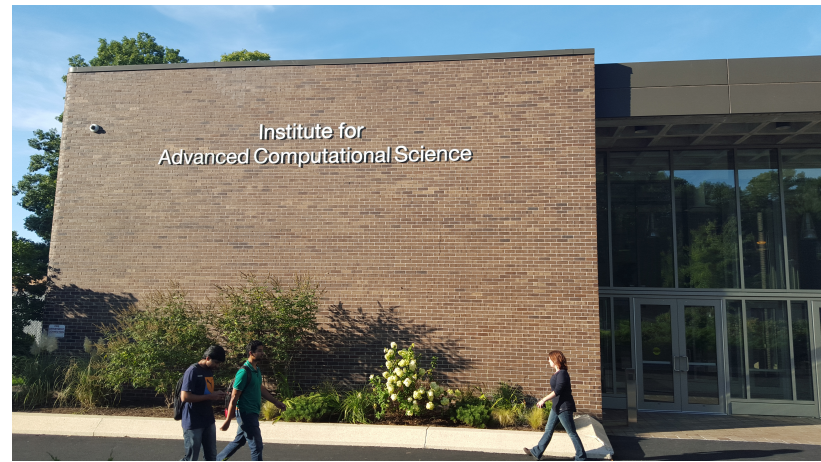# Institute for Advanced Computational Science

