



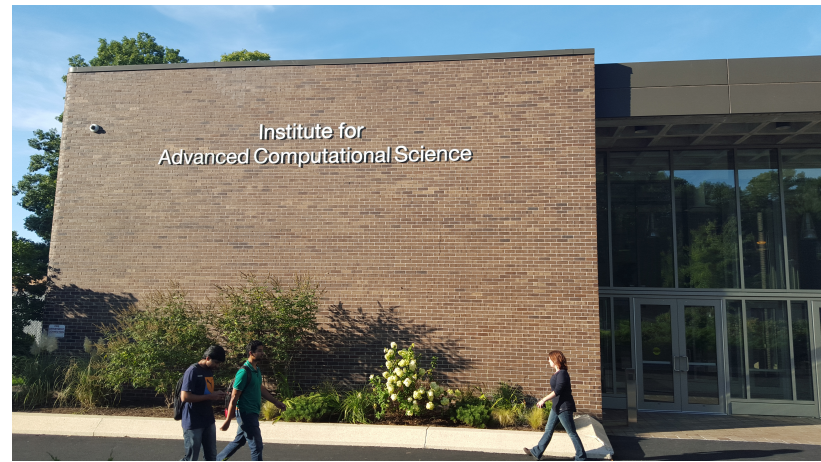
Institute for Advanced Computational Science

