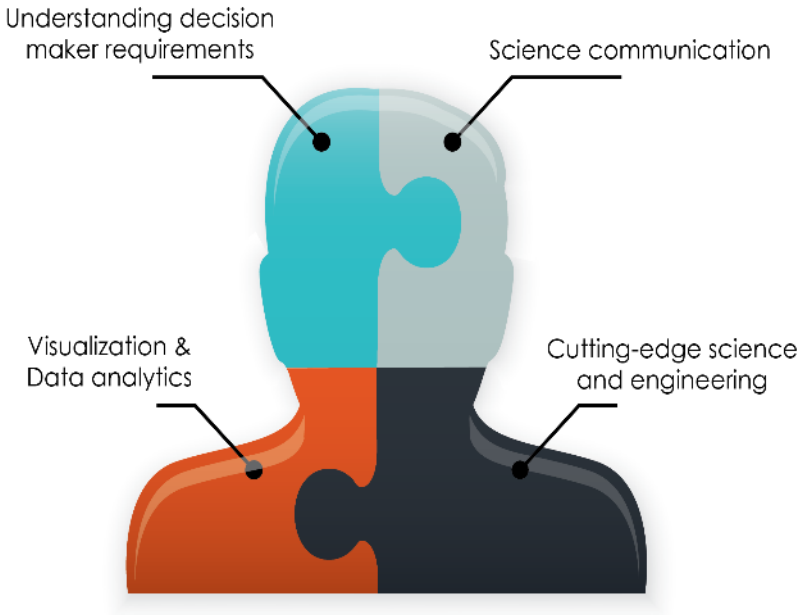
✧ 60 general courses

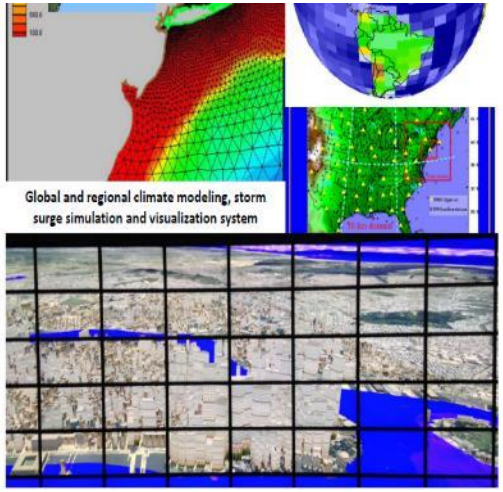
STRIDE



Science Training and Research to Inform DEcisions

Science Training & Research to Inform DEcisions (STRIDE)





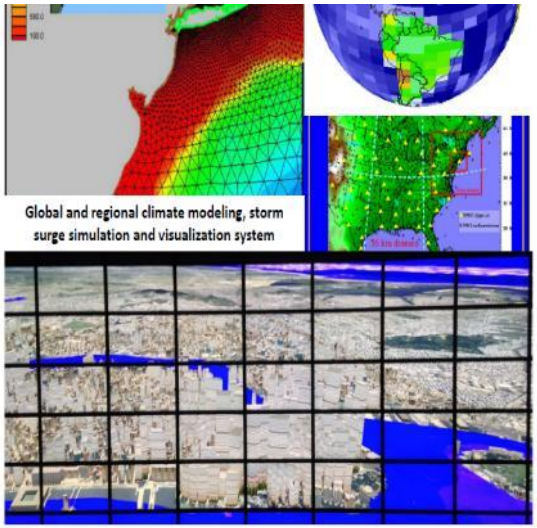
Vertically-integrated graduate training:

- 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



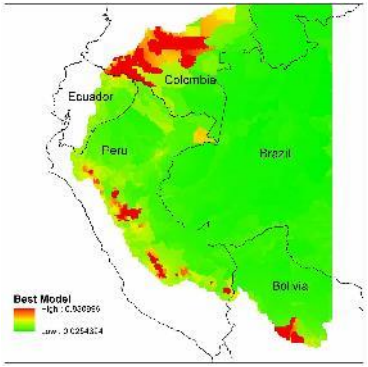
Decision-making often requires a rapid response ➤ Need experts that straddle the traditional divide between data-science and policy

