Institute for Advanced Computational Science

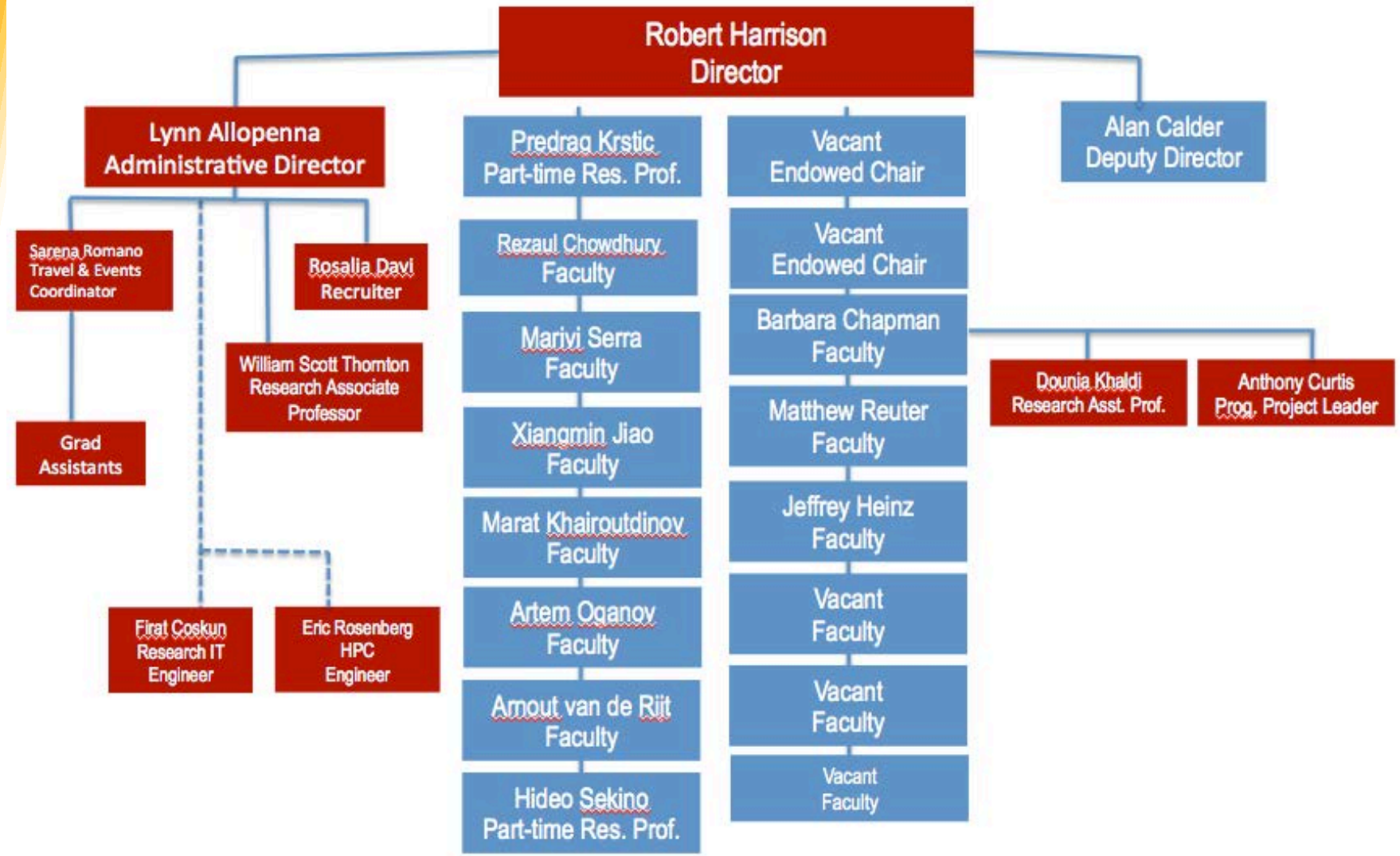
Robert J. Harrison, Director

robert.harrison@stonybrook.edu

What is IACS?

- A multidisciplinary institute with a focus on computational and data science
- $20M endowment to support 3 endowed chairs and operations (~$13M)
- 12 core faculty, 32 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

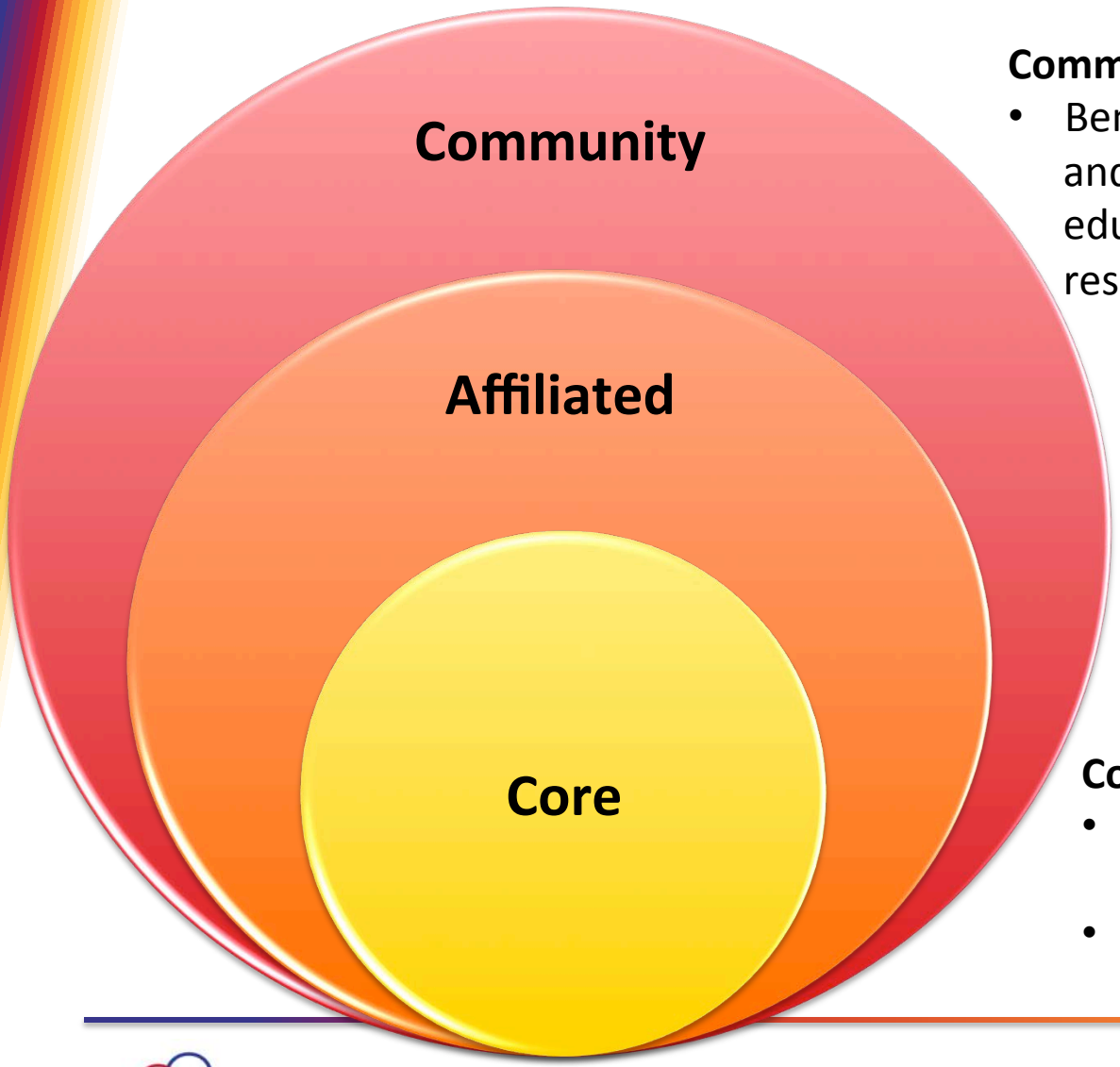
IACS Organizational Chart



Vision

Our vision is to be an internationally recognized center in data and computational science, having vibrant multidisciplinary research and education programs, with broad leadership and benefit across Stony Brook and SUNY, and with demonstrated economic benefit to New York State.

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

- Predrag Krstić

- Xiangmin Jiao (app. math.)

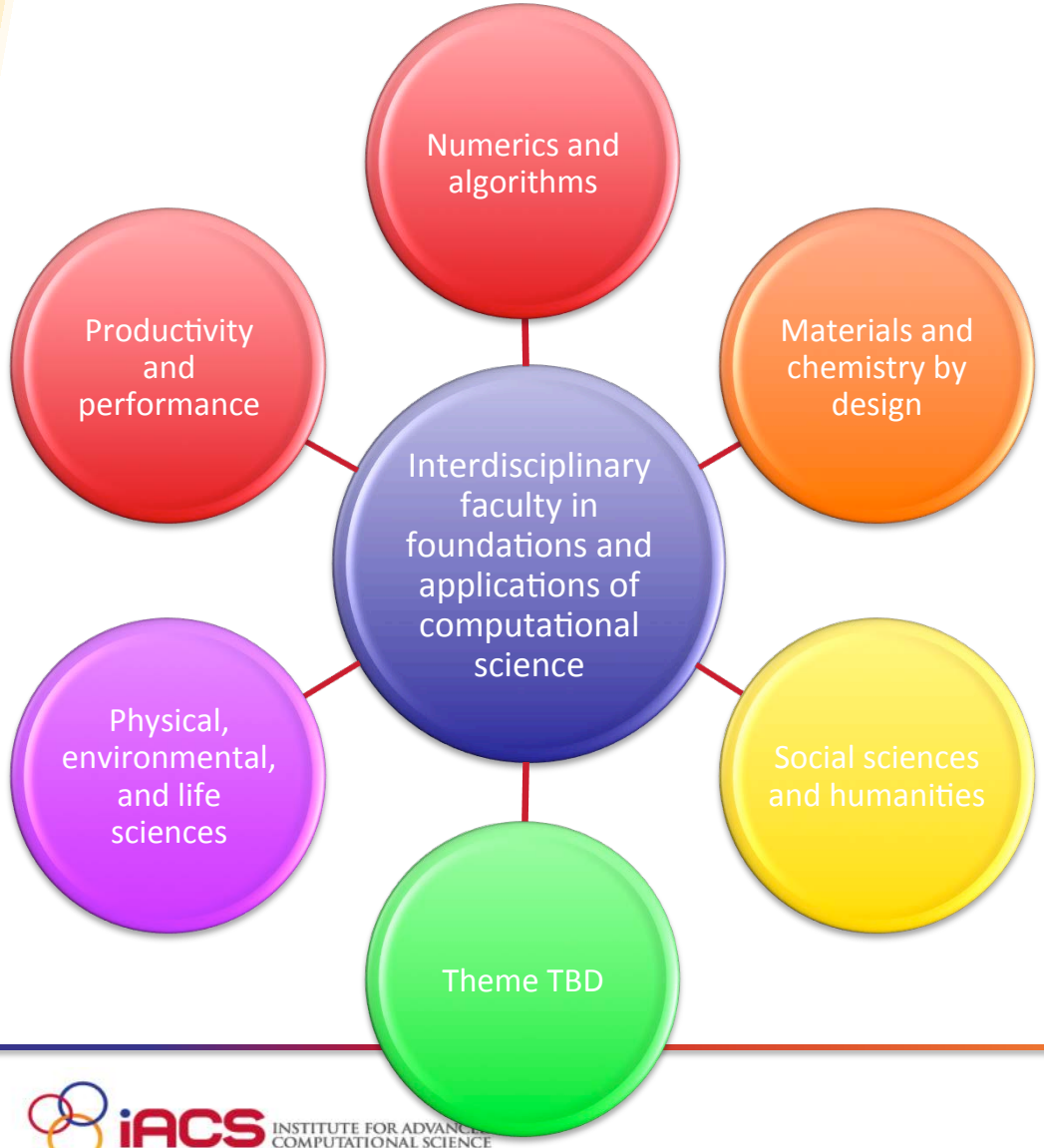
- Marat Khairoutdinov (atmos. sci.)