Robert J. Harrison, Director

robert.harrison@stonybrook.edu
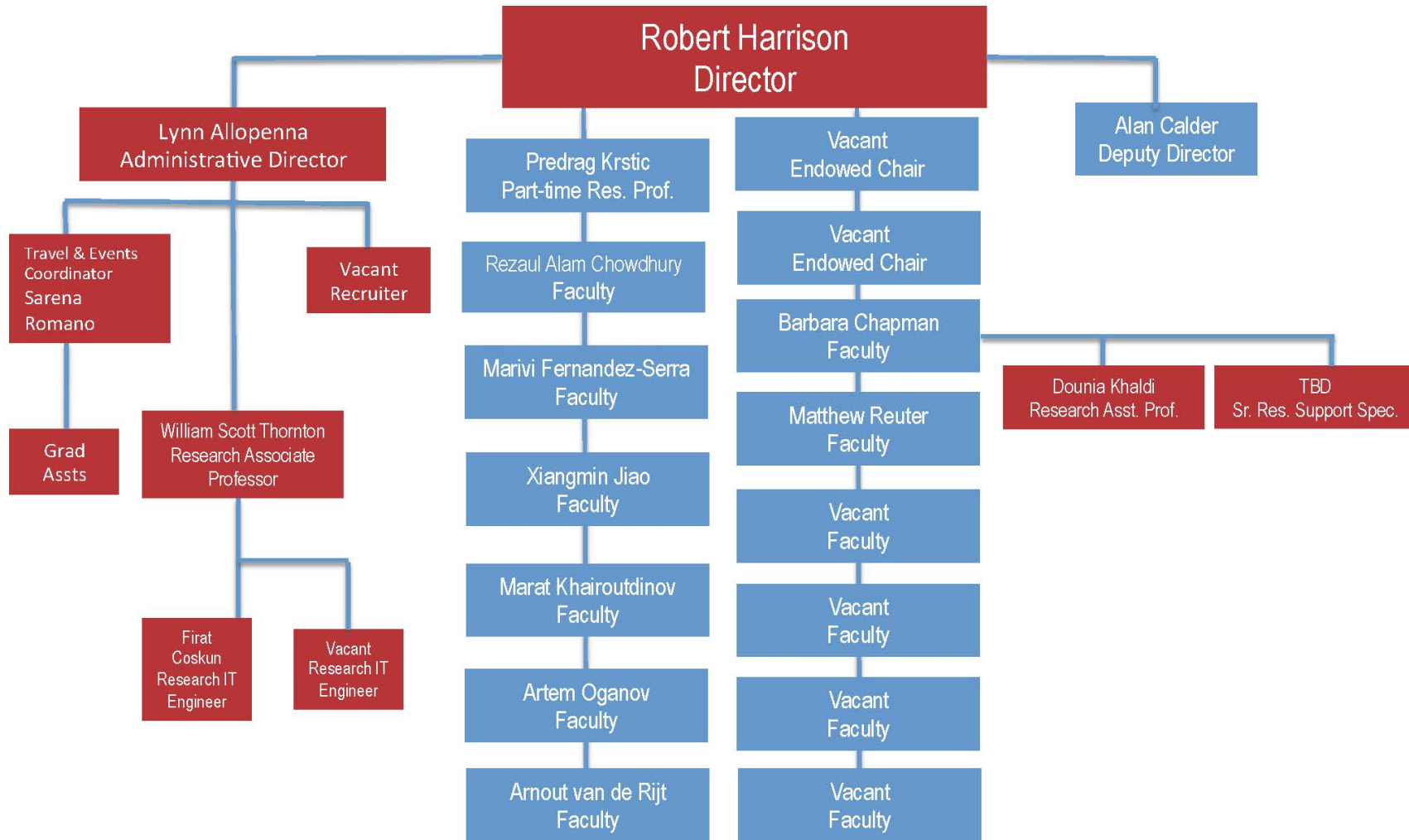
Stony Brook University
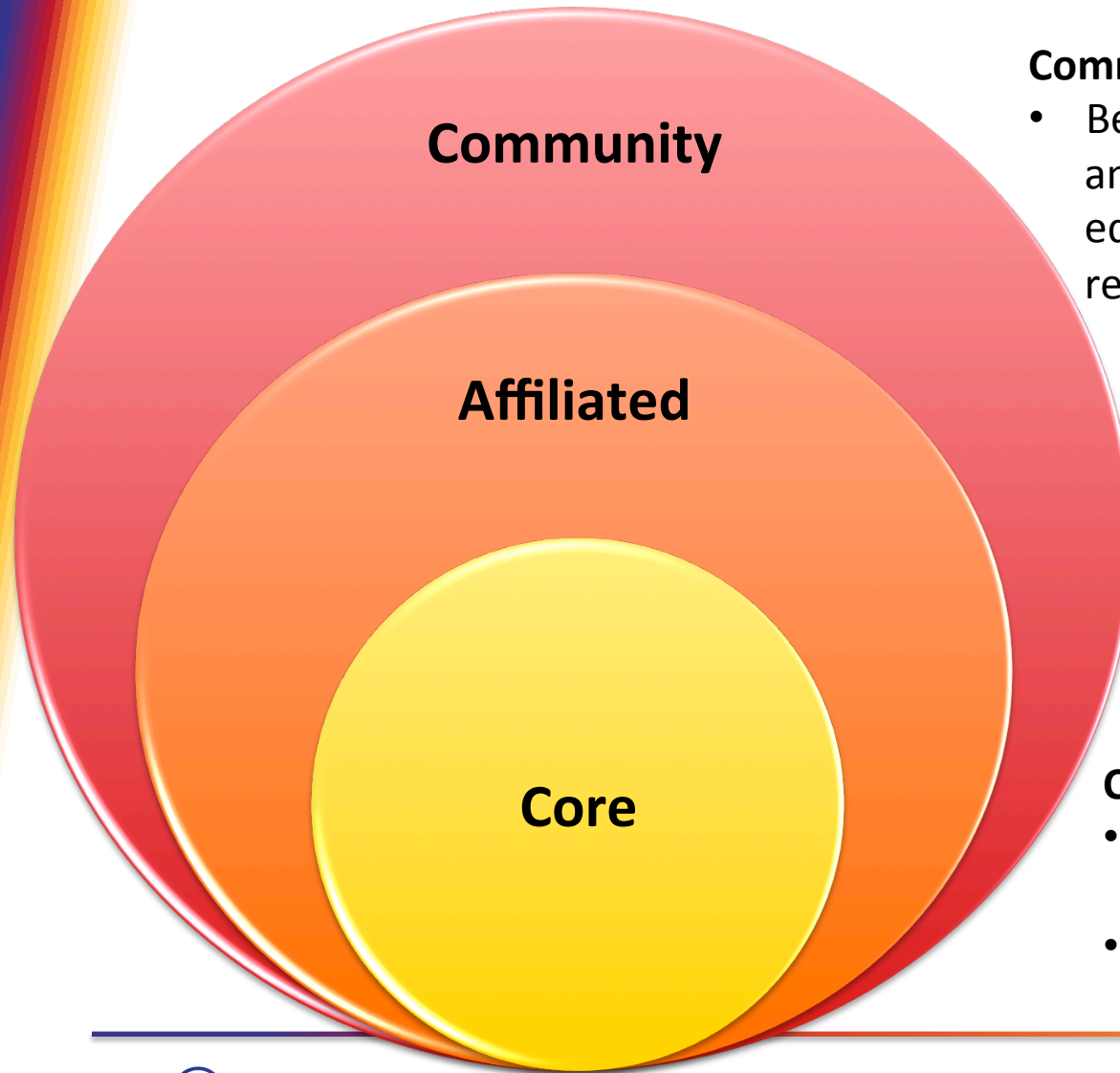
# What is IACS?