Research Themes

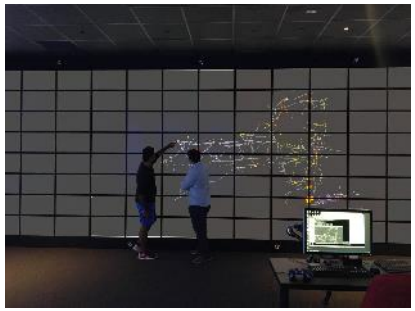
Climate Change and Coastal Resilience

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

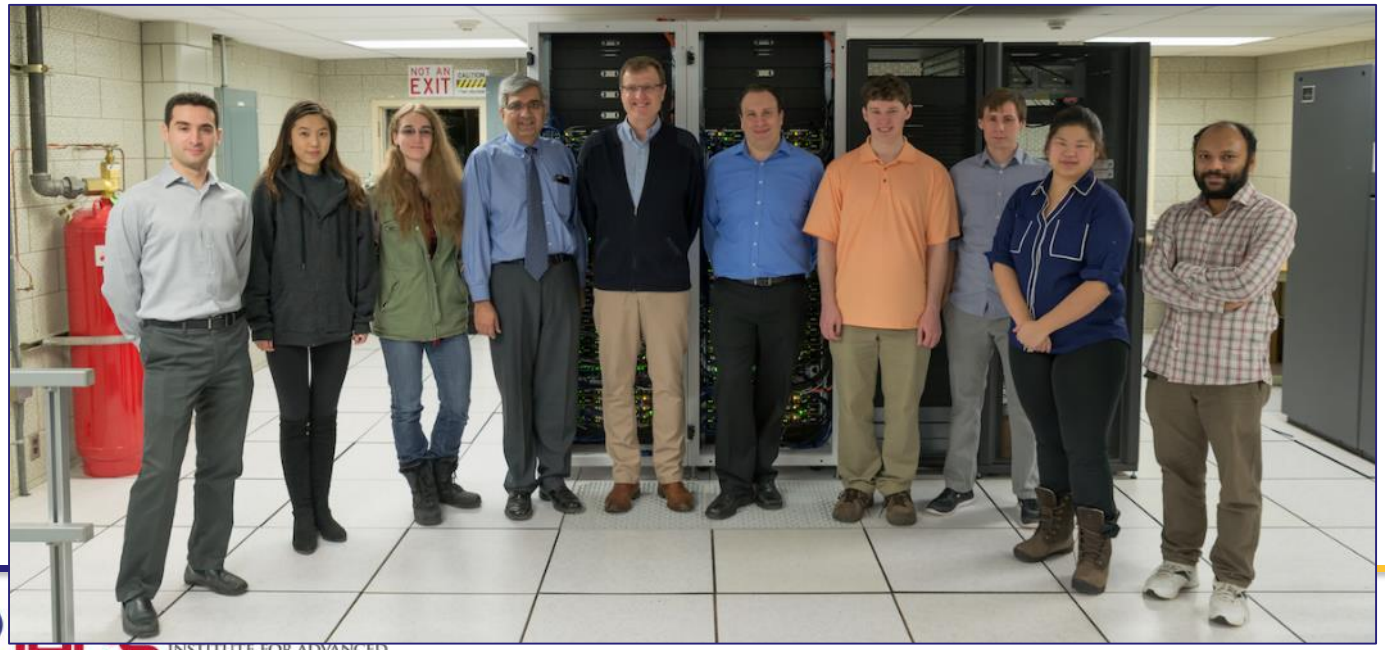
Carlos Simmerling
Laufer Center

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

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

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

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 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*

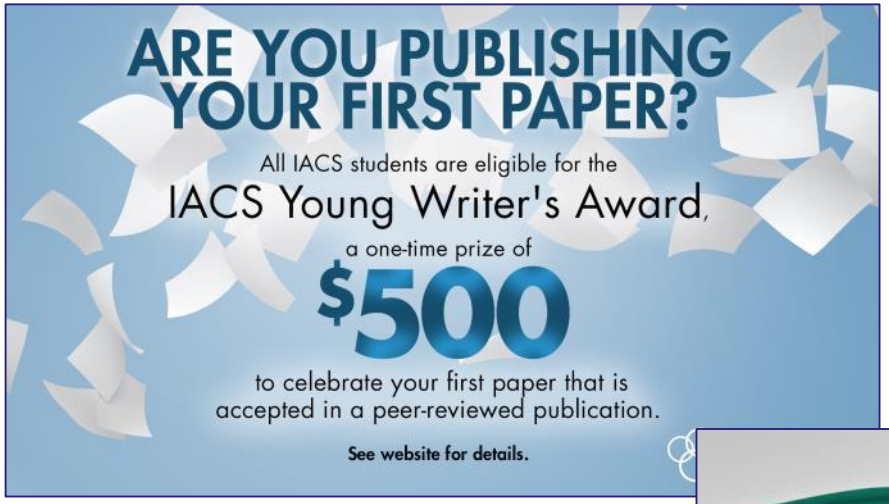
Maria Barrios Sazo (PHY) – *Simulations of Black Widow Pulsars and White Dwarf Mergers using Castro*