Robert J. Harrison, Director
robert.harrison@stonybrook.edu

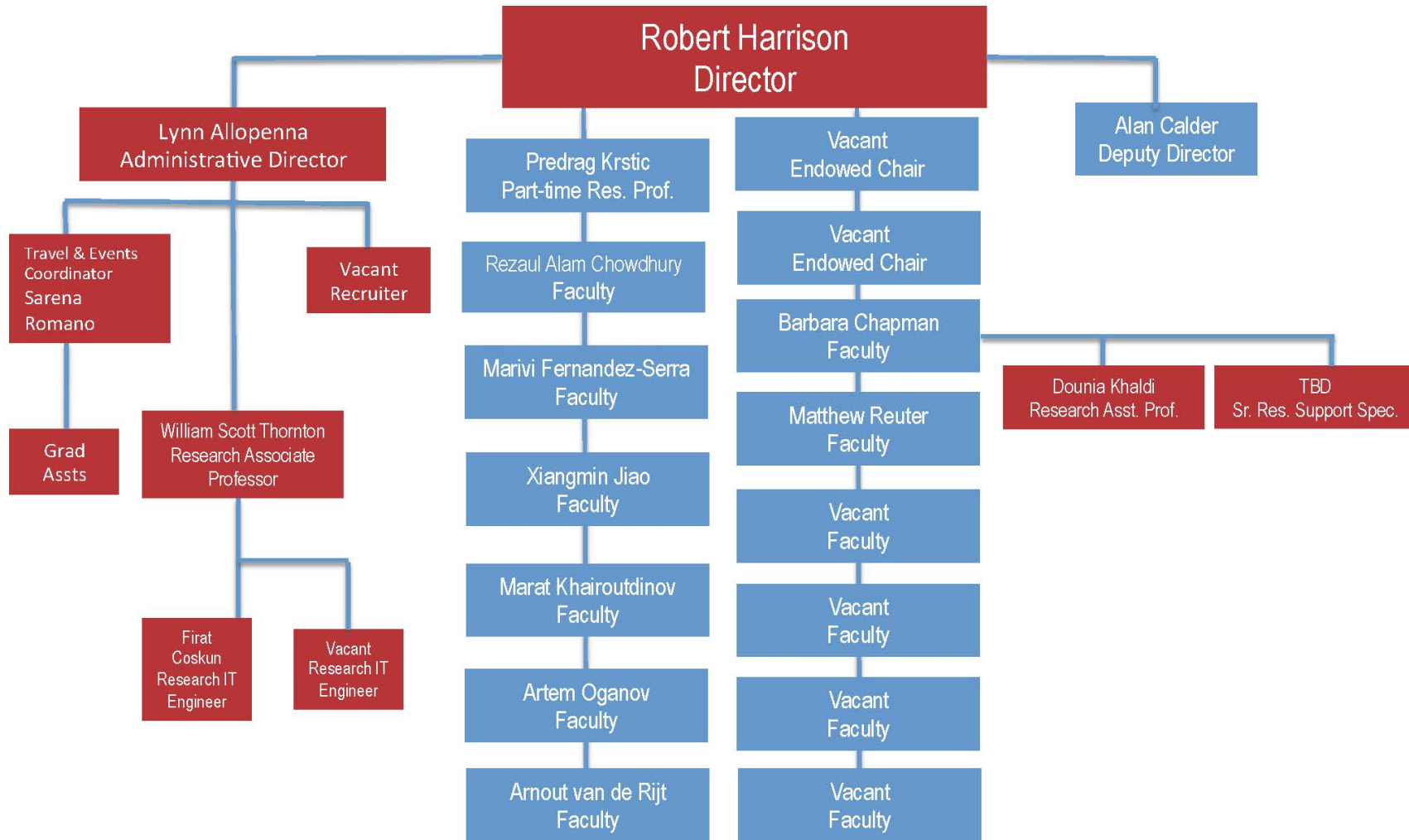


Stony Brook University

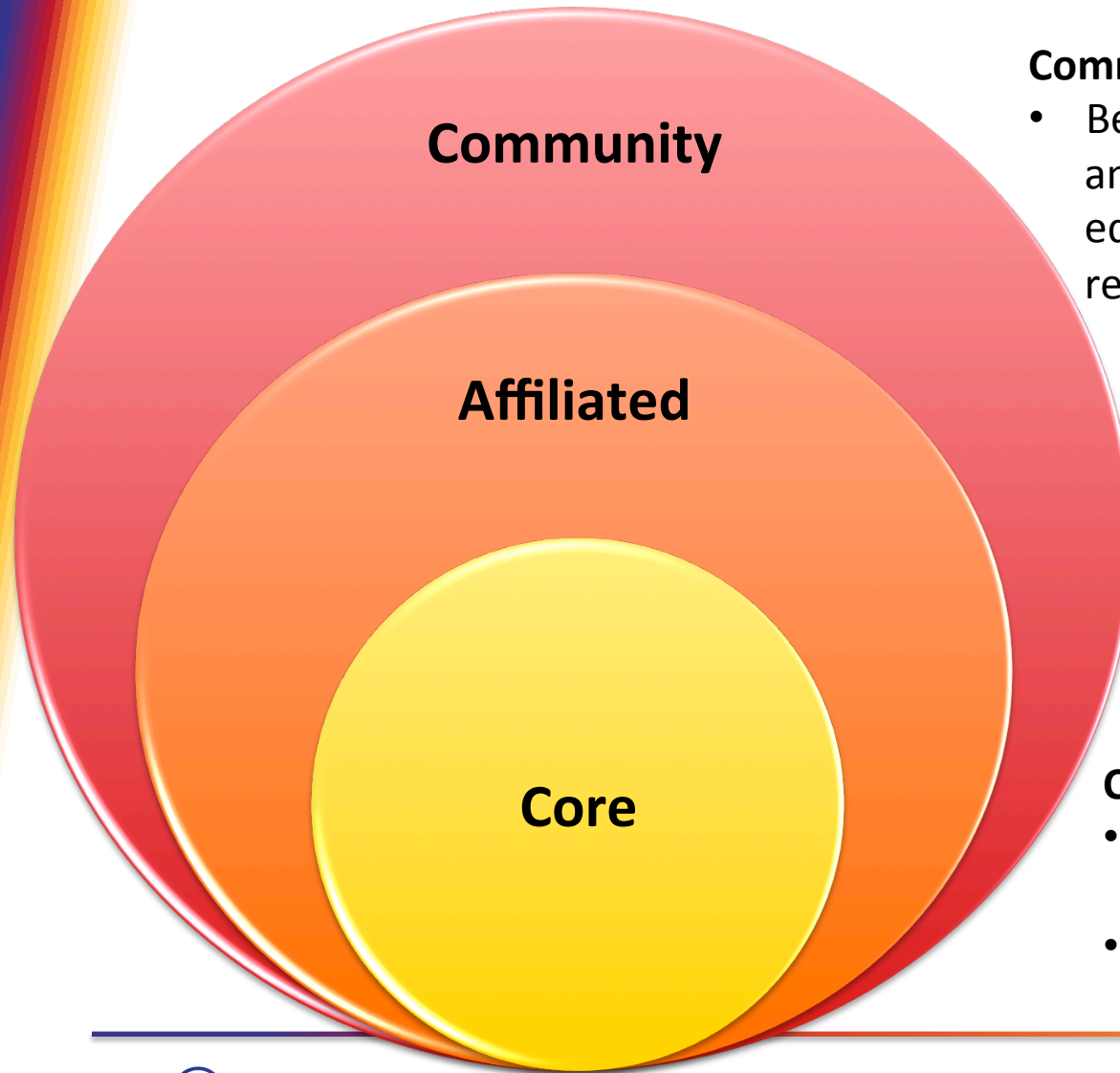
What is IACS?