- A multidisciplinary institute with a focus on computational and data science

- $20M endowment to support 3 endowed chairs and operations (~$13M)

- 11 core faculty, 25 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

iACS INSTITUTE FOR ADVANCED COMPUTATIONAL SCIENCE

# Institute for Advanced Computational Science
## Organization Chart

**Stony Brook University**

**iACS — INSTITUTE FOR ADVANCED COMPUTATIONAL SCIENCE**

**Robert Harrison**
Director

**Lynn Allopenna**
Administrative Director

**Alan Calder**
Deputy Director

Predrag Krstic
Part-time Res. Prof.

Vacant
Endowed Chair

Travel & Events Coordinator
Sarena Romano

Vacant
Recruiter

Rezaul Alam Chowdhury
Faculty

Vacant
Endowed Chair

Grad Assts

William Scott Thornton
Research Associate Professor

Marivi Fernandez-Serra
Faculty

Barbara Chapman
Faculty

Dounia Khaldi
Research Asst. Prof.

TBD
Sr. Res. Support Spec.

Xiangmin Jiao
Faculty

Matthew Reuter
Faculty

Firat Coskun
Research IT Engineer

Vacant
Research IT Engineer

Marat Khairoutdinov
Faculty

Vacant
Faculty

Artem Oganov
Faculty

Vacant
Faculty

Arnout van de Rijt
Faculty

Vacant
Faculty

Vacant
Faculty

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# IACS Faculty and Community

**Community**

**Affiliated**

**Core**

**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

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# IACS Affiliate Faculty

- Leman Akoglu, Computer Science
- Philip Allen, Physics & Astronomy
- Yuefan Deng, Applied Math & Statistics
- Dilip Gersappe, Materials Science & Engineering
- James Glimm, Applied Math & Statistics
- Thomas Graf, Linguistics
- Jennifer Heerwig, Sociology
- Jason Jones, Sociology
- Patricia Kovatch, Icahn School of Medicine @ Mount Sinai
- Yan Li, American Physical Society
- Heather Lynch, Ecology & Evolution
- Sotirios Mamalis, Mechanical Engineering
- Marek Michalewicz, A*STAR Singapore
- Alexander Orlov, Materials Science &
  Engineering
- Joel Saltz, Bioinformatics
- Roman Samulyak, Applied Math & Statistics
- Steve Skiena, Computer Science
- Allen Tannenbaum, Computer Science
- Jason Trelewicz, Materials Science & Engineering
- Lee Warren, The College of New Rochelle
- Michael White, Chemistry
- Song Wu, Applied Math & Statistics
- Shinjae Yoo, Brookhaven National Laboratory
- Dantong Yu, Brookhaven National Laboratory
- Wei Zhu, Applied Math & Statistics
- Michael Zingale, Physics & Astronomy