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



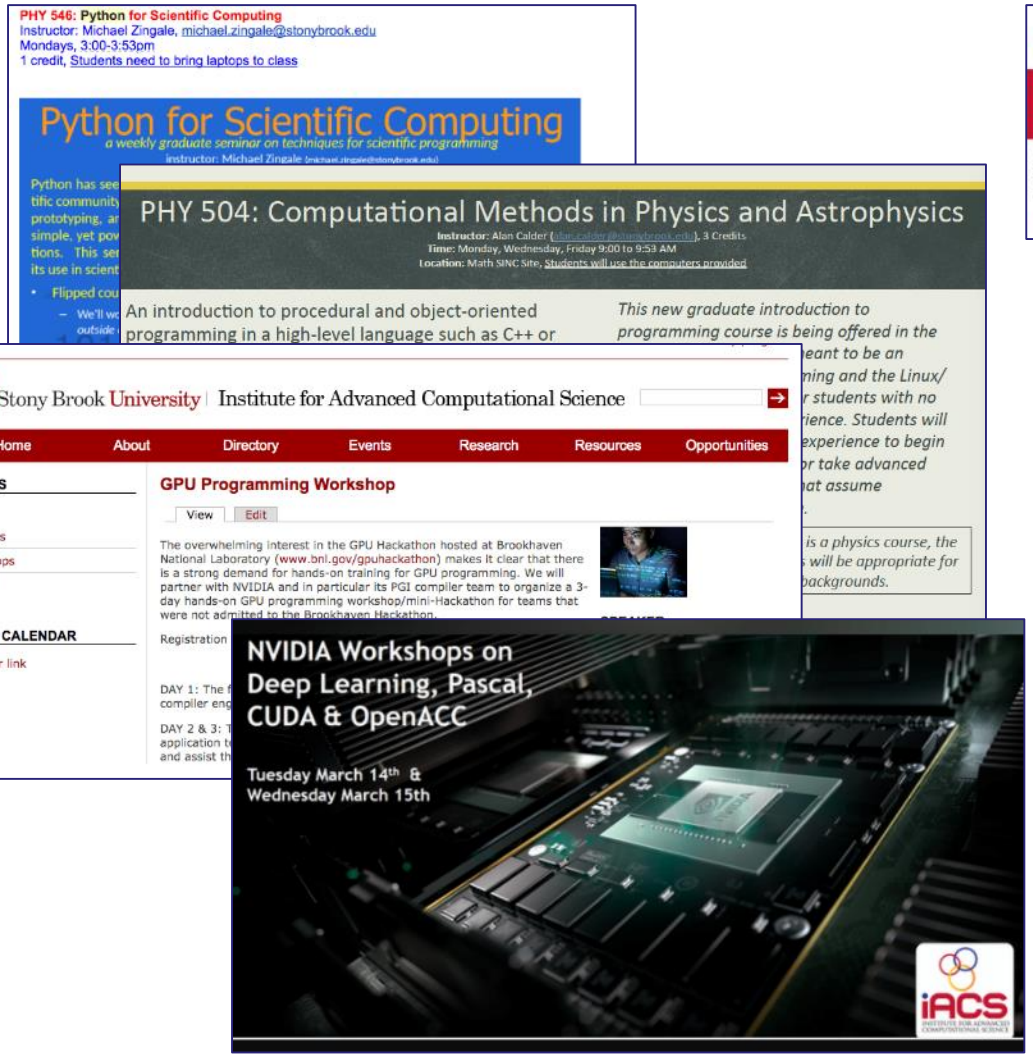
Writing

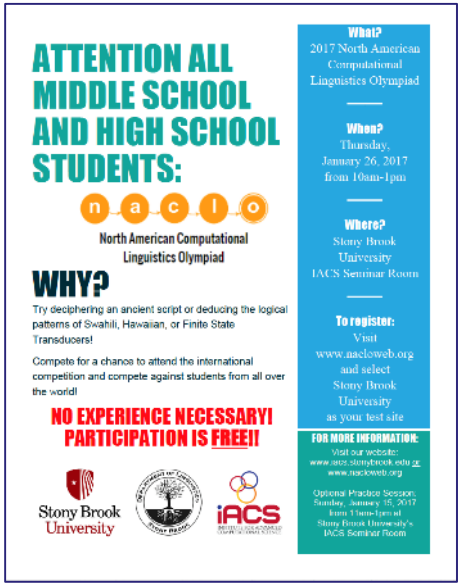
6 awarded in CY 2015
11 awarded in CY 2016
6 awarded in CY 2017 (so far)

Travel

7 awarded in 14/15
4 awarded in 15/16
8 awarded in 16/17

Workshops, Tutorials, Courses





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

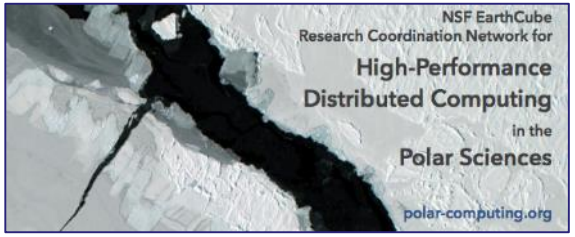
Adrian Soto-Cambres, Jr. Researcher Award Winner