- 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 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

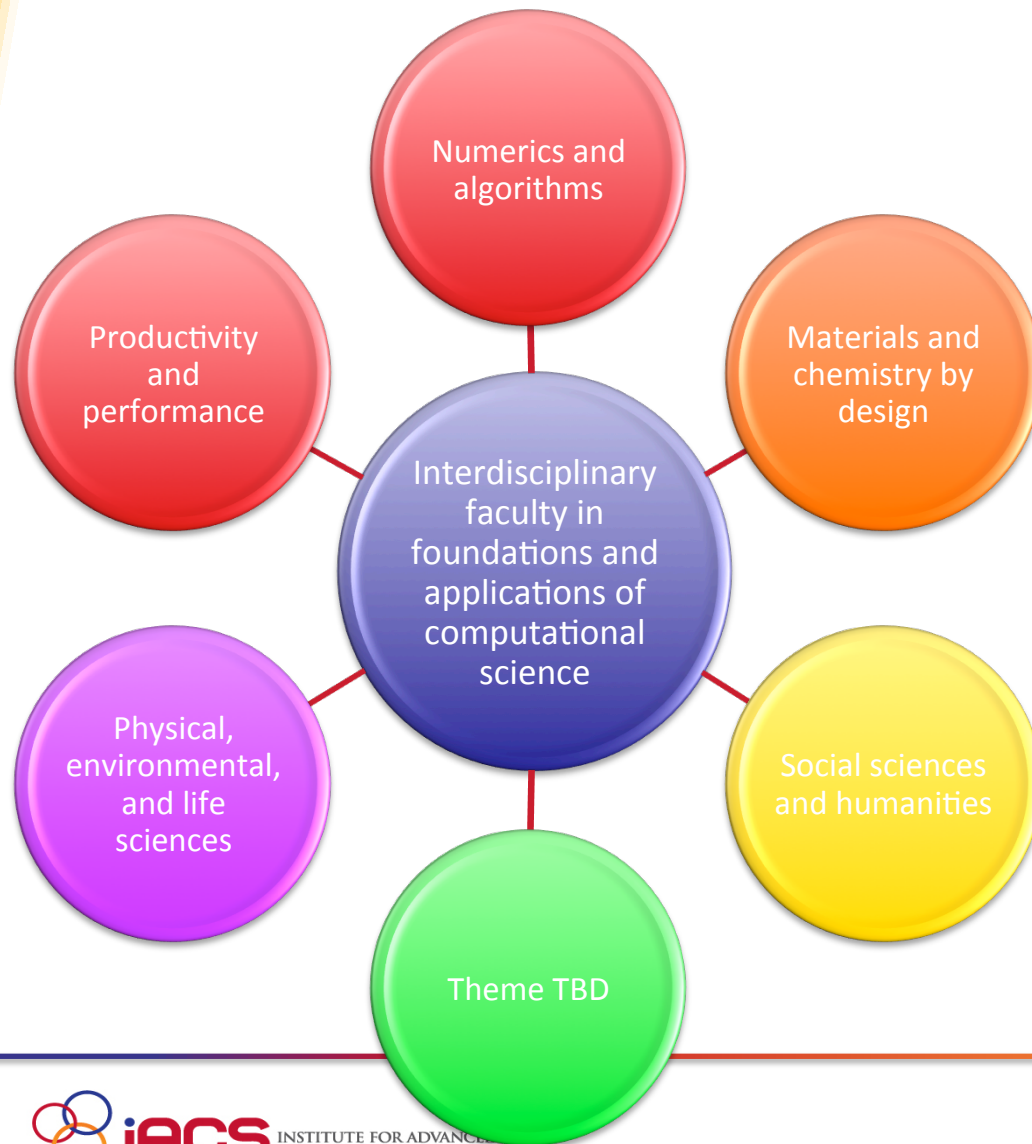
Core faculty and students

- 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

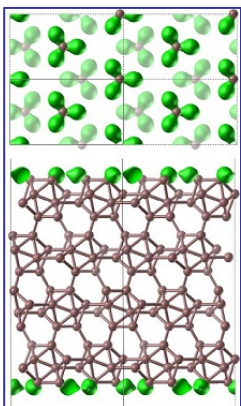
- Handy – startup funds
 - 40 dual-socket Sandybridge nodes, 2 GPUs, 2 KNC, 250 TB disk
- LI-red – \$1M grant from regional economic development council
 - 100 dual-socket Haswell nodes, 250 TB disk
 - 1 quad-socket Haswell node with 3 TB memory
 - 1 IBM Power8 node
- Sea-wulf – \$1.4M NSF MRI + \$300 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