IACS Core Faculty - III

- Artem Oganov (materials)

- Matt Reuter (math/chem. phys.)
- Arnout van de Rijt (sociology)

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)

Publications by year

- 30 publications to date in CY 2016
- 49 publications in CY 2015
- 44 publications in CY 2014
- 35 publications in CY 2013
- 33 publications in CY 2012

IACS Core Faculty Grants

20 grants submitted in CY 2014

- ✧Total value $33,738,224
- ✧7 grants awarded
- ✧Total value $2,484,214

20 grants submitted in CY 2015

- ✧Total value $66,373,306
- ✧10 grants awarded
- ✧Total value $5,352,131

IACS Core Faculty Grants

10 grants submitted to date in CY 2016

- ✧Total value $8,392,613
- ✧6 grants awarded to date
- ✧Total value $4,849,704

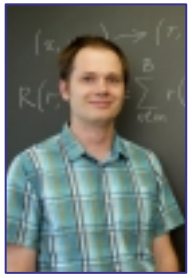
New IACS Core Faculty

Jeffrey Heinz, Linguistics –
starting F17

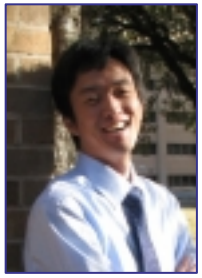
Hideo Sekino
Part-time Research Professor

New IACS Affiliate Faculty

Stephen Irle
Nagoya
University



Dima Kozakov
AMS



Il Memming Park
Neurobiology

Meg Schedel
Music

Fotis Sotiropoulos
CEAS

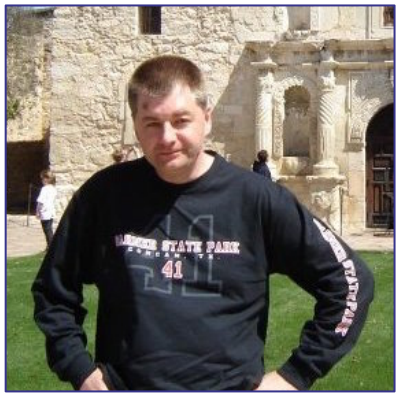
Minghua Zhang
SOMAS

New staff

Rosalia Davi
Diversity Outreach Coordinator

Eric Rosenberg
Systems Administrator

Dounia Khaldi
Research Asst. Professor



Tony Curtis
Programming Project Leader

IACS Computer Resources

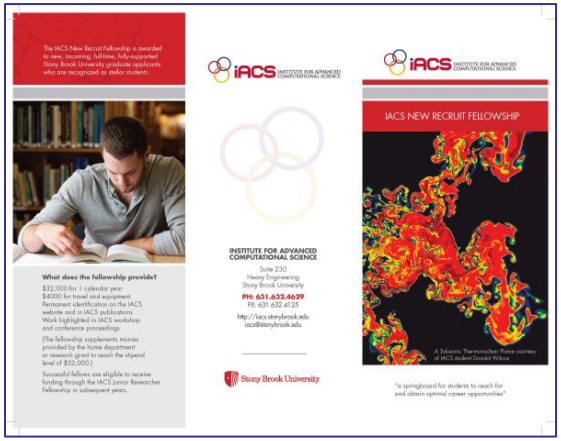
- Handy – startup funds
  - 40 dual-socket Sandybridge nodes, 2 NVIDIA K20 GPUs, 2 Intel KNC, 250 TB disk
- LI-red – $1M grant from regional economic development council
  - 100 dual-socket Haswell nodes, 250 TB disk
  - 1 quad-socket Haswell node with 3 TB memory
  - 1 IBM Power8 node
- Two Intel KNL 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

Seminar Series

16 seminars held in CY 2015
24 seminars planned for CY2016

Speakers:
Joel Saltz
William Tang
Dima Kozakov
Michele Benzi
Fotis Sotiropoulos
Dongbin Xiu
Il MemmingPark
Stephan Irle
Huan Liu
Hongyuan Zha
Richard Tapia
Roberto Car
Thomas Graf
Martin Deneroff
Ann Almgren
Krishna Kavi
Angela Shiflet
Mark Ratner

IACS Researcher Awards



Five awarded in 2016, total value $71,570

- 1 new recruit award
- 4 junior researcher awards

(2 new and 2 renewed for 2nd year)

IACS Awards

New Recruits

- Eric Raut, AMS – Computation Fluid Dynamics

Junior Researchers

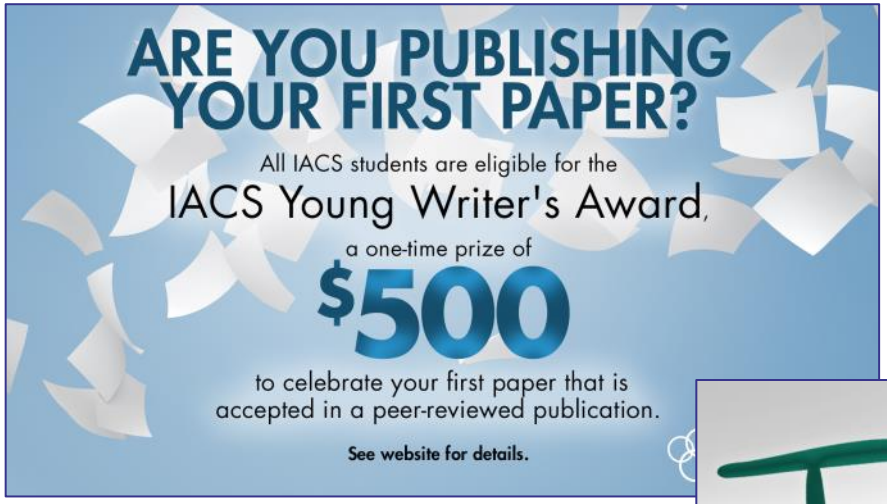
Philip McDowall (EE) – *computer-vision enabled spatial ecology of seabird coloniality*

Adrian Soto Cambres (PHY) – *computation of dark matter - electron scattering rates for direct detection experiments*

Aditi Ghai (AMS) – *robust numerical computation on meshes*

Zeyang Ye (AMS) – *global optimization and massively parallel algorithms*

IACS Travel & Writing Awards



Writing

Six awarded in CY 2015

Nine awarded in CY 2016 (so far)

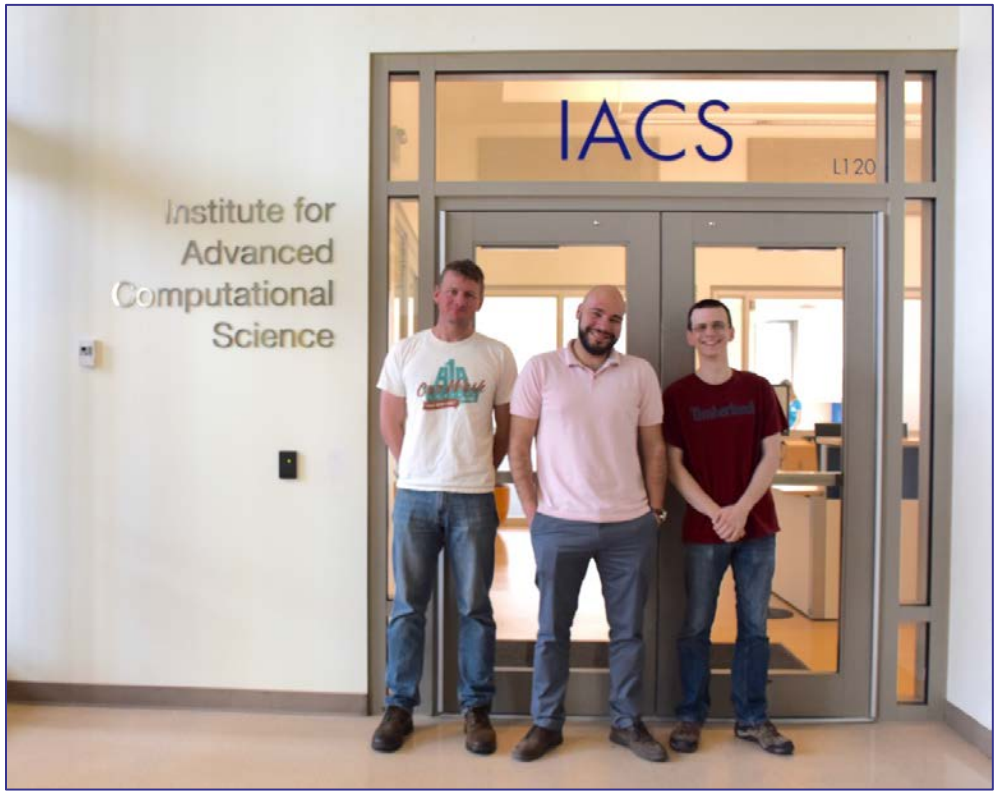
Travel

Seven awarded in 14/15

Four awarded in CY 2016 (so far)

IACS Student Association

What do Matchmaking, Patents and Science Have in Common?