Can Machine Learning Settle the Debate of the Dual Microscopic Character of Water?

Aditi Ghai, Jr. Researcher Award Winner
Towards Adaptive Hybrid Multigrid Method for PDE Based Systems

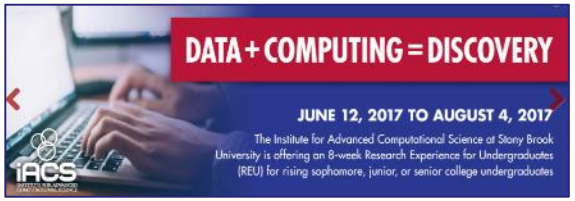
Associate Professor Marivi Fernandez-Serra
Understanding Water/Solid Functional Interfaces for Photocatalysis and Electrochemical Applications

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

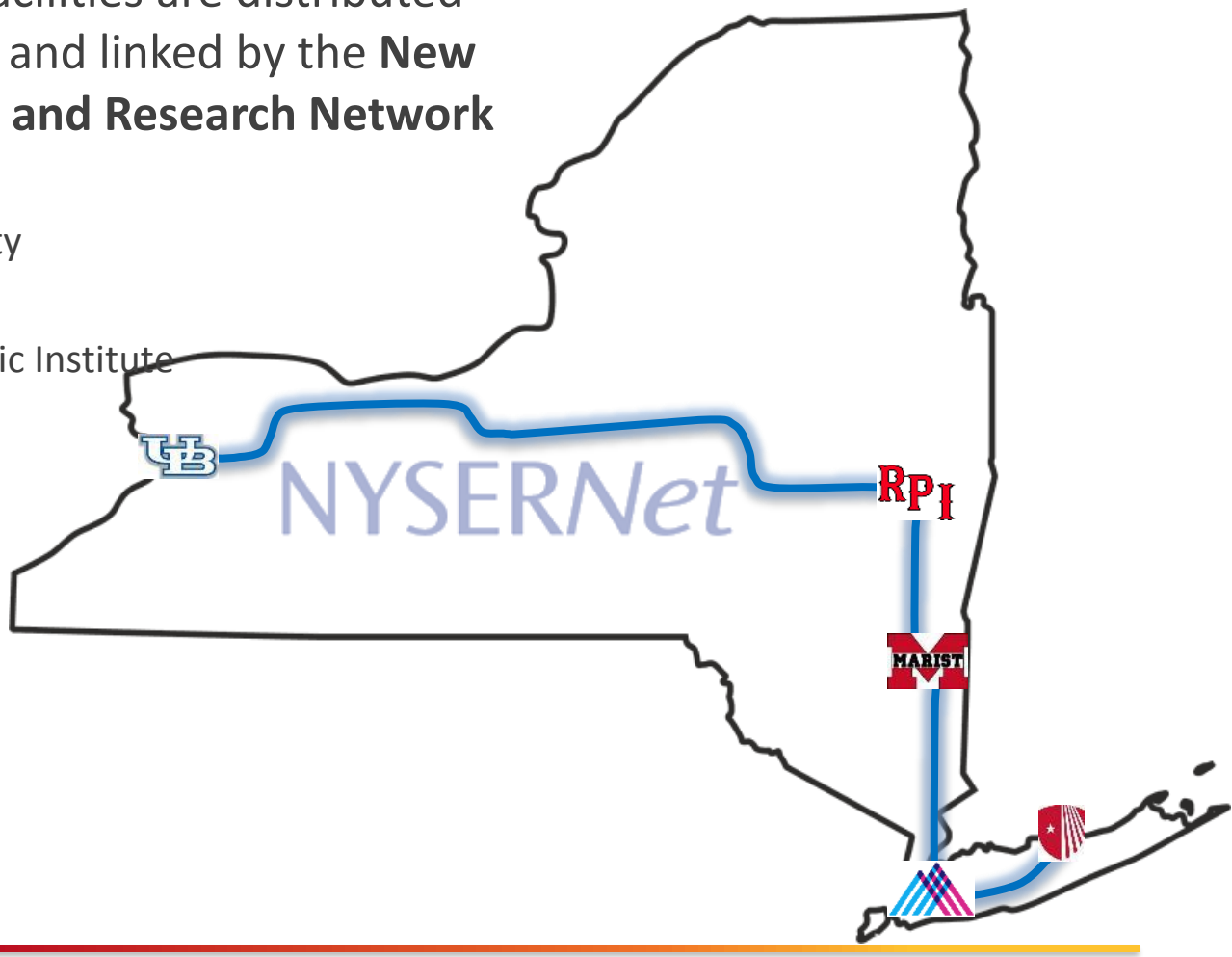
Institute for Advanced Computational Science