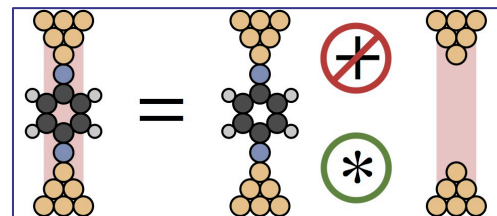
35 publications in 2013
44 publications in 2014



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

Grant Highlights

Major Research Instrumentation (MRI)

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

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

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

Grant Highlights

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



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

Tuesday, November 18, 2014
IACS Staff



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

Research Summary

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

IACS Events

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

Seminar Series


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

iACS INSTITUTE FOR ADVANCED COMPUTATIONAL SCIENCE

INFINICORTX: ANOTHER PATH TO REACH EXASCALE SUPERCOMPUTING

DR. MAREK MICHAŁEWICZ
A*STAR COMPUTATIONAL RESOURCE CENTRE

THURS. AUG. 27th
iACS SEMINAR ROOM 1:00 PM



The Infinicortex is a metaphor of a human brain-scale system. The cortex is a dense, concurrent supercomputing across the globe utilizing heterogeneous hardware and software. We have integrated four separate important and interesting concepts to realize Infinicortex:

- (i) High bandwidth intercontinental connectivity between Asia (Singapore, Japan), Australia, the USA and Europe (France).
- (ii) High bandwidth intercontinental connectivity between Asia (Singapore, Japan), Australia, the USA and Europe (France).
- (iii) High bandwidth intercontinental connectivity between Asia (Singapore, Japan), Australia, the USA and Europe (France).
- (iv) Connecting separate interlinked sub-nets with different node topologies to create a single computational resource Galaxy of Supercomputers.

to Workflow and applications on such a concurrent, distributed computational infrastructure, especially using HPC/Cloud framework.

This year, at SC15 in Austin, TX, we will demonstrate the most extensive Infinicortex demonstration to date – comparing the world's first communication by Infinicortex, with most of the world's top 500 supercomputers. Applications are being tested from many sites and will include genomics, various bioinformatics, medical image analysis, plasma reactor simulation, superconducting device simulation, etc. It is planned to screen for network traffic direction at the node and connection, and for network bandwidth data as well as visual display of applications from all partners.

Dr. Marek Michałewicz is the Chief Executive Officer at A*STAR Computational Resource Centre. Marek holds a PhD degree in Theoretical Physics from the Institute of Advanced Studies, The Australian National University, Australia, and an MSc in Theoretical Physics from La Trobe University, Australia. He is a computational scientist, entrepreneur and inventor. Between 1980-90s he was at the University of Minnesota where he worked on computational research using Minnesota Supercomputer Center's Cray 2, which at the time was the most powerful computer in the world. Marek has extensive first-hand experience with vector, parallel, vector parallel, MIMD & SIMD supercomputers and large scale clusters.

iACS INSTITUTE FOR ADVANCED COMPUTATIONAL SCIENCE

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

DR. MARGARET SCHEDEL
STONY BROOK UNIVERSITY

THURS. NOV. 5th
iACS SEMINAR ROOM 1:00 PM



Big data is one of the defining problems of our time: we are interested in a torrent of information from scientific discoveries, news, social circles, and the devices we carry. The challenge is to distill all this abstract data into useful conclusions. The Data Sensorium was launched in 2011 to foster novel kinds of collaborations to yield new insights. Collaborations are not merely fashionable: they are critical to tackling modern scientific and engineering challenges. However collaborations are typically thought of in terms of bleeding across conventional discipline boundaries. While these "weary" interactions (e.g. between physicists and chemists) are undoubtedly valuable, the Data Sensorium instead explores how seemingly disparate disciplines such as the arts and the sciences can interact to mutual benefit.

Margaret Anne Schedel is a composer and artist specializing in the creation and performance of technologically interactive media whose works have been performed throughout the United States and abroad. While working towards a PhD in music composition at the University of Cincinnati College Conservatory of Music, her interactive multimedia opera, A King's Lullaby, premiered at the Cincinnati Contemporary Arts Center and was profiled by *Playboymag*. She is a joint author of *Electronic Music* and recently edited an issue of *Organized Sound* on the aesthetics of digital music. Her research focuses on digital music, the sustainability of technology in art, and verification of data. She has been the beneficiary of the International Computer Music Association, and is a regular editor for *Organized Sound*. From 2009-2011 she helped co-organize the *Willamberg-Gallery* focused on the intersection of art, science, new media, and design. In 2010 she co-chaired the International Computer Music Conference. She is SUNY's first Coursera Massive Open Online Course (MOOC), an introduction to computational arts. As an Associate Professor of Music at Stony Brook University, she serves as Co-Director of Computer Music and is the Director of iACS, the consortium for digital art, culture and technology.