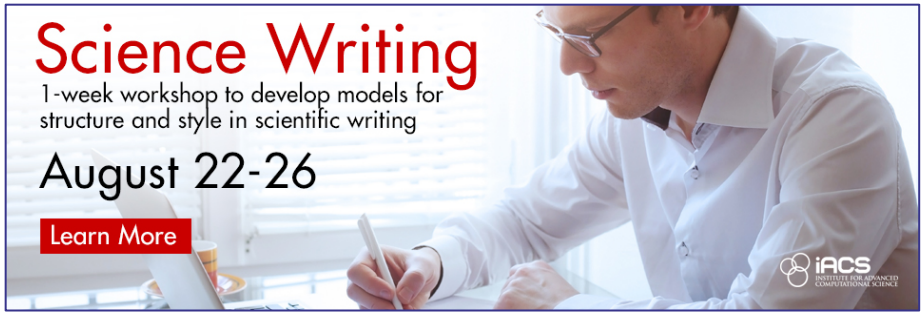


Research Events
- IACS Student Seminar Series
- Brown-Bag Lunch Sessions

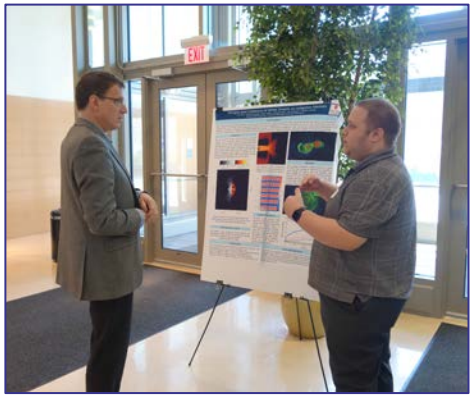
Professional Development
- Scientific Communication Workshop
- Patents Workshop

Social Events
- Student-Faculty Dinners
- Group Outings to NYC

Workshops and Tutorials



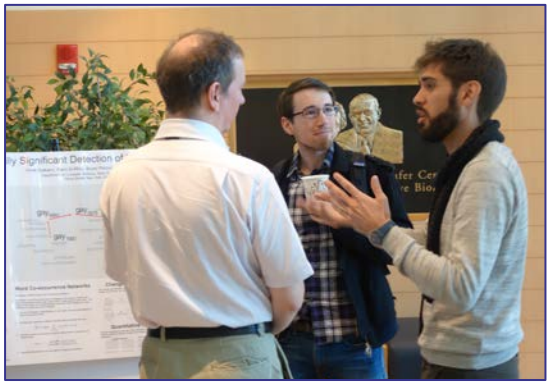
IACS Research Day



08:30 am- 09:00 am 2015 Student Award Winner Presentation
Adrian Soto, Physics and Astronomy
Direct Detection of Sub-GeV Dark Matter via Single-Electron Excitations in Crystals

09:00 am-09:30 am IACS Faculty Presentation
Barbara Chapman, AMS
Programming Next-Generation Computers:
A Large Scale Challenge

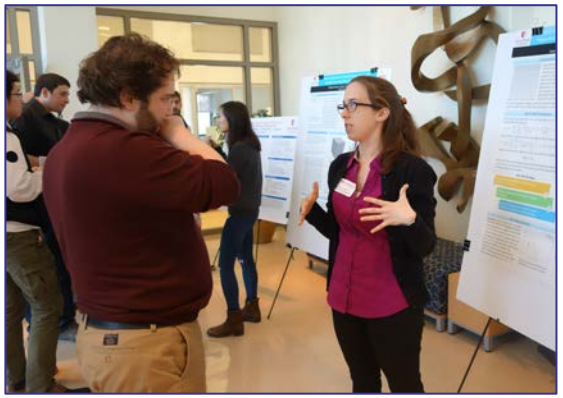
4 student presentations
3 faculty presentations
13 posters presented



09:30 am-10:00 am
2014 Student Award Winner Presentation
Bryan Perozzi, Computer Science
Deep Learning for Social Media

10:00 am-10:30 am IACS Faculty Presentation
Marat Khairoutdinov, School of Marine and Atmospheric Sciences
Aggregation of Convection and Tropical Climate

IACS Research Day

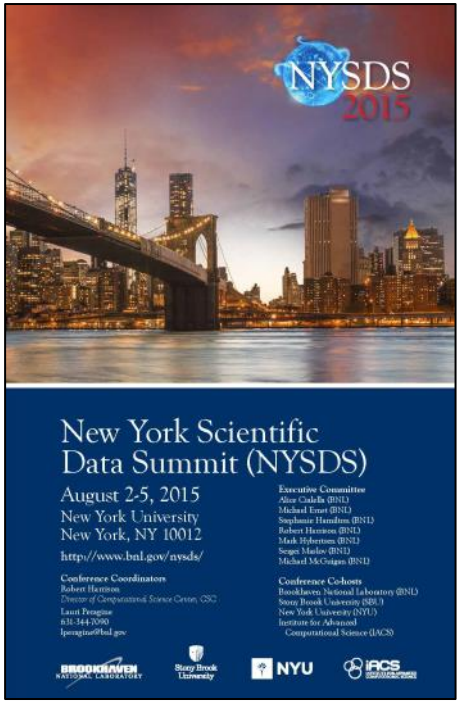


10:45 am-11:15 am 2015 Student Award Winner Presentation
Philip McDowall, Ecology and Evolution
Escaping Flatland: Adventures in 3D Ecology

11:15 am–11:45 am IACS Faculty Presentation
Xiangmin Jiao, Applied Mathematics & Statistics
Robust, Flexible, High-Order Numerical Methods

11:45 am-12:15 pm 2014 Student Award Winner Presentation
Adam M. Jacobs, Physics and Astronomy
Tiny Exploding Dwarfs in the Sky

Conferences and workshops



NY Scientific Data Summit
August 15-17, 2016
New York University
www.iacs.stonybrook.edu/event/events/2016-new-york-scientific-data-summit-nysds

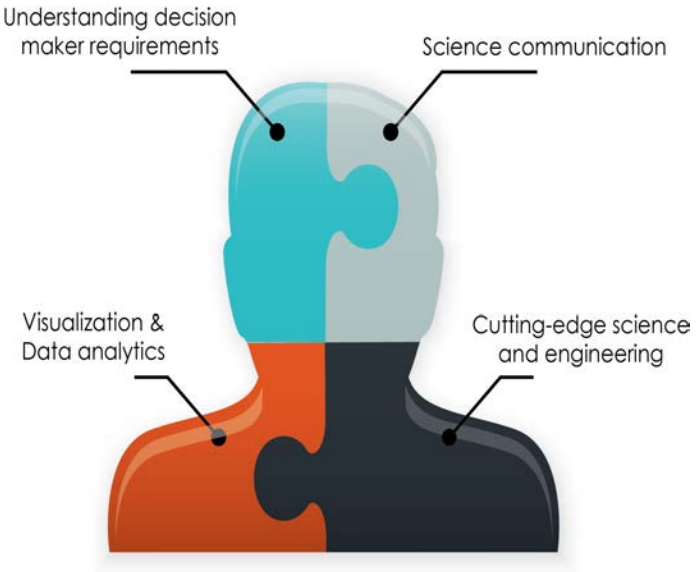
MultiResolution Analysis (MRA) Summer School
August 1-12, 2016
IACS @ SBU
www.iacs.stonybrook.edu/event/other/multiresolution-analysis-mra-summer-school

What's on the Horizon?

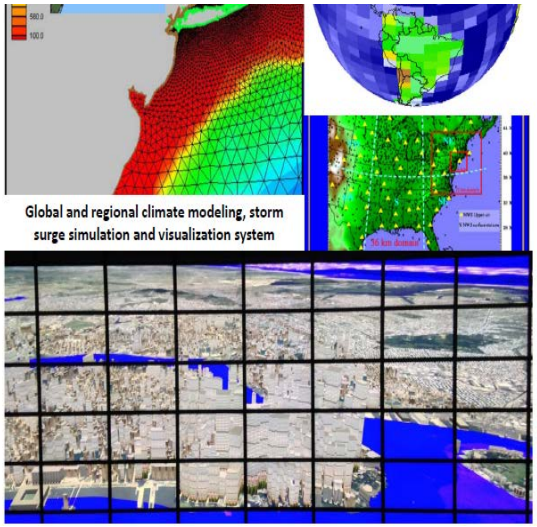
- Two advanced graduate certificates
  - STRIDE; CDCSE
- Recruiting: Additional faculty and staff
  - Two endowed chairs
  - Two junior faculty
  - More interdepartmental joint lines
  - Grants budget manager
- DATA SUNY
- IDIME
- Robust internship program
- Significant increase in diversity

Science Training & Research to Inform DEcisions **(STRIDE)**

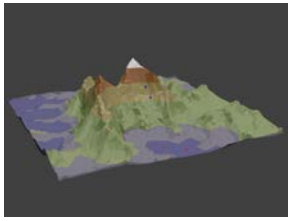
L Dávalos, RJ Harrison, AE Kaufman, HJ Lynch, J Nye,
C O'Connell, J Saltz, E Zadok and M Zhang
Ecology and Evolution, Applied Mathematics, Journalism, Computer Science, Marine and Atmospheric Sciences, Biomedical Informatics



E.g., Probabilistic modeling of climate change for adaptation & mitigation



Vertically-integrated graduate training
Connects research to decision support
Prepares students for high-impact careers
Connects science to real-world applications



Decision support challenges include:

- *Climate change and coastal resilience* –communicate uncertainties to stakeholders
- *Marine resource management* –communicate uncertainties & enable scenario planning
- *Tracking and targeting illegal deforestation* –model and communicate priorities to UN
- Other themes include smart grid energy infrastructure, population health, and more!

CDCSE - Certificate in Data and Computing for Scientists and Engineers

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, intro courses
- ✧ 60 general courses

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

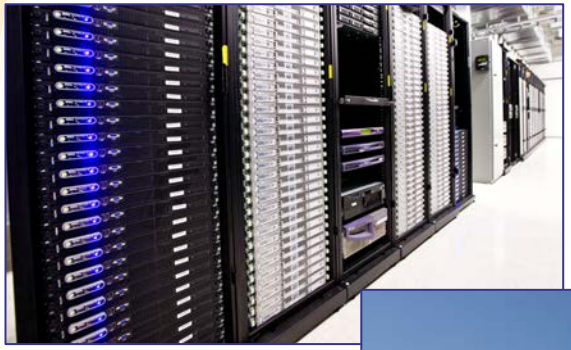
Recruiting Plan

- 4 positions in foundations of computation
  - Positions advertised simultaneously
    - Senior endowed, IACS named chair in CS & AMS
    - Junior faculty in CS and AMS
  - Interviews of 1st three candidates in November/ December
  - Hires now expected summer 2017; some joint with BNL
- 2 interdepartmental joint hires
  - Jason Trelewicz, MSE; Heather Lynch, E&E
- Staff: P/T Grants Budget Manager

DATA SUNY

- DATA SUNY is the planned deployment of a multi-campus and multi-institutional data analytic and computational framework that will transform and support academics across SUNY.
- The SUNY-wide high-speed networking will be a lasting legacy of the project that will greatly enhance SBU's (inter)national competitiveness.
- The proposed modern cyberinfrastructure connected by advanced networks to the world at large is essential to the education and preparation of a workforce prepared for careers in a data-enabled future driven by ever-changing technologies.
- SBU's pot = $4.5M

Long Island Institute for Data-Enabled Applications (LI-IDEAS)



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

Sited in Stony Brook University's R&D Park

Co-locate industry staff, and staff/faculty from SBU, BNL, CSHL and other LI research institutions

Access for both private industry and public research

60,000 gross sq. ft. building
5,000 sq. ft. computer room
27,000 sq. ft. office & lab space

Funding Request: $75M
(matched with $75M from SBU, federal grants, and private donations for operations)

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

iACS INSTITUTE FOR ADVANCED COMPUTATIONAL SCIENCE

In the process of being funded, but now re-envisioned as the following:

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

- 150 new and 30 retained jobs
- 70,000 square feet, SBU R&D Park, $75M state capital construction investment
- $200M over 5 years, including external funding resulting in 2:1 match
- 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
- Planned to be on the October agenda of the ESD, Empire State Development

Internships

- STRIDE internships with IBM Research (8/year)
- STRIDE internships with BNL (8/year)
- STRIDE internships with NOAA (6/year)
- Talks underway with ANL, ORNL, LANL for internship MOU
- Additional sites to be approached:
  - Intel; Penguin Computing; NVIDIA, Dell

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.