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

- HPC^2 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

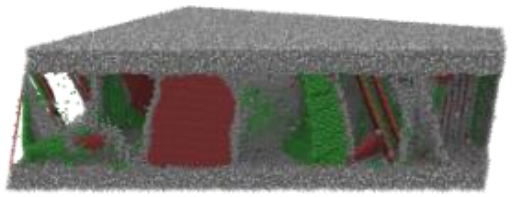


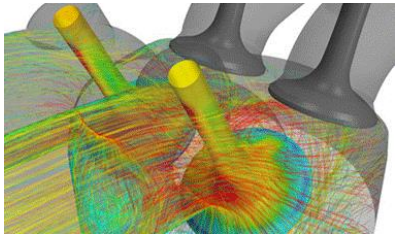
Powered by ESD/NYSTAR

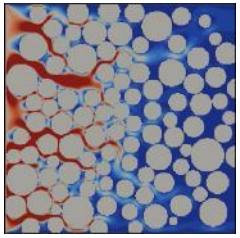
NYSTAR
Empire State Development
Division of Science, Technology & Innovation

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

innoveering
innovative engineering solutions

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

PIGTRONIX
FUTURISTIC AUDIO TECHNOLOGY

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.

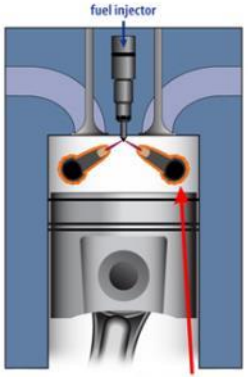
Success Story: Innoveering

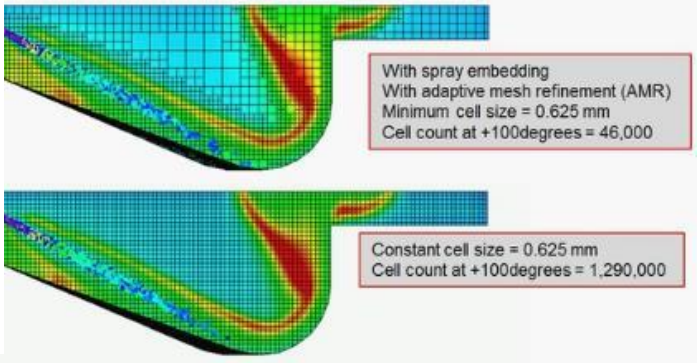
innoveering
innovative engineering solutions