Stony Brook University

iACS INSTITUTE FOR ADVANCED COMPUTATIONAL SCIENCE

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



The Big data world in the Earth Sciences so far exists primarily for disciplines that generate massive volumes of observational or computed data using large-scale, shared instrumentation such as global sensor networks, satellites, or high-performance computing facilities. These data are typically highly standardized, and managed and curated by well-supported community data facilities. In many other Geoscience domains, especially those where data are primarily acquired by individual investigators or small teams (known as Long Tail science communities), data are poorly shared and integrated, lacking a community-based data infrastructure that ensures persistent access, quality control, standardization, and integration of data, as well as appropriate tools to fully explore and mine the data within the context of broader Earth Science datasets. In this presentation I will offer some insights from my long-term work with data systems in geochronology, describing technical and cultural achievements, challenges, and opportunities to advance data science in a long-tail Geoscience domain.

Kerstin Lehnert is Senior Research Scientist at the Lamont-Doherty Earth Observatory of Columbia University, where she directs the NSF-funded data facility *Earth Data (Interdisciplinary Earth Data Alliance)*. Her background is in petrology and geochemistry, holding a PhD in petrology from the University of Freiburg in Germany. Over the past 15 years, her research interest has centered on Geoinformatics with particular emphasis on the development of data infrastructures for the solid Earth sciences and Earth science samples. Kerstin is currently member of the NSF Advisory Committee for Cyberinfrastructure, President of the Earth and Space Science Informatics Focus Group of the American Geophysical Union, President of the IGSN e.V., and elected member of the EarthCube Leadership Council.

Stony Brook University

iACS INSTITUTE FOR ADVANCED COMPUTATIONAL SCIENCE

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



Scientific simulation comprises a complex mixture of mathematical components, such as models for scientific and engineering problems, discretization algorithms, and software libraries interacting with a computer science software stack that is our interface to the hardware. In this talk, I will look at how we have navigated this complex system in the case of numerical methods for partial differential equations on structured grids to obtain successful simulations across a broad range of fields. I will also discuss how the coming changes in processor architecture due to power limitations is causing the approach we have taken over the years to break down, and describe some new ideas we are pursuing to remedy this problem.

Dr. Phillip Colella received his AB (1976), MA (1976) and PhD (1978) degrees from the University of California at Berkeley. He has been a staff scientist at the National Laboratories and at the Lawrence Livermore National Laboratory in the Mechanical Engineering Department at the University of California, Berkeley.

Dr. Colella is Group Leader for the Applied Numerical Algorithms Research Division at the Lawrence Berkeley National Laboratory, and is the Electrical Engineering and Computer Science Department.

Stony Brook University

IACS Fellowships

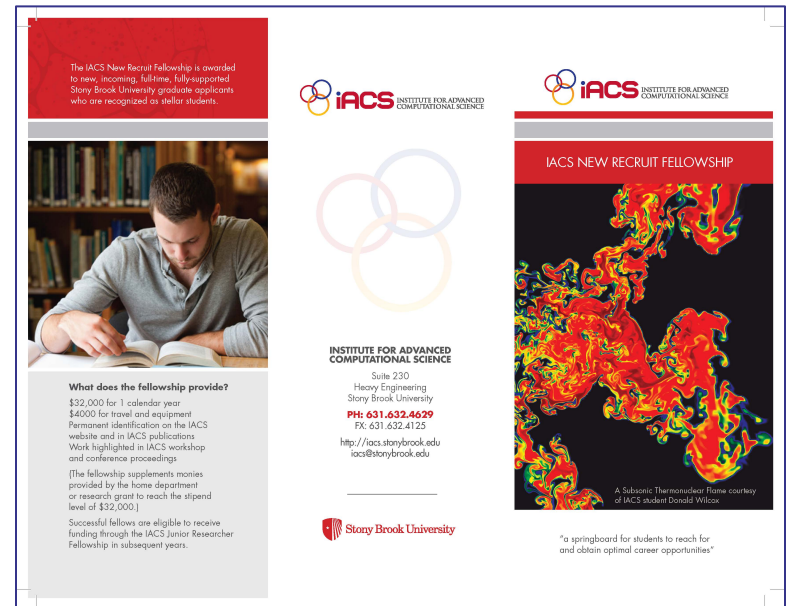


iACS INSTITUTE FOR ADVANCED COMPUTATIONAL SCIENCE

JUNIOR RESEARCHER FELLOWSHIP

This \$34K fellowship is awarded to continuing graduate students who are recognized as outstanding junior researchers.