Appendix

- Faculty Research
  - Arnout van de Rijt
  - Marat Khairoutdinov
  - Artem Oganov
  - Alan Calder
  - Marivi Fernandez-Serra
  - MattReuter
  - Jim Jiao
  - Rezaul Chowdhury
- HPC^{ny}

Rich-Get-Richer in Crowdfunding

Arnout van de Rijt

Projects on www.kickstarter.com

random assignment

Experimental condition

Raised from others:

$294

Control condition

Raised from others:

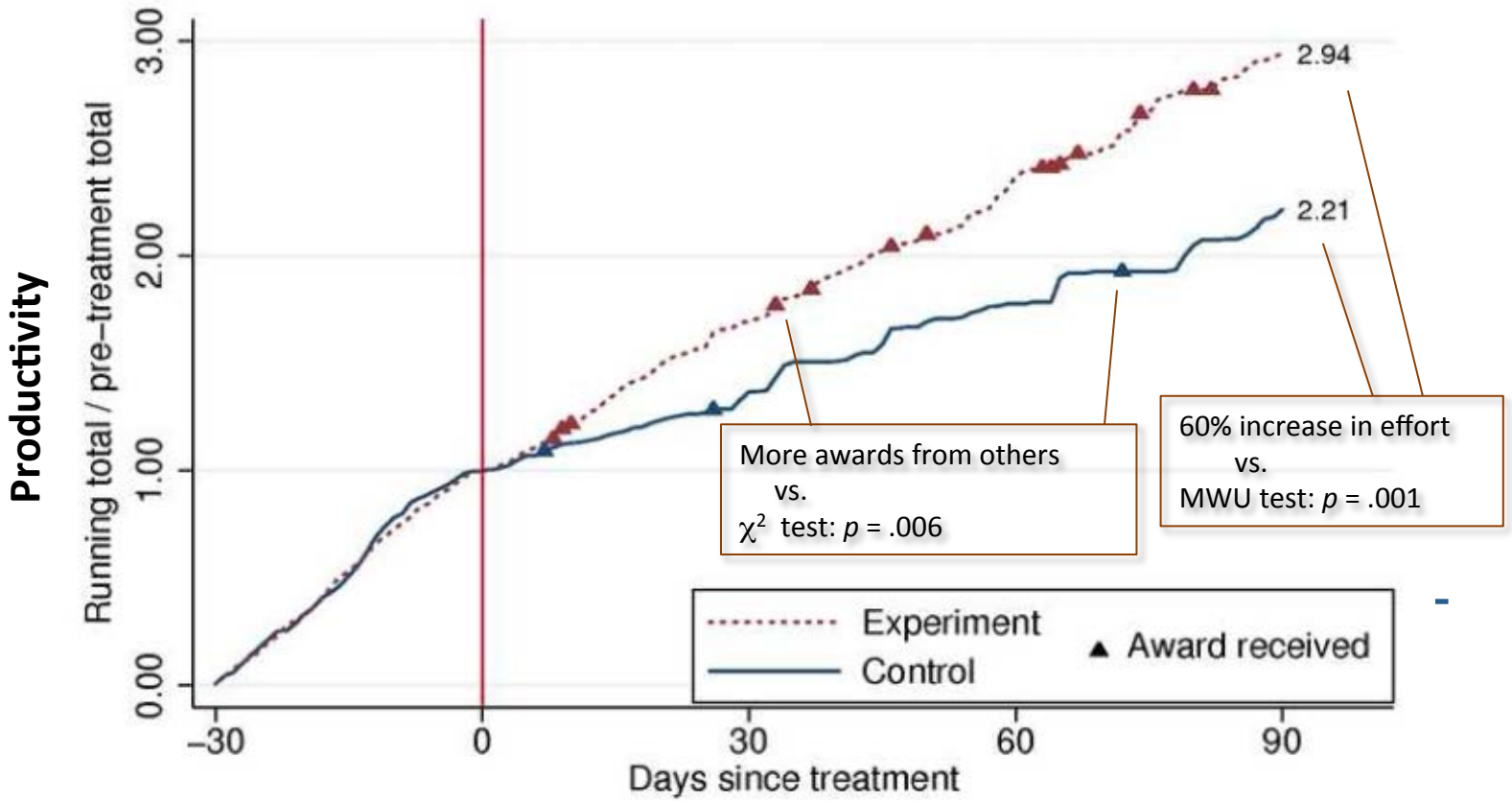
$103

Source: *Van de Rijt et al. in **PNAS** (2014)*

Funding: ***NSF** grants SES-1340122*

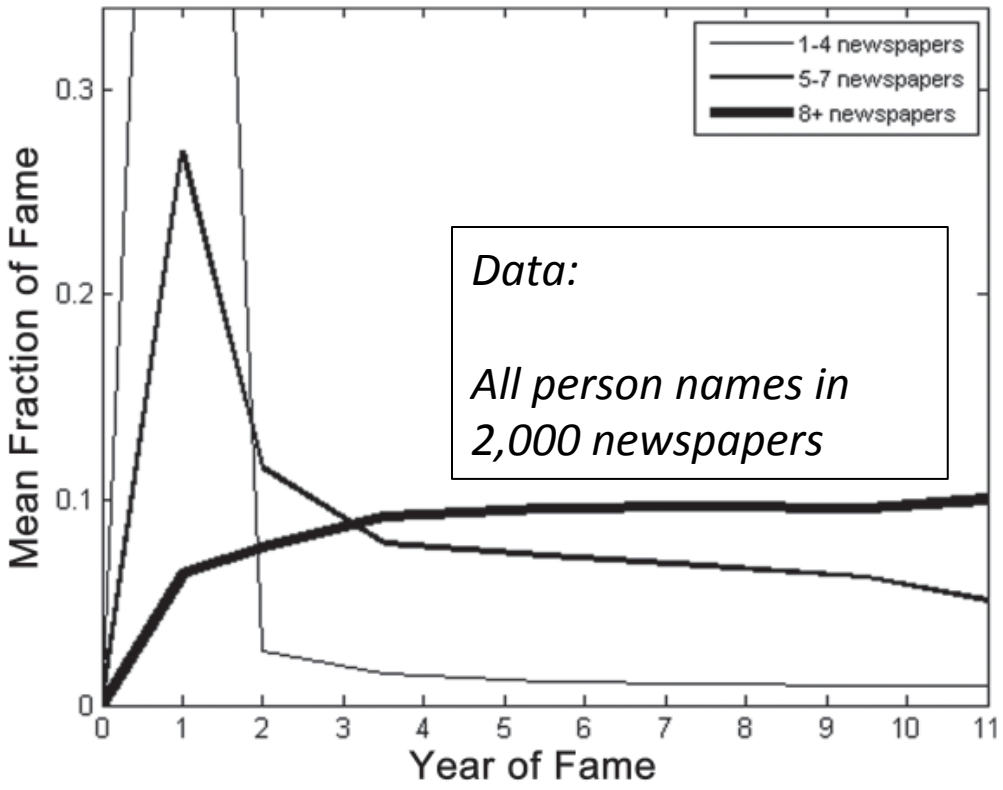
Press: *Economist, Time Magazine, National Geographic, WAMC*

Wikipedia Volunteer Editors Increase Effort after Virtual Awards Given by Researchers



Source: *Restivo & Van de Rijt in* ***PLOS ONE*** *(2012)*

Only Fifteen Minutes?



Source: *Van de Rijt et al. in **American Sociological Review** (2013)*
Press: *LA Times, NBC News, Toronto Star, Globe and Mail, Yahoo News, Pacific Standard, Politiken (front page)*

Computer Simulations of clouds and climate

Marat Khairoutdinov

Paleoclimate simulations using advanced climate model

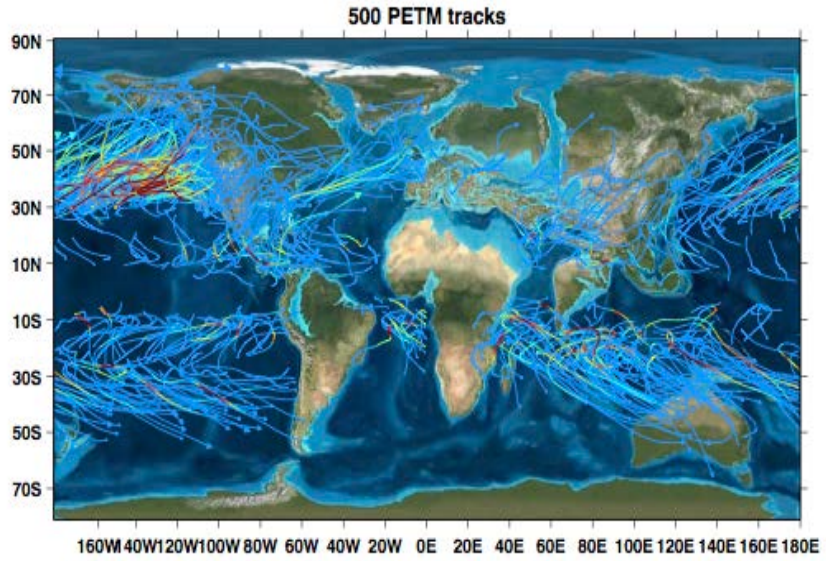
According to paleo reconstructions, it has been tens of millions of years since the Earth had the levels of CO_2 and corresponding radiative forcing that we may experience in just 100 years from now.

Perhaps we can use the past to tell us what is awaiting us in the future ...

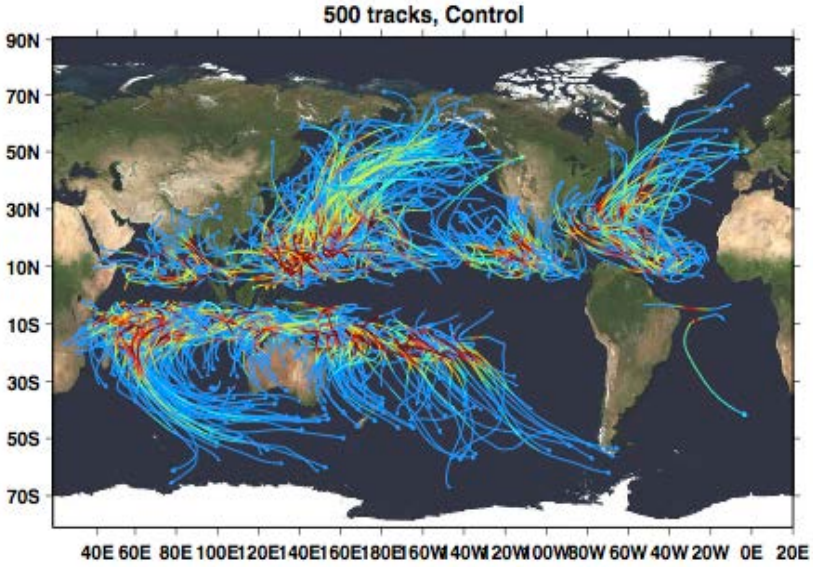
Unlike simulations of the future, there are observational constraints on simulations of the past...