- 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

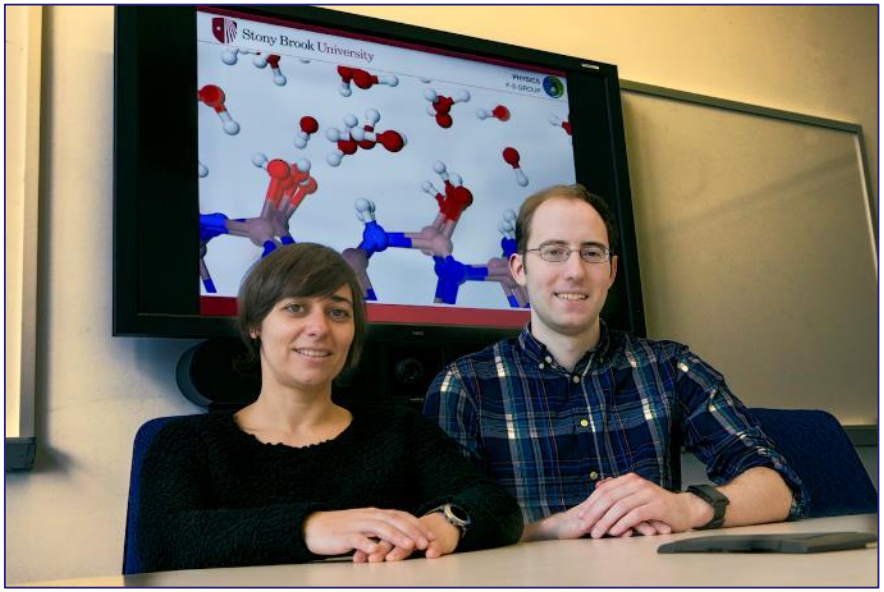
Jason R. Trelewicz

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



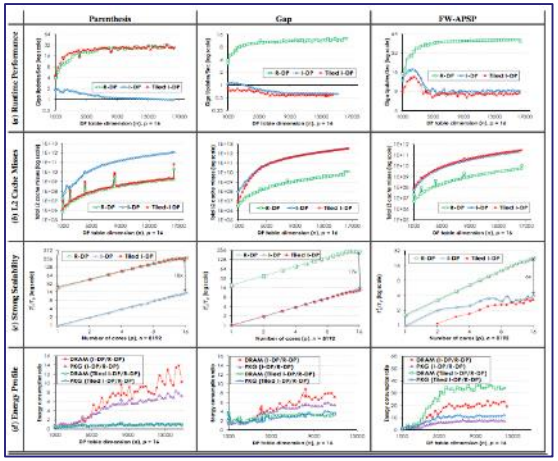
Marivi Fernandez Serra

Nature Communications

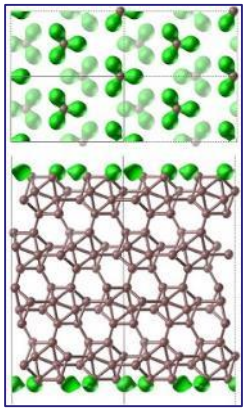
The Hydrogen-bond Network of Water Supports Propagating Optical Phonon-like Modes

Rezaul Chowdhury, PPoPP 2016

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

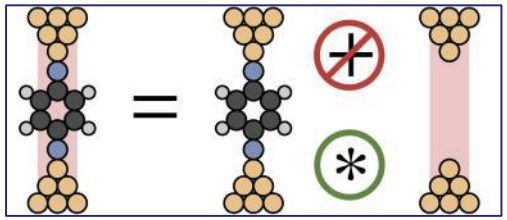


IACS Core Faculty Publications



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 syn 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