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# IACS Research Themes
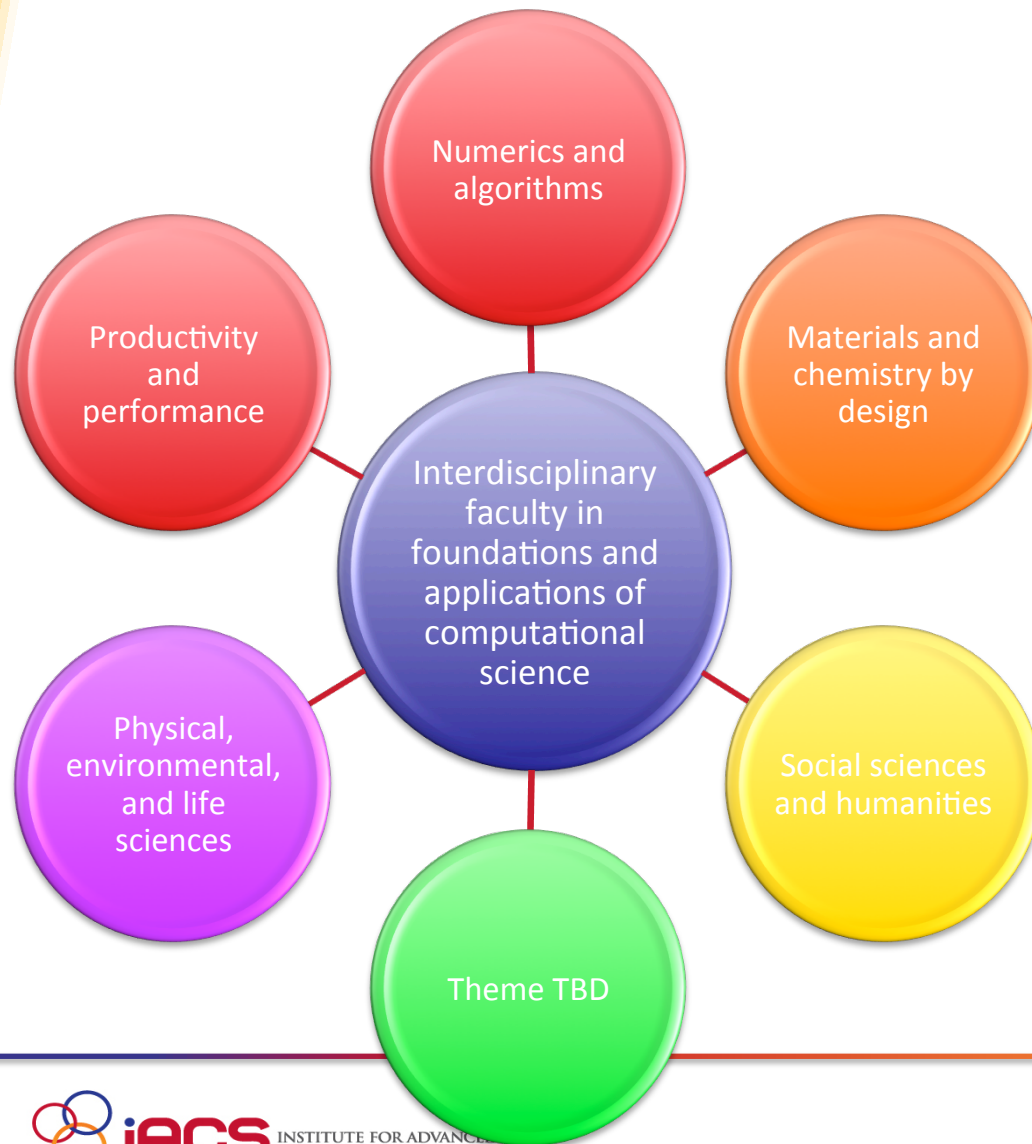


**Numerics and algorithms:**
Jiao, Chowdhury, Harrison, (all)

**Materials and chemistry by design:**
Fernández-Serra, Oganov, Krstić, Harrison, Reuter

**Social sciences and humanities:**
van de Rijt (and affiliates)

**Physical, env. and life sciences:**
Calder, Fernández-Serra, Reuter, Khairoutdinov, Oganov, Krstić

**Productivity and performance:**
Chapman, Chowdhury, Harrison (all)

# 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 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 directs Center for Data Driven Discovery and is chief computational scientist

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# 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


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# IACS Computer Resources

- Handy – startup funds
  - 40 dual-socket Sandybridge nodes, 2 GPUs, 2 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

- Sea-wulf – $1.4M NSF MRI + $300 NYSTAR + $300 SBU internal including $67K from IACS
  - 160+ dual-socket Haswell (?) nodes, 1PB disk, 32 GPUs

- Seed institutional approach to computing – more later

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# Year in Review

- Accomplishments
  - Publications, grants
- Events
- Fellowships and awards
-  Workshops and tutorials

# IACS Core Faculty Publications

35 publications in 2013
44 publications in 2014
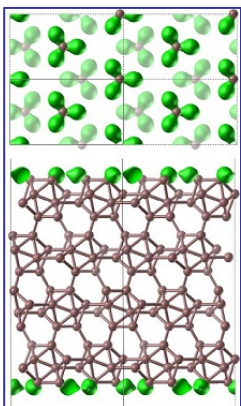
Artem Oganov, *Phys. Rev. Lett.*
*Unexpected Reconstruction of the α-Boron (111) Surface*