Earth 55 million years ago during Paleocene-Eocene Thermal Maximum (PETM)
Simulated possible tracks of hurricanes

55 million years ago



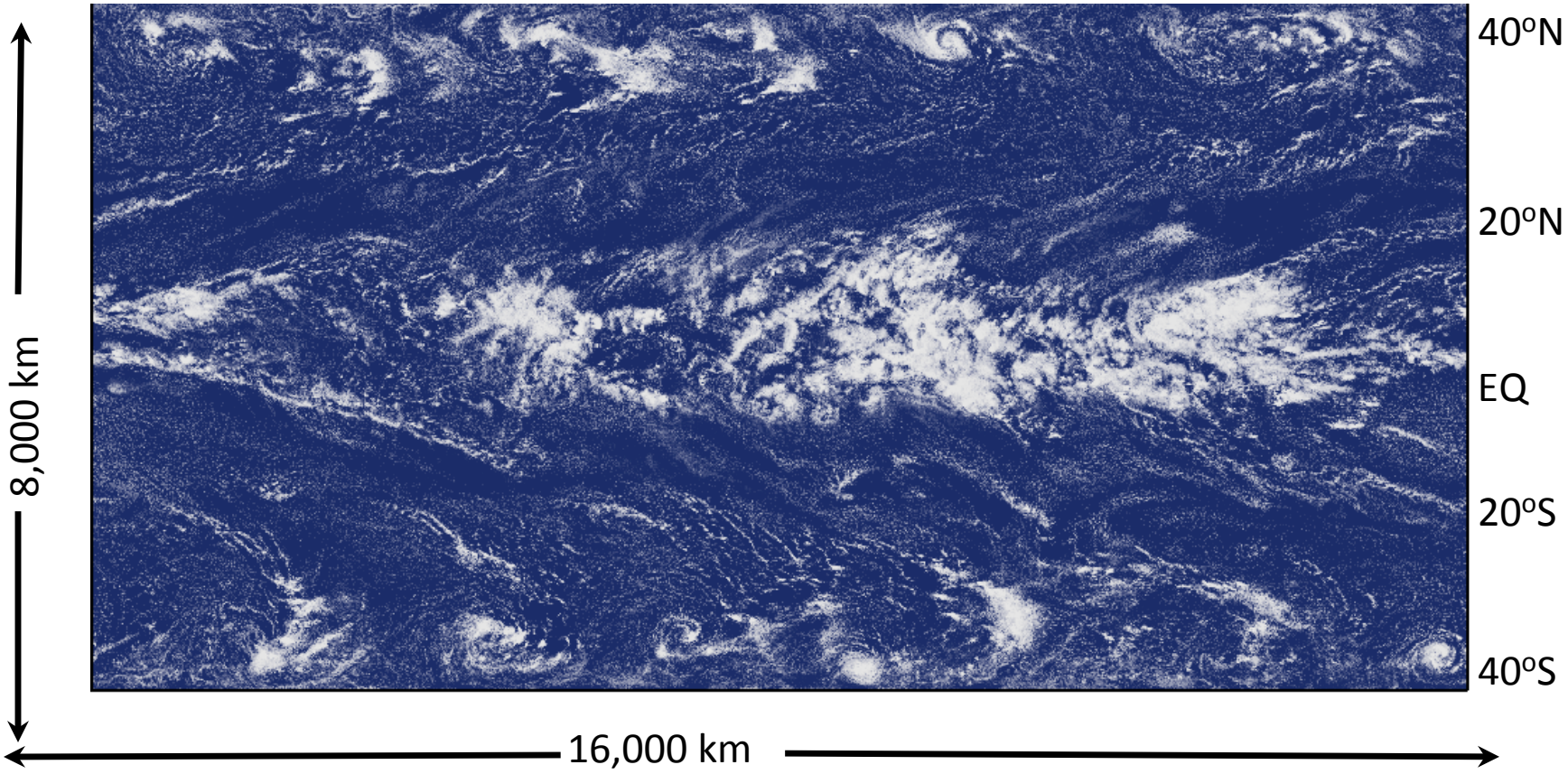
Today



Cloud-resolving simulation of tropical weather systems

Simulations like that help us to understand how climate regulates itself, how cloud systems organize on large scales, and what can happen in the warmer world.

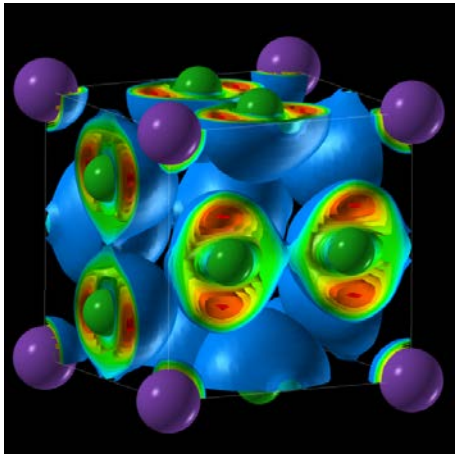
Simulated view of a cloud field in Tropics as would be seen from a satellite



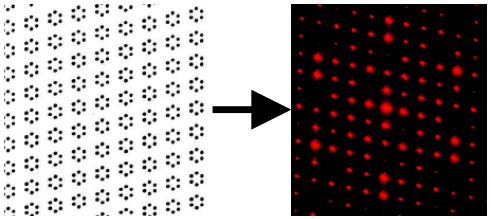
Each pixel of this image represents 4x4 grid cells of the numerical grid. A 100 day-long simulation takes about one month of nonstop computations using 2,048 processors of the IBM BlueGene/L supercomputer. It would take more than 150 years for a home desktop PC to produce such a simulation.

Predicting “forbidden” chemistry and novel materials with the USPEX method/code

Artem R. Oganov

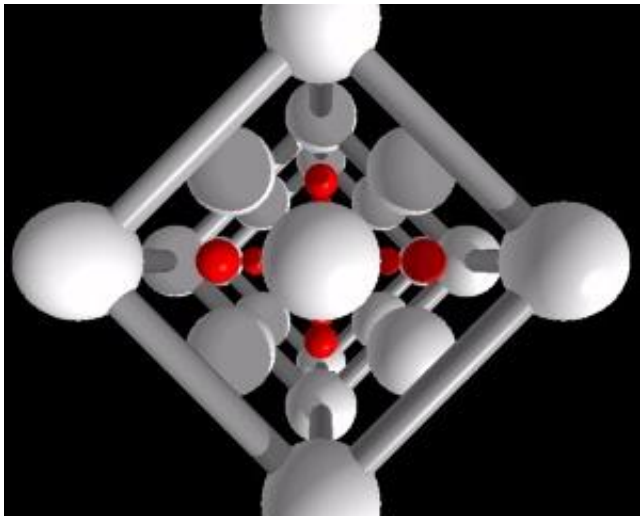


Can Periodic Systems change at extreme conditions?
What is the chemical formula of sodium chloride?
What is the most inert element?
What is the cleanest fuel material?
Why does some dust cause lung cancer?



Structure **Diffraction**

Zincblende ZnS.
One of the first structures solved by Braggs in 1913.



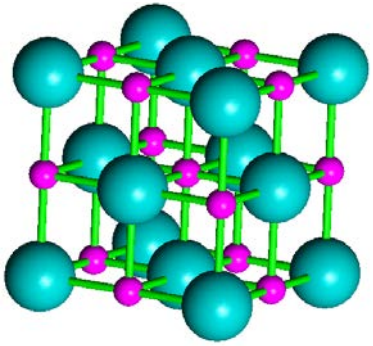
Example: “Crazy” sodium chlorides

Na-Cl

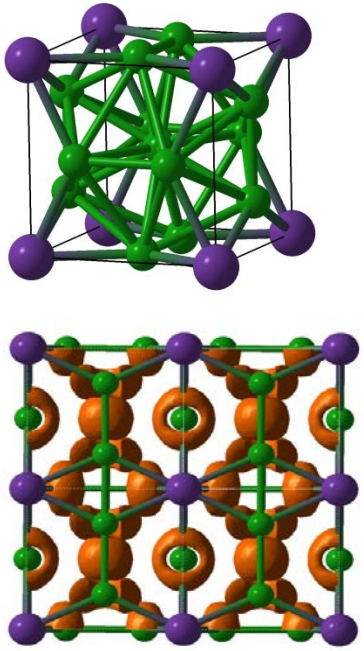
Salt as we know it:

Peculiar Na-Cl compounds:

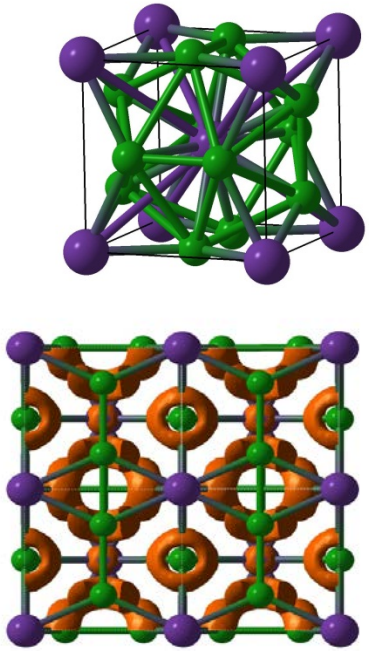
- NaCl7: some Cl atoms have POSITIVE Bader charge (+0.07).
- Na3Cl: 2D-metal



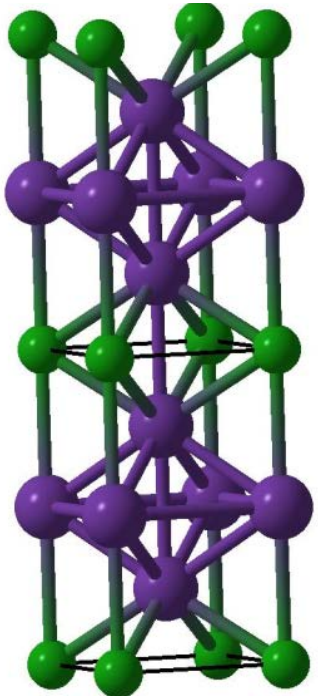
NaCl



$NaCl_7$



$NaCl_3$

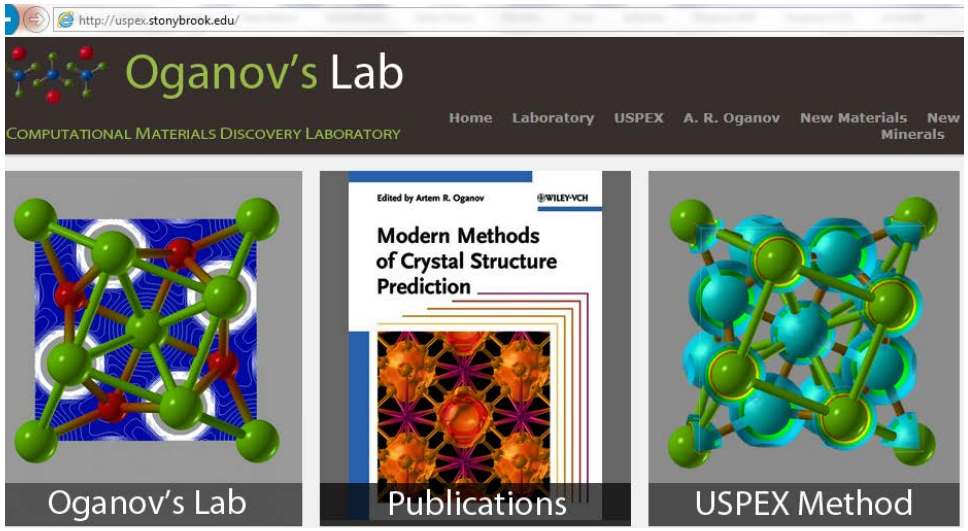


Na_3Cl

[Zhang, ARO, et al., Science (2013)]

The USPEX (Universal Structure Prediction: Evolutionary Xtallography) project

http://uspex.stonybrook.edu



- The most popular code for computational materials design in the world (>1700 users)
- The largest, the most versatile, the fastest and the most reliable code in this field.