See website for details.



The IACS New Recruit Fellowship is awarded to new, incoming, full-time, fully-supported Stony Brook University graduate applicants who are recognized as stellar students.

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iACS NEW RECRUIT FELLOWSHIP

A Subsonic Turbonuclear Reactor courtesy of IACS student Donald Wilcox

"a springboard for students to reach for and obtain optimal career opportunities"

INSTITUTE FOR ADVANCED COMPUTATIONAL SCIENCE

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Stony Brook University

What does the fellowship provide?

- \$32,000 for 1 calendar year
- \$4000 for travel and equipment
- Permanent identification on the IACS website and in IACS publications
- Work highlighted in IACS workshop and conference proceedings

[The fellowship supplements monies provided by the home department or research grant to reach the stipend level of \$32,000.]

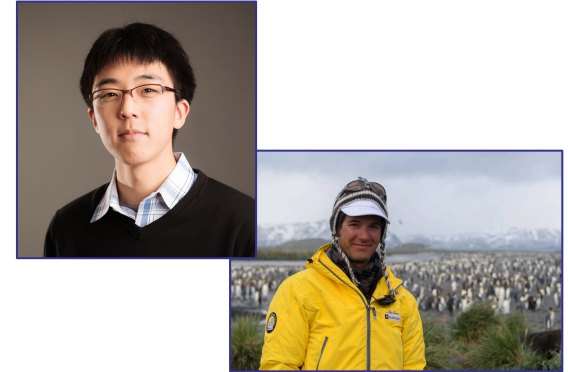
Successful fellows are eligible to receive funding through the IACS Junior Researcher Fellowship in subsequent years.

- 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

ARE YOU PUBLISHING YOUR FIRST PAPER?

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

\$500

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

See website for details.

Writing

Five awarded in 14/15

Two awarded in 15/16 (so far)

Travel

Seven awarded in 14/15

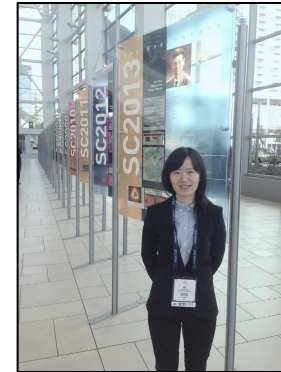
Two awarded in 15/16



IACS Travel Grants to SC1X

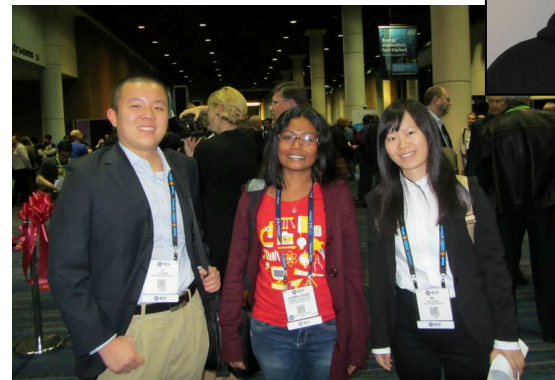
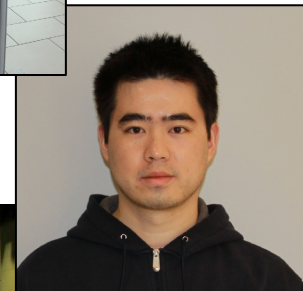
SuperComputing13