Matthew Reuter, ACS Nano
*Quantitative Interpretations of Break Junction Conductance Histograms in Molecular Electron Transport*
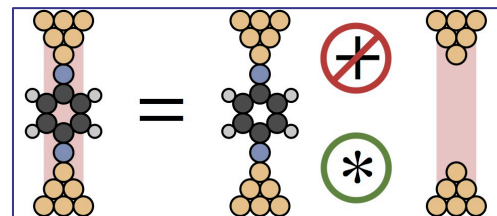
# IACS Core Faculty Grants

20 grants submitted in 2014 (15 NSF, 3 DoE, 1 NYSTAR, 1 BNL)

- ✧ Total value $33,738,224
- ✧ 6 grants awarded
- ✧ Total value $2,001,422

16 grants submitted to date in 2015 (9 NSF, 4 DoE, 1 NYSTAR, 1 EIP, 1 Silicon Mechanics)

- ✧ Total value $10,496,891
- ✧ 6 grants awarded to date
- ✧ Total value $4,031,934

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# 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

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# 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 Events

- IACS Seminar Series
- Workshops
- Networking
- Training
- Conferences

# Seminar Series

13 seminars held in 14/15
15 seminars planned for 15/16

BNL
LBNL
A*STAR
NYSERNet
Columbia U
Nanyang TU

NIST
Fudan U
U Buffalo
UT Austin
U Toronto
Ohio State

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## INFINICORTEX: ANOTHER PATH TO REACH EXASCALE SUPERCOMPUTING

DR. MAREK MICHALEWICZ
A*STAR COMPUTATIONAL RESOURCE CENTRE

THURS, AUG 27TH
IACS SEMINAR ROOM
1:00 PM

## TRADEOFFS IN THE DESIGN OF HIGH-PERFORMANCE COMPUTATIONAL SIMULATIONS IN SCIENCE AND ENGINEERING

DR. PHILLIP COLELLA
LAWRENCE BERKELEY NATIONAL LABORATORY

THURS, APRIL 2ND
LAUFER CENTER
ROOM 101 | 1:00 PM

## THE DATA SENSORIUM: MULTIMODAL EXPLORATION OF SCIENTIFIC DATA SETS

DR. MARGARET SCHEDEL
STONY BROOK UNIVERSITY

THURS, NOV. 5TH
IACS SEMINAR ROOM
1:00 PM

## MAKING SMALL DATA BIG: INSIGHTS FROM A LONG-TAIL GEOSCIENCE DOMAIN

DR. KERSTIN LEHNERT
LAMONT-DOHERTY EARTH OBSERVATORY
COLUMBIA UNIVERSITY

THURS, APRIL 9TH
LAUFER CENTER
ROOM 101 | 1:00 PM

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# IACS Fellowships



- Two awarded in 2014,
  total value $20,375
- Six awarded in 2015, total value $59,280
  - 2 new recruit fellowships
  - 4 junior research fellowships (2 new and 2 renewed for 2nd year)

# IACS Fellowships

## New Recruits

- DW Han, Physics
- Alex Borowicz, Ecology & Evolution
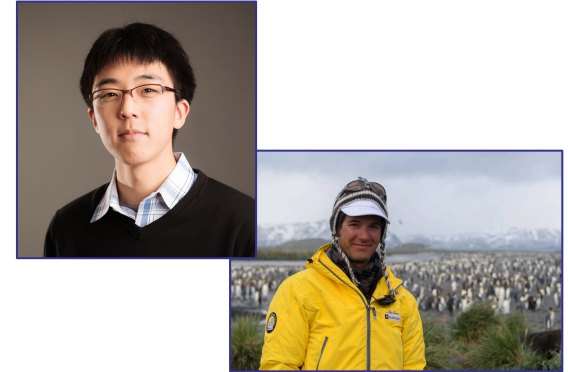
## Junior Researchers

Bryan Perozzi (C/S) - *machine learning techniques & graph algorithms for Big Data analysis applied to large-scale text and network data*

Adam Jacobs (Phys.) — *low-mach number modeling of explosive burning in double-detonation type Ia progenitors*

Philip McDowall (EE) — *computer-vision enabled spatial ecology of seabird coloniality*

Adrian Soto Cambres (Phys.) — *computation of dark matter - electron scattering rates for direct detection experiments*