Many of its capabilities are unique. 3D-, 2D-, 1D-, 0D- systems can be treated

- THE CODE IS FREE
- Effort of ~50 man-years
- ~200 publications, 2 US patents

Nuclear Astrophysics

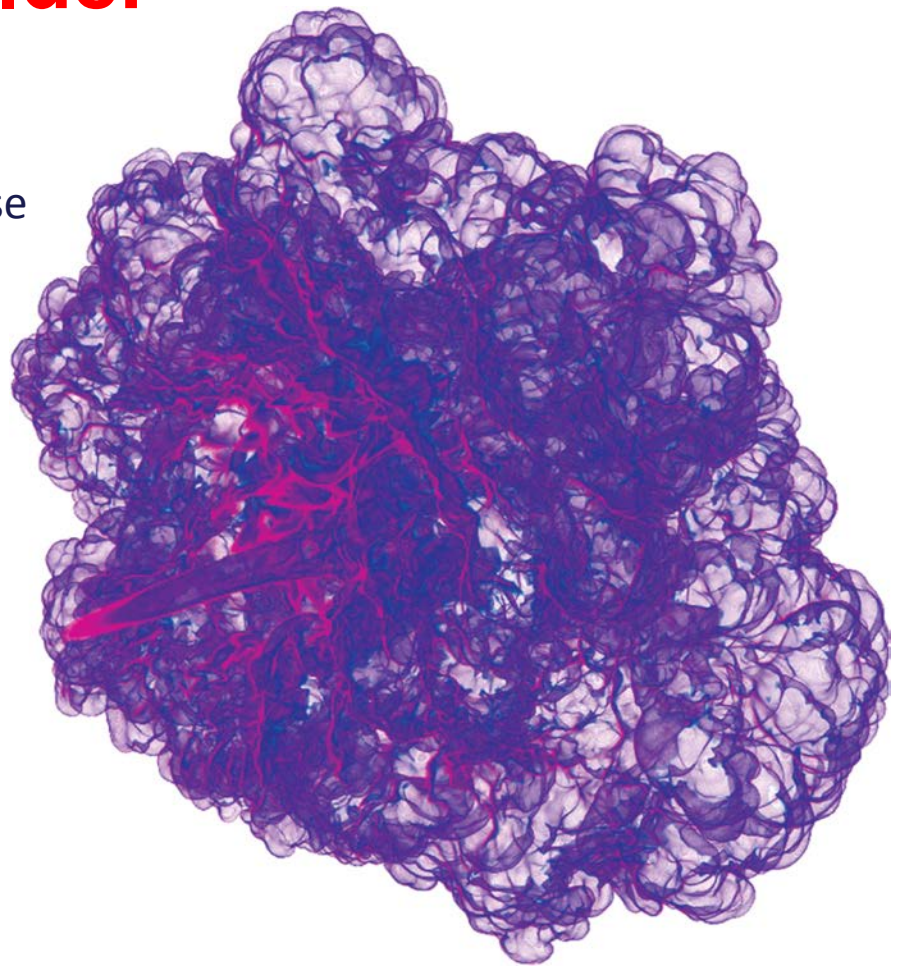
Alan Calder

Stellar Explosions:

- Thermonuclear (type Ia) and core collapse supernovae
- Classical novae
- Neutron stars and X-ray bursts.

Computational Science:

- Hydrodynamics and radiation hydrodynamics
- Verification, validation, and uncertainty quantification
- Basic Physics of turbulent combustion
- Computational Science Education



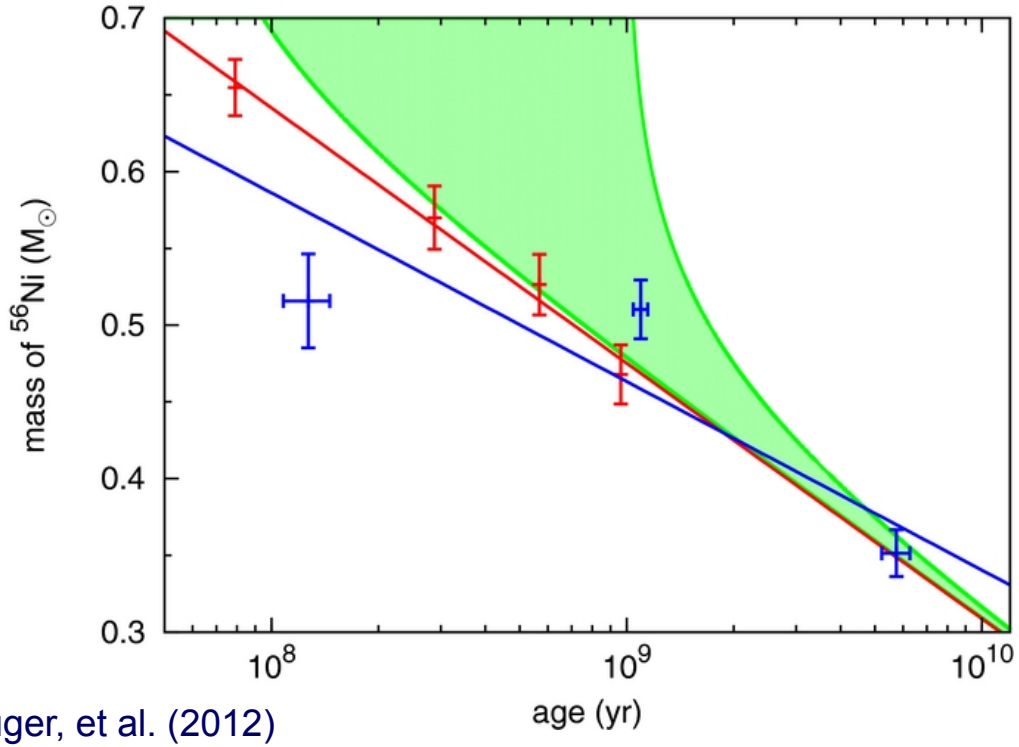
Type Ia Supernovae

Thermonuclear (Type Ia) Supernovae are bright explosions that serve as distance indicators for cosmological studies.

Research focuses on understand the mechanism of the explosion and determining systematic effects on the brightness and the intrinsic scatter.

Figure: mass of radioactive nickel, the source of brightness, vs. age of progenitor (red points).

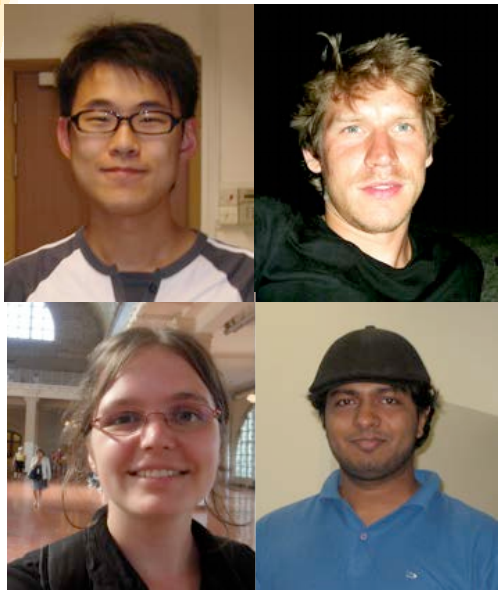
The study provided the first theoretical explanation for the observed trend of dimmer supernovae in older galaxies (blue points).



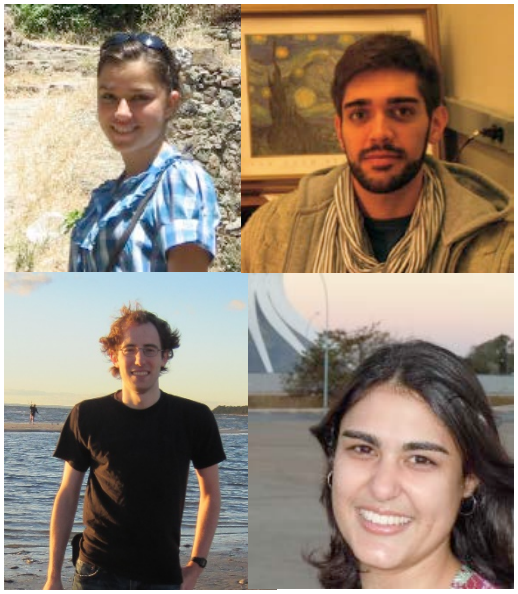
Kruger, et al. (2012)

Marivi Fernandez-Serra

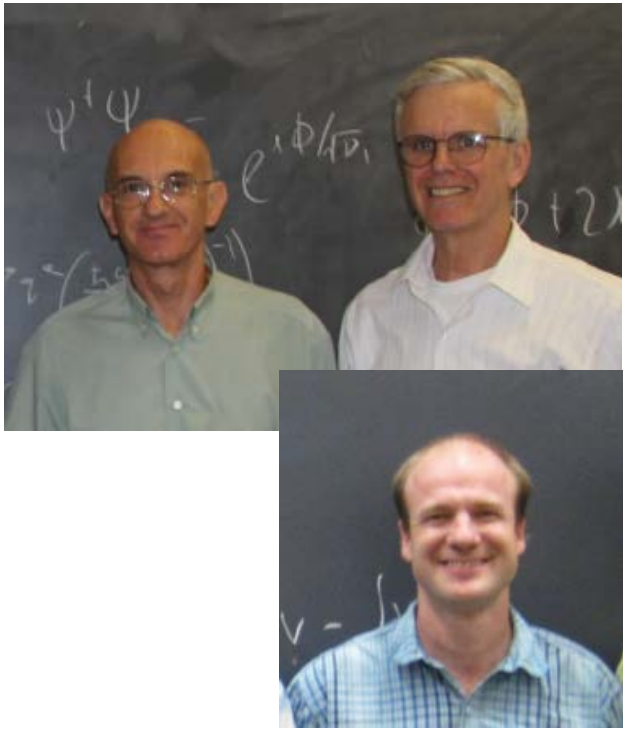
Past Members



Current Members



Close Collaborators



Madrid: Rafa Ramirez
San Sebastian: Emilio Artacho, Fabiano Corsetti
SIESTA team

DOE Early Career DE-SC0003871
DOE: DE-FG02-09ER16052

siesta

iACS INSTITUTE FOR ADVANCED COMPUTATIONAL SCIENCE

Water/interfaces by first principles

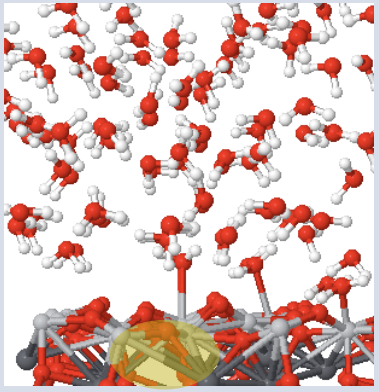
Ferroelectric Surfaces:
Investigating the role of polarity on water/substrate interactions