Gao Chao; Na Zhang;
Yufei Ren



SuperComputing14

Li Zhang; Jesmin Tithi



SuperComputing15

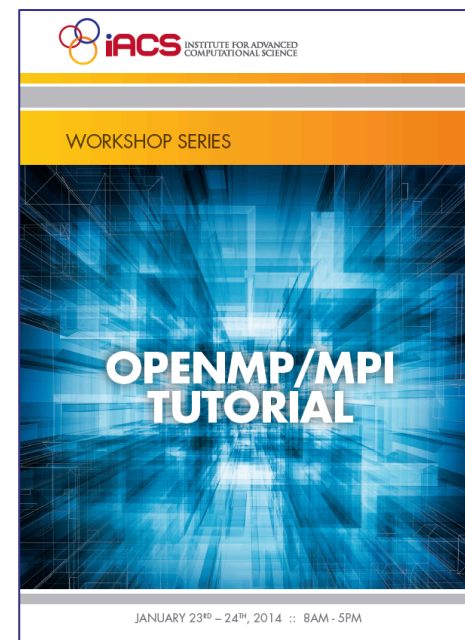
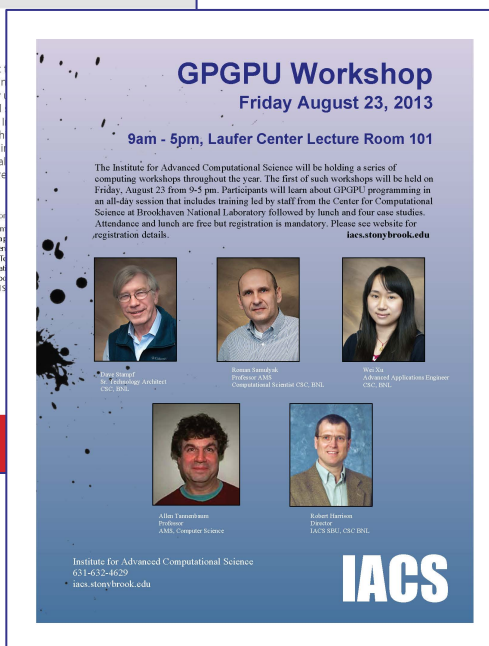
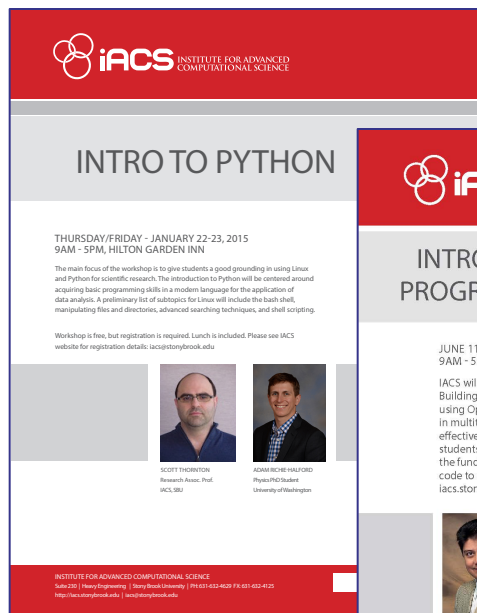
Na Zhang



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

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 Sarena Romano 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,
enjoy some tasty snacks like a finger or two!
Students & faculty, come to our party this night,
the most creative costume will win best fright!*



*IACS Pre-Halloween Costume Party
Costume Contest
First Prize: \$150
Friday, October 23, 2015 6 - 9 pm
IACS Seminar Room*

Training

iACS INSTITUTE FOR ADVANCED COMPUTATIONAL SCIENCE

DEVELOPING MODELS FOR STRUCTURE AND STYLE IN SCIENTIFIC WRITING

MONDAY AUGUST 17-21, 2015
9AM - NOON, IACS MULTIMEDIA ROOM

This workshop will focus on improving structure and organization of professional writing for graduate students in computational science. We will be working on basic writing 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 own 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 from your specific field to examine and emulate. Special emphasis will be placed on the logical presentation of information for your particular audience, including organizational features such as thesis statements, topic sentences and paragraphing to accommodate an outside reader.

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

Jennifer Albanese is currently the Interim Associate Director of the Writing Center where she has taught for sixteen years. Beginning in 2014, she will also be Director of the campus Writing Center. She has developed writing courses for the Graduate Chemistry program and the Center for Communicative Science at Stony Brook University.

JENNIFER ALBANESE
Interim Associate Director
Stony Brook University
Writing & Rhetoric Program

INSTITUTE FOR ADVANCED COMPUTATIONAL SCIENCE
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The Institute for Advanced Computational Science at Stony Brook University is offering a one-week programming workshop for high school rising juniors and seniors. Students must be 15 years old or older. This hands-on, 5-day camp introduces students to the programming skills and software/computer technologies that drive advances in science, industry, business and society. Starting with no assumed prior knowledge of programming, the camp introduces programming using the Python language and emphasizes development of algorithmic thinking and problem solving. From faculty and graduate students, participants will learn about using big-data analytics and high-performance computing to solve problems in science and engineering, and will then participate in team projects motivated by these same 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 future choices for education and careers. Ideally students will use their own laptops (Mac, PC, or a Linux are acceptable; a few are available for loan) so they can continue to use the camp's open-source software programming environment and tools.



