Institute for Advanced Computational Science

Robert J. Harrison, Director
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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
Institute for Advanced Computational Science
Organization Chart

Robert Harrison
Director

Lynn Alloppena
Administrative Director

Predrag Krstic
Part-time Res. Prof.

Vacant Endowed Chair

Rezaul Alam Chowdhury
Faculty

Vacant Endowed Chair

Marivi Fernandez-Serra
Faculty

Barbara Chapman
Faculty

Matthew Reuter
Faculty

Xiangmin Jiao
Faculty

Vacant
Faculty

Maret Khairoutdinov
Faculty

Vacant
Faculty

Artem Oganov
Faculty

Vacant
Faculty

Arnout van de Rijt
Faculty

Vacant
Faculty
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 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
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
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 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
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

*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
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
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
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

INTRO TO PYTHON

THURSDAY/FRIDAY - JANUARY 22-23, 2015
9AM - 5PM, HILTON GARDEN INN

The main focus of the workshops is to give students a good grounding in using Linux and Python for scientific research. The introduction to Python will be centered around acquiring basic programming skills in a modern language for the application of data analysis. A preliminary list of subtopics for Linux will include the bash shell, manipulating files and directories, advanced searching techniques, and shell scripting.

Workshop is free, but registration is required. Lunch is included. Please see IACS website for registration details: iacs@stonybrook.edu

THURSDAY/FRIDAY - JANUARY 22-23, 2015
9AM - 5PM, HILTON GARDEN INN

INTRODUCTION TO PARALLEL PROGRAMMING USING OPENMP

JUNE 11, 2015
9AM - 5PM, IACS BUILDING

IACS will hold a 1-day, free, hands-on workshop at Building featuring tutorials on parallel programming using OpenMP. OpenMP is one of the most widely used in multiprocessor programming and is an essential effective program today. Students will get an introduction to OpenMP and will experience hands-on parallel programming code to solidify their understanding of the material. For more information, see the workshop website:

http://iacs.stonybrook.edu

INTRO TO PYTHON

SCOTT THORNTON
Research Assoc. Prof.
IACS, SBU

ADAM RICHIE
HALFORD
Physics PhD Student
University of Washington

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

Student backgrounds:
SoMAS
Comp. Sci.
AMS
EE
Geosciences
Physics
Chemistry
BME
Social Networking

IACS 1st Annual Apps & Ale Social

Welcome!
Let’s start off the semester with a toast!
Join us for apps and ale as we welcome back old friends, welcome new friends and toast to a great year!
Friday, September 11, 2015, 3:00pm – 5:00pm
IACS, Seminar Room

Please RSVP to Serena Romanos using the link provided by August 31st

IACS Students and Postdocs Networking Social

May 5, 2015
4:30-7 PM
Bliss Restaurant
766 New York 25A, Setauket
(631) 941-0430

Come socialize and network with your IACS colleagues over free dinner and drinks

By Invitation Only
RSVP: A Must

Join us if you dare.....

Eyeballs, bloody cocktails and witches brew, and some many more (like a finger or two).
Students de facundo, come to our party this night, the most creative costume will win best fright.

IACS Pre-Halloween Costume Party
Costume Contest
First Prize $100
Friday, October 23, 2015, 6-9 pm
IACS Seminar Room
Training

This workshop will focus on improving structure and organization of professional writing for graduate students in computational science. Through critical analysis and writing exercises, we will explore the relationship between words and sentences, and our understanding of grammar and effective writing. We will work together to develop a heightened sensitivity to the relationship between words in a sentence. We'll use these discussions of grammar to develop better style – more concise and more effective writing, which better communicates complex ideas. This practice in English grammar will also encourage a more logical presentation of ideas, and a tighter structure for your written work.

We will also spend considerable time finding examples and models in the journals and databases students already use for secondary research. We will look at some published articles together in class and ask students to choose appropriate published work to use as models and to develop your own work from those examples.

In the process, I hope to encourage you to draft and revise, to recognize the importance of reading and revising your own work to find opportunities for improvement.

**MONDAY AUGUST 17-21, 2015**

**9AM - NOON, IACS MULTIMEDIA ROOM**

**INSTITUTE FOR ADVANCED COMPUTATIONAL SCIENCE**

Stony Brook University

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**DEVELOPING MODELS FOR STRUCTURE AND STYLE IN SCIENTIFIC WRITING**

**JENNIFER ALBANESE**

Interim Associate Director
SBU Writing & Rhetoric Program

Jennifer Albanese is currently the Interim Associate Director of the Writing & Rhetoric Program where she has taught for sixteen years. Beginning in Fall 2015, Dr. Albanese will also be Director of the Campus Writing Center. She has taught courses for the Graduate Chemistry program and the Center for Communicating Science at Stony Brook University.

**The Institute for Advanced Computational Science at Stony Brook University is offering a one-week programming workshop for high school students and seniors. Students must be 15 years old or older. The workshop, 'edge' camp, introduces students to the programming skills and software/computer technologies that drive advances in science, industry, business and society. Students will learn how to use Python, a high-level, easy-to-learn language, to solve problems in science and engineering, and will take part in team projects motivated by these science research challenges. By the end of the camp, students will have sufficient programming skills and awareness of the field to pursue further independent study and to inform their college search for admission and majors. Ideally students will use their own laptops (Python, C++, or a Java type are acceptable), but if they are available for loan they can continue to use the camp’s open-source software programming environment and tools.”

**1-week summer camp**

18 colleges represented

34 students participated

**1-week writing course**

15 students participated

**2-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

- 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

- 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

- 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

- 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.

Associate Professor
Robert J. Harrison

• 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
Xiangmin Jiao

• 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

- 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

- 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
Artem R. Oganov

- 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

- 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
Arnout van de Rijt

- 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
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
Located next to Laufer Center
Our new space