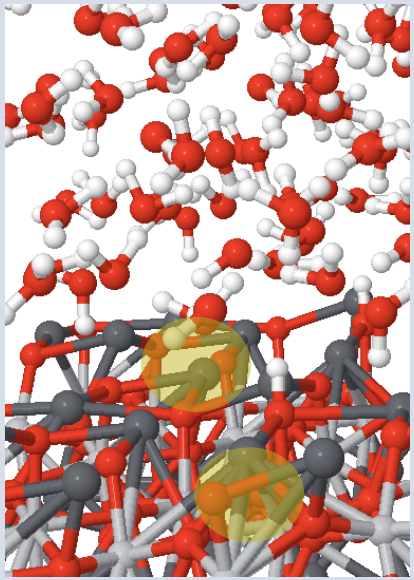
PbO Surfaces

dissociation+OH^- in solution

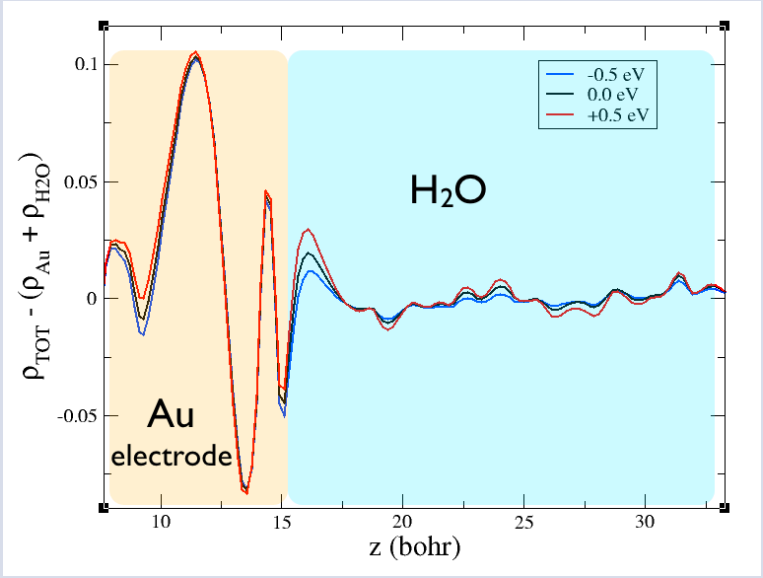
TiO_2 Surfaces

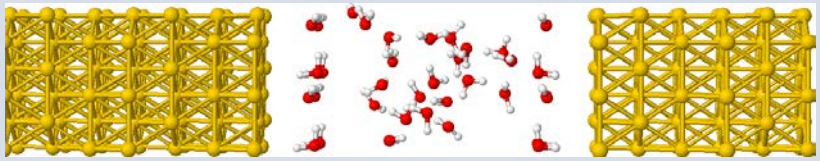
No dissociation





Electrochemical interface: metal/ water under applied bias coupling non equilibrium transport methods with molecular dynamics

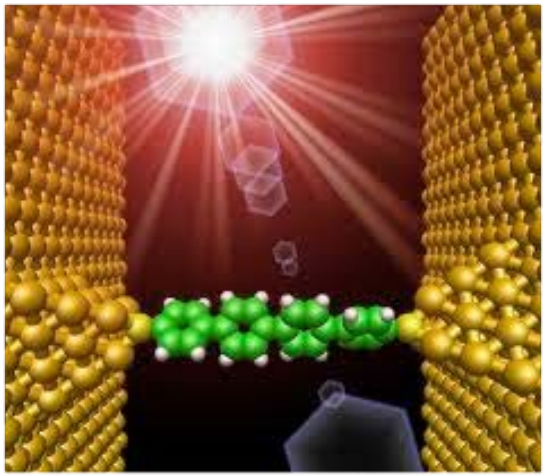




Matthew Reuter

Electron transport through molecules:

- How does electric current traverse a **quantum** system?
- What is the conductance of a single molecule?
- What physics determines this behavior?
- What effects lack classical analogs?



Applications include:

- Photovoltaics
- Scanning probe microscopies
- Molecular electronics

Our goals:

- Provide better interpretations of experimental data
- Develop & implement more accurate computational frameworks

Ratner, Nature Nanotech. **8**, 378 (2013).

Improving Computation

Ab initio simulations are common

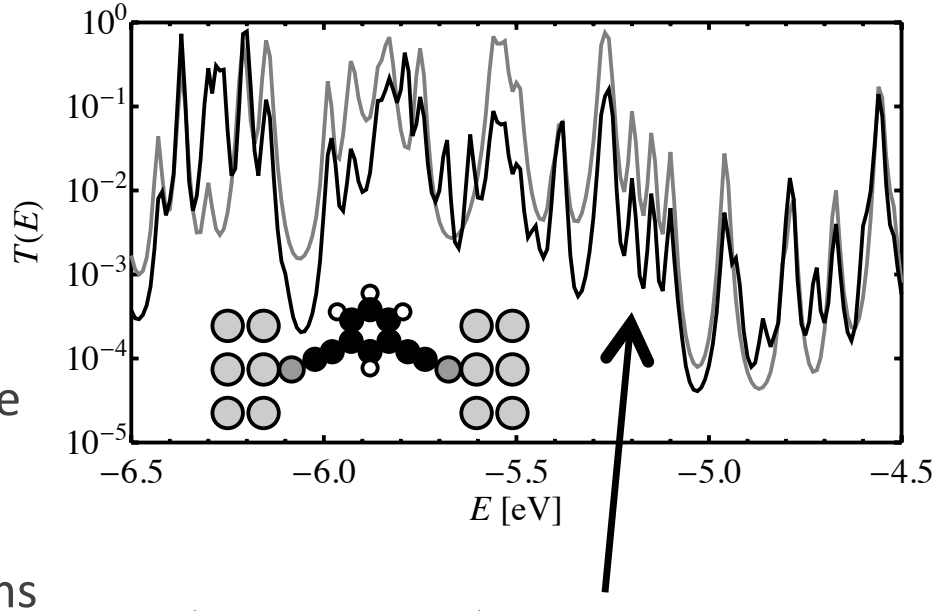
- Several known "white elephant" problems:
- Numerical artifacts
- Unphysical behavior (e.g., ghost transmission)

→ Transmissions are usually too large

Our work:

- Diagnose causes for these problems (e.g., poor system partitioning)
- Implement computational tools that are not plagued by these problems

→ More accurate simulations!



Preliminary results:
Gray line — Common formalism
Black line — Our tools

Although these issues sound pedanti c, they have big effects!

Reuter & Harrison. J. Chem. Phys. **139**, 114104 (2013); **140**, 177104 (2014).

Jim Jiao

NumGeom Group in Computational & Applied Mathematics

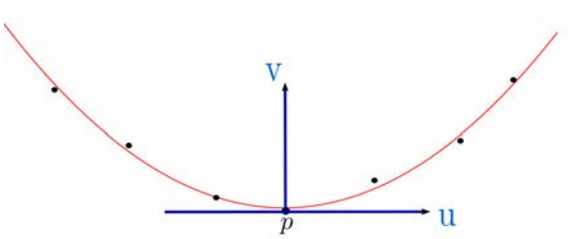
NumGeom group focuses on high-performance numerical and geometric computations

- **Numerical methods**: accurate and stable methods for general approximations or solving PDEs
- **Geometric algorithms**: methods for dynamic surfaces; data structures and algorithms for meshing; interfaces in multiphysics coupling
- **HPC**: efficient and scalable multigrid solvers; high-productivity programming environment

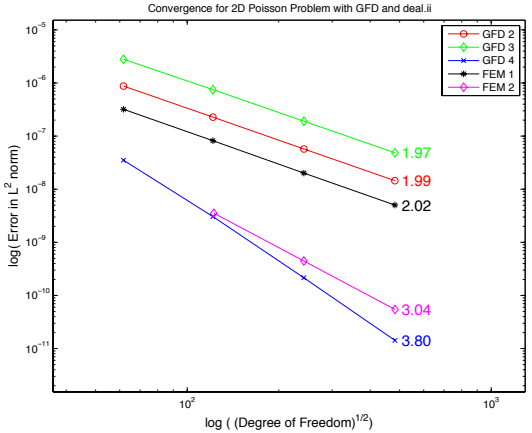
From left to right: Tristan Delaney, Hongxu Liu, Cao Lu, Prof. Xiangmin Jiao, Navamita Ray, Rebecca Conley, and Xinglin Zhao

Highlights 1: Unified Theoretical Framework of Numerical Methods

- **WLS**: Weighted least squares provides more flexible framework than interpolation for accurate and stable methods over point clouds or unstructured meshes
- **GFD**: Based on WLS, GFD generalizes finite-difference methods to unstructured meshes, delivering higher-order accuracy and stability (student participants: Hongxu Liu, Rebecca Conley, et al.)



WLS generalizes interpolation, with more flexibility and better stability.



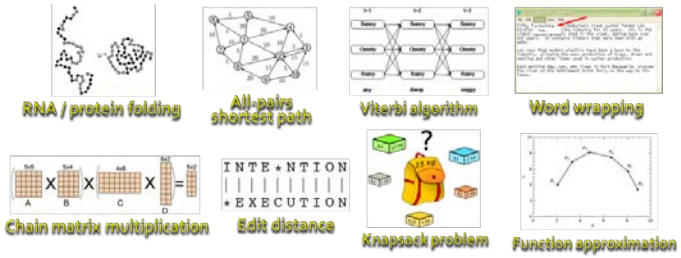
GFD delivers higher order convergence than other state-of-art methods.