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iACS INSTITUTE FOR ADVANCED COMPUTATIONAL SCIENCE

IACS COMPUTES!

SUMMER CAMP 2015

Software-Development Summer School for Computational Chemistry and Materials Modeling

(SICM)2 Summer Program in NY



DATE
Monday, July 7, 2014 to Friday, July 18, 2014

TIME
9 am - 5:30 pm

LOCATION
Stony Brook University

MEDIA
Facebook page
Video recordings

The second annual Software-Development Summer School for Computational Chemistry and Materials Modeling will be held at Stony Brook University in Stony Brook, NY July 8-18, 2014. The 2014 workshop will focus on junior-level chemistry and materials science graduate students in U.S. research groups who have an interest in modern programming methods and software development techniques. This summer school is part of the sustainable software initiative led in chemistry by the (SICM)2 (<http://www.s2i2.org/school.php>).

Students interested in attending were required to fill out an "Expression of Interest" form that was due March 31.

On the information from the "Expression of Interest" form, qualified students will be sent an email asking for application documents to be sent to iacs@stonybrook.edu by May 1. Those who qualify must send:

- a letter of support from their current research advisor;
- their CV;
- and a 1-page statement of how their research (or planned research) requires programming skills.

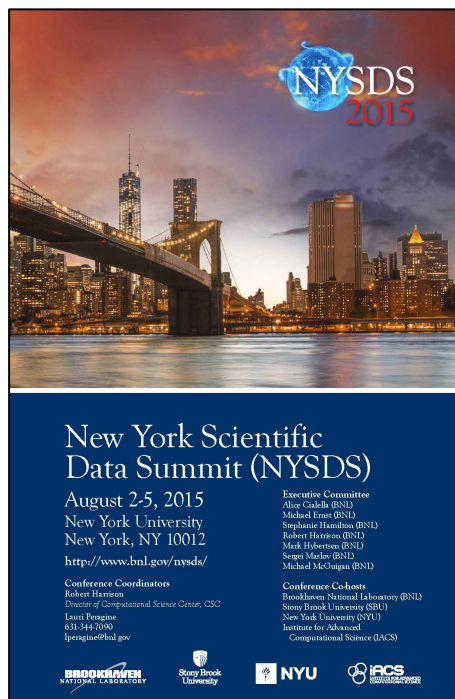
Documents should be in pdf form and sent to iacs@stonybrook.edu by May 1.

Students who are selected will be contacted via email. Lodging and meals will be provided for all accepted registrants. Travel to and from the program will be reimbursed up to \$500 per registrant. To learn more about the program, visit <http://www.s2i2.org/school.php>.

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

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.

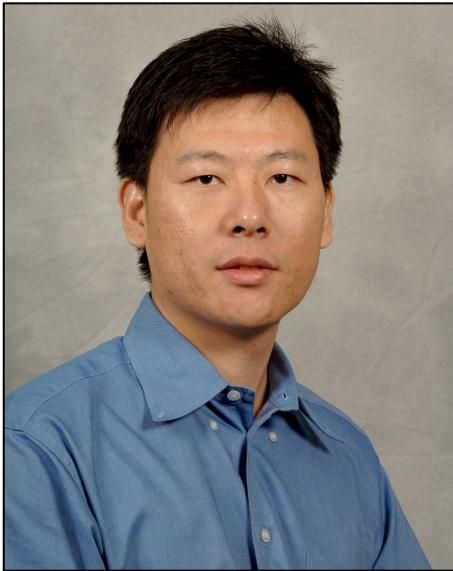
Robert J. Harrison



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

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

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

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

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



OPEN AREA SEAT COUNT:
MEDIUM DENSITY SEATING (8'-0" OF LINEAR DESK)
38 CPU WORKSTATIONS AT 300W EACH

PRIVATE OFFICES = 17 TOTAL

OPEN WORKSTATIONS = 3 ADMIN WORKSTATIONS

SYMBOL LEDGEND

	DUPLEX RECEPTACLE
	QUAD RECEPTACLE
	1 CAT6 (DATA), 1 CAT6 (VOICE)

ARCH. DESIGN BY TS/A/PL	CHECKED HQA	SHEET NUMBER 37A3
MECH. DESIGN BY HQA	CHECKED HQA	
ELEC. DESIGN BY JG	APPROVED GJ	
PROJECT NO. 10000	NOTE AS NOTED	
D.E. NAME _____ DATE _____		

37A3

REV 0 12/22/11

Our new space