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

Tuesday, November 18, 2014
IACS Staff

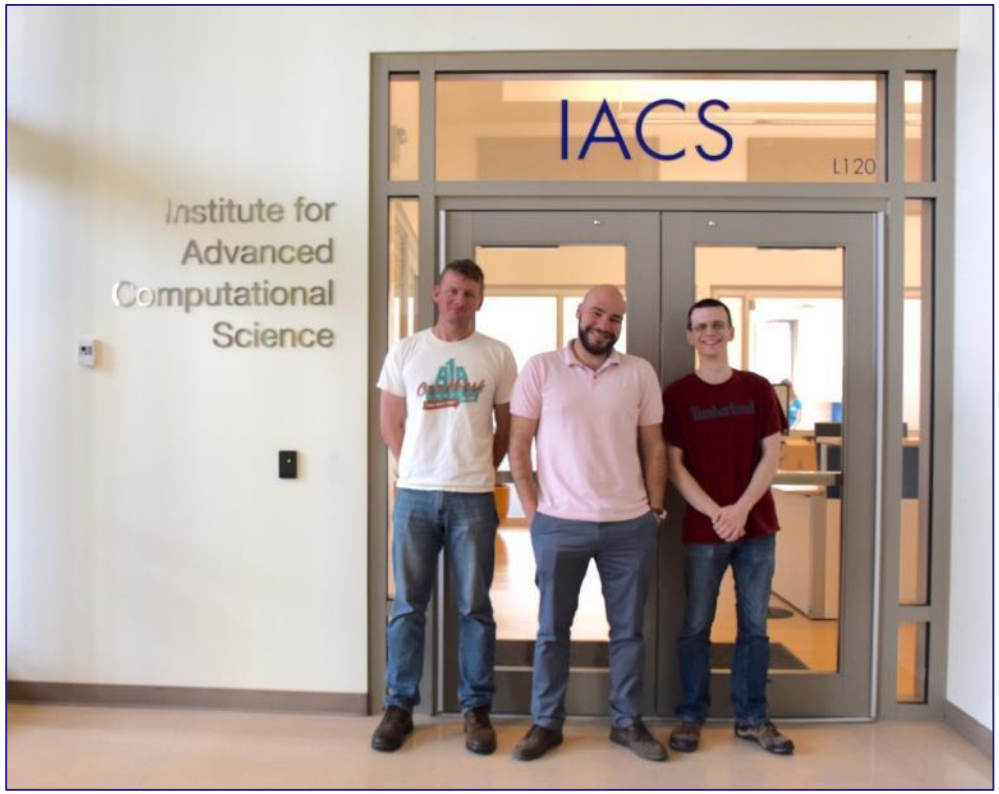
IACS Director Robert Harrison was awarded 15,000,000 processor hours, from the Department of Energy's INCITE Leadership Computing program, on Argonne National Laboratory's IBM Blue Gene/Q for his proposal entitled Dynamic and Adaptive Parallel Programming for Exascale Research. Along with Harrison, the 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

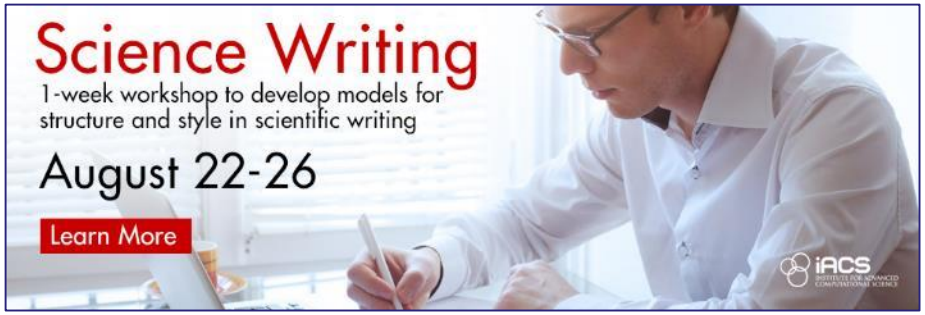
- Student-Faculty Dinners
- Group Outings to NYC

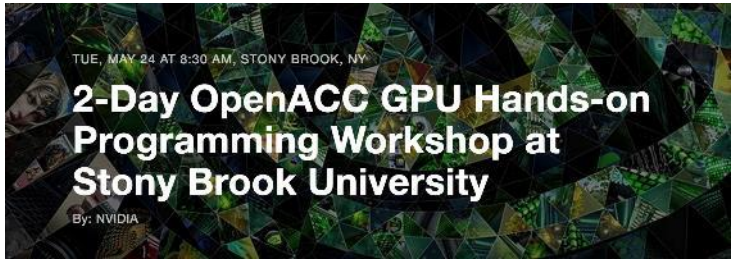
Social Networking

Drawing Diversity to Academia

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





IACS Travel Grants to SC1X

SuperComputing13

Gao Chao; Na Zhang;

Yufei Ren

SuperComputing14

Li Zhang; Jesmin Tithi

SuperComputing15

Na Zhang