Automatic Discovery of Cache-oblivious Parallel Recursive Algorithms for Dynamic Programs

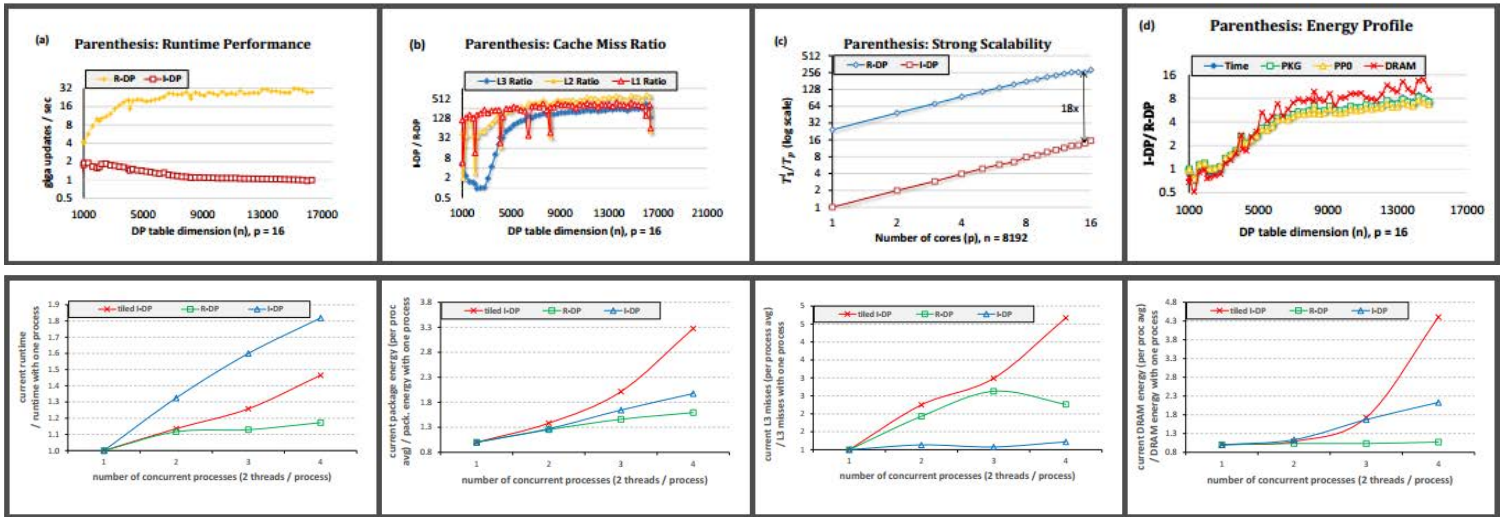
(with MIT and Fudan University)

Rezaul Chowdhury

- *Dynamic Programs (DP)*
  - arise in many application areas
  - traditionally implemented using inefficient nested loops

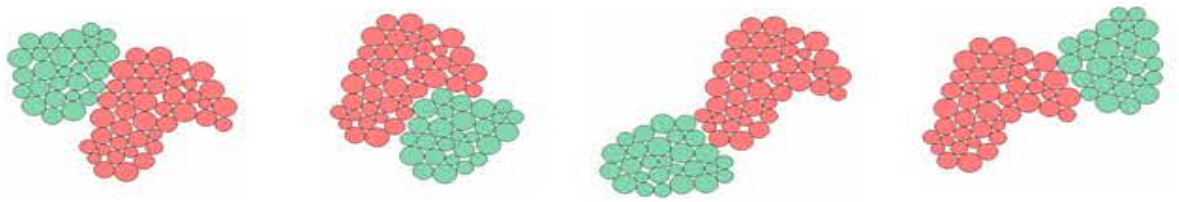


- Given an inefficient iterative DP implementation (I-DP), we automatically generate a *high-performing energy-efficient resource-oblivious parallel recursive algorithm* (R-DP) for solving the DP



F²Dock: Rigid-body Protein-Protein Docking

(with UT Austin and SCRIPPS Research)



- employs many novel ideas for ranking/filtering docked positions
  - outperforms other rigid-body docking software in accuracy
- first docking software to employ
  - non-uniform (error-bounded) & sparse uniform FFT
  - octree based tunable approximations (speed-accuracy tradeoff)
- parallelization
  - multithreaded
  - MPI-based distributed implementation
- front-end
  - graphical user interface
  - client-server mode (submits jobs to UT PRISM2 cluster by default)
- open source

HPC^{NY} @ Stony Brook

Jason Trelewicz and Robert J. Harrison

Overview

STONY BROOK UNIVERSITY

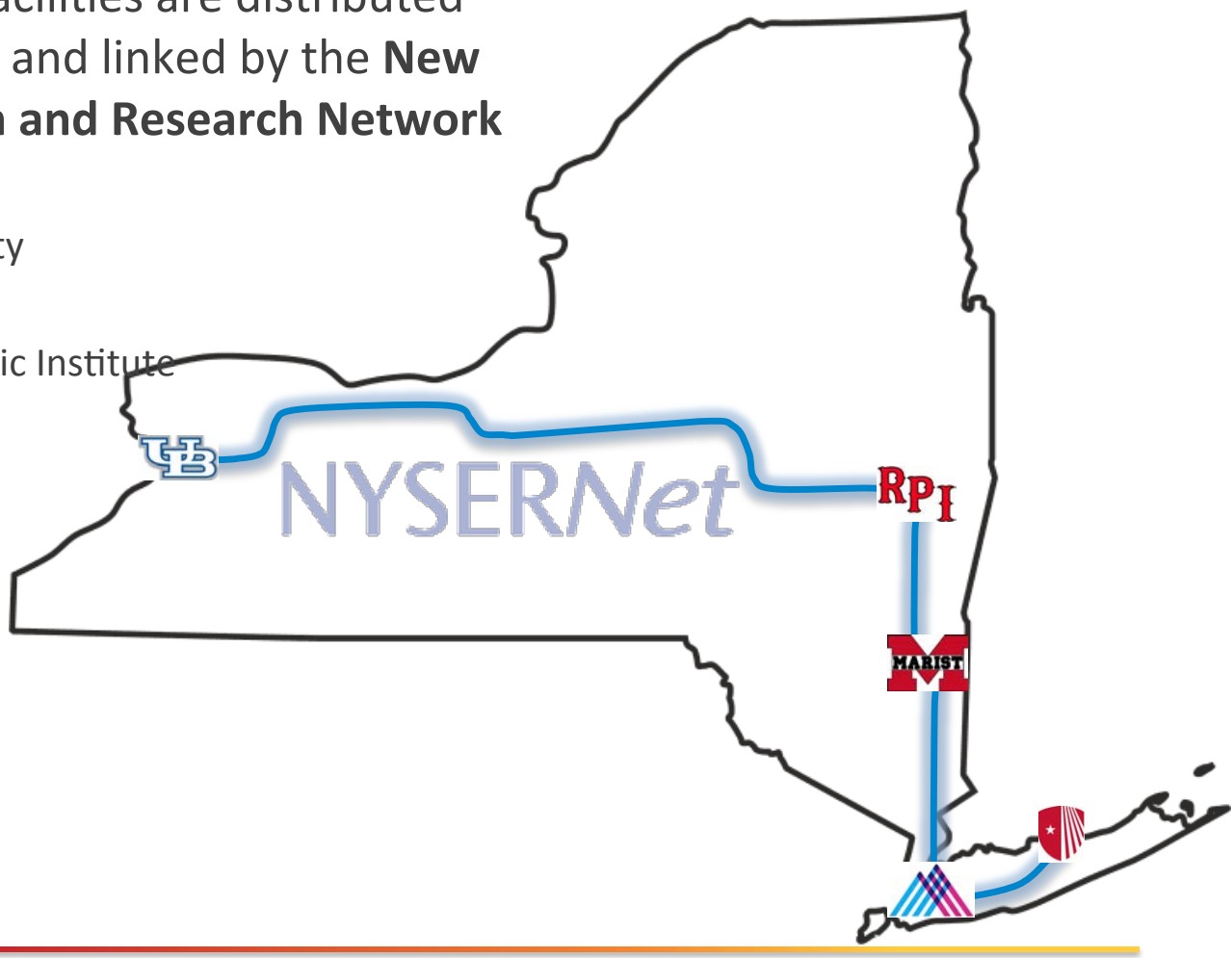
Institute for Advanced Computational Science

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

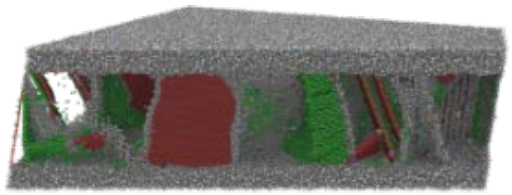


Powered by ESD/NYSTAR

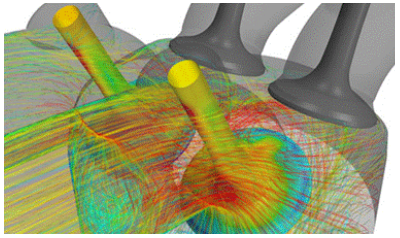
NYSTAR
Empire State Development
Division of Science, Technology & Innovation

The SBU HPC^{NY} team

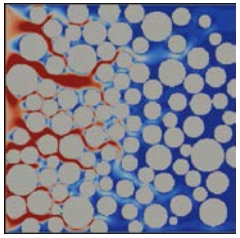
- A team of SBU faculty and staff with expertise in computational science, engineering, scientific programming, data analysis and database design, animation and visualization, and marketing.
  - Faculty include mechanical, chemical, and materials engineers, computational chemists, and computer scientists 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

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

Motiff Technologies: Supercomputing Audio

Modeling of Hybrid Batteries for Grid Storage

TheoretiK

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

Paralab Computing

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

Measuring Economic Impact

- Jobs created/retained in New York State at company
  - New Jobs – Credited jobs must be permanent, full-time positions
  - Retained Jobs – Address jobs at risk and that the collaboration was a significant reason for their retention.
- Increased company revenues
  - Retained sales – In some cases, NYSTAR may credit impact for retained sales with company through retention of a specific customer that it would have otherwise been lost (e.g., due to quality control).
- Cost savings realized by company
  - Production process improvements, the value of accessing specialized equipment, expertise or analytical testing, and other research savings.
  - Valuing Research Savings –NYSTAR partner is providing services such as access to computational resources or research expertise that otherwise would have to be done by the company in-house.
- Funds acquired by the company
  - Venture capital, other business investments, and federal or non-NYS grants.
- Capital expenditures by the company
  - Infrastructure improvements, purchases of new capital equipment, and construction where NYSTAR partner played a substantive role in leading the company to make these investments.

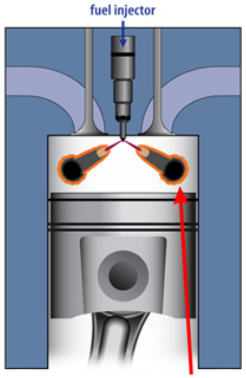
Success Story: Innoveering

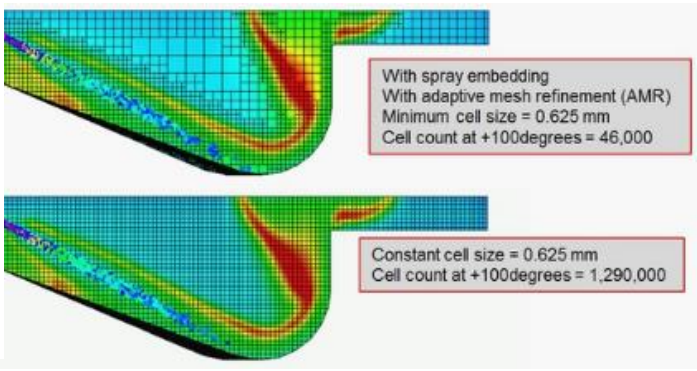
innoveering
innovative engineering solutions

- Exploring a partial fuel reformation technique to improve combustion efficiency and reduce CO and UHC emissions in heavy-duty diesel engines.