# IACS Awards to Students



**Writing**

Five awarded in 14/15

Two awarded in 15/16 (so far)
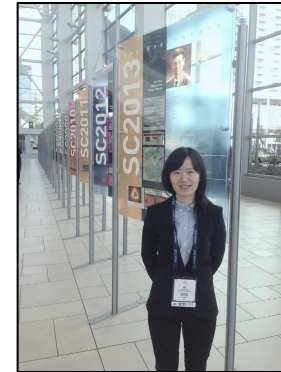
**Travel**

Seven awarded in 14/15
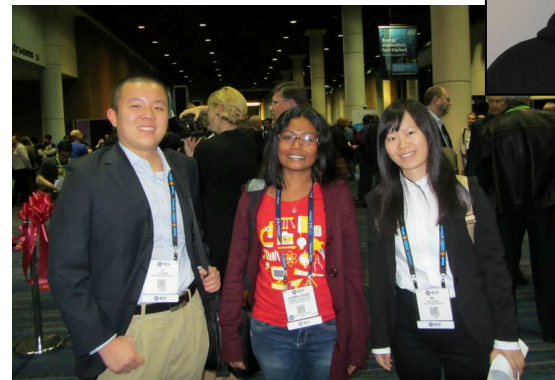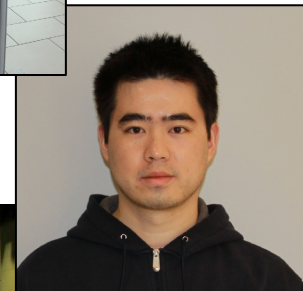
Two awarded in 15/16

# IACS Travel Grants to SC1X

SuperComputing13

Gao Chao; Na Zhang;
Yufei Ren

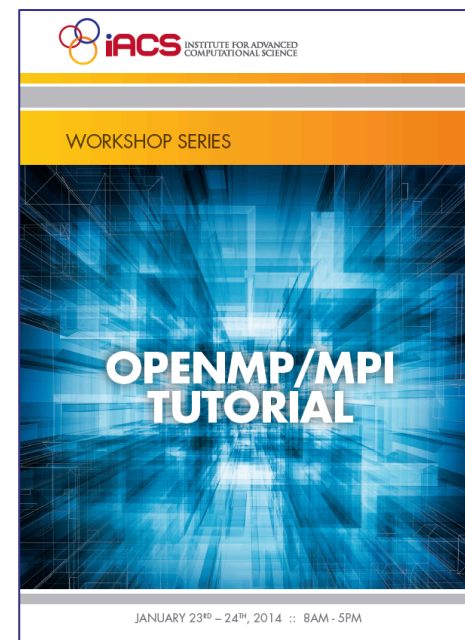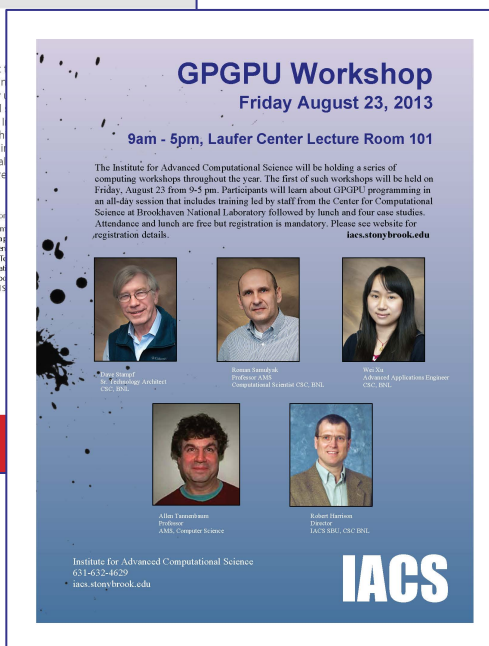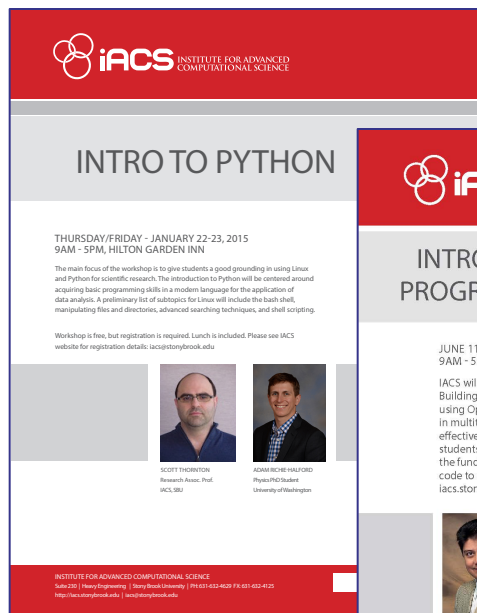SuperComputing14

Li Zhang; Jesmin Tithi

SuperComputing15

Na Zhang

# Workshops and Tutorials



Student backgrounds:

| | |
|---|---|
| SoMAS | AMS |
| Comp. Sci. | Geosciences |
| EE | Chemistry |
| Physics | BME |

Joint with BNL
Average attendance 40
Registration full in ~1 hour!
Preregister from CIE members; survey for topics

# Social Networking

# Training



2-week summer camp
18 colleges represented
34 students participated

1-week writing course
15 students participated

1-week summer camp
8 high schools represented
10 students participated
2 scholarships awarded

# Conferences
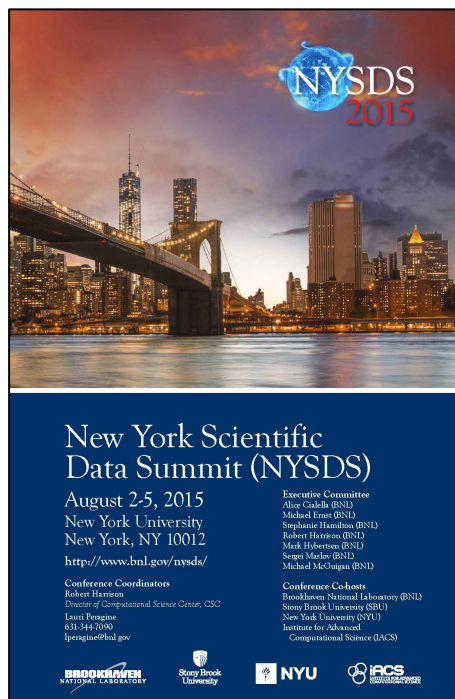


NY Scientific Data Summit
August 2-5, 2015
New York University



Sensitivity, Error and Uncertainty
Quantification for Atomic, Plasma
and Material Data
November 5-7, 2015
IACS @ SBU



Sustainable Software for Chemistry & Materials
March 28-30, 2014
SBU Manhattan

# 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

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# Rezaul Alam Chowdhury



Assistant Professor

- Computer Science Department

- Leads the Theoretical and Experimental Algorithmics (TEA) Group

- Research involves cache-oblivious algorithms and data structures, shared-memory parallelism, structural bioinformatics

- 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 National Science Foundation

# 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.

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# 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

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# Xiangmin Jiao
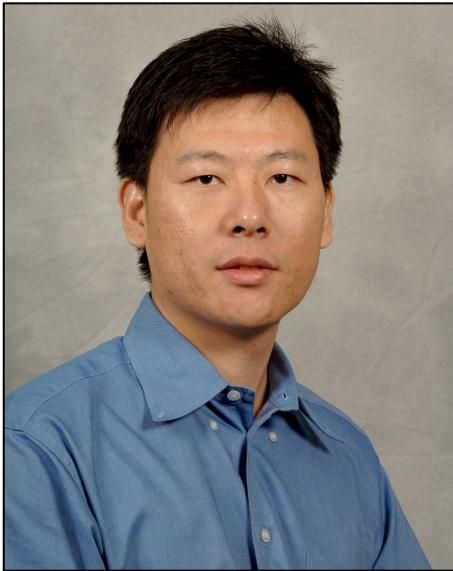


Associate
Professor

- 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.

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# 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

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# 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

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# Arnout van de Rijt

Associate
Professor

- Sociology Department
- Research exploits novel data collection opportunities enabled by present-day communication technology to answer longstanding questions about the origins of social order and societal inequality
- For contributions to social network analysis, received the 2010 Freeman Award for Distinguished Junior Scholarship
- Research is supported by the National Science Foundation and has been published in American Sociological Review, American Journal of Sociology, and PNAS

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# Supporting Hires

- Arnout van de Rijt
  - 5-years graduate student support

- Jason Jones
  - 2 months summer salary for 2 years

- Matthew Reuter
  - 1 year salary

- Jennifer Heerwig
  - Affiliate status

- Dima Kozakov
  - $60K of compute nodes

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# Located next to Laufer Center

# Our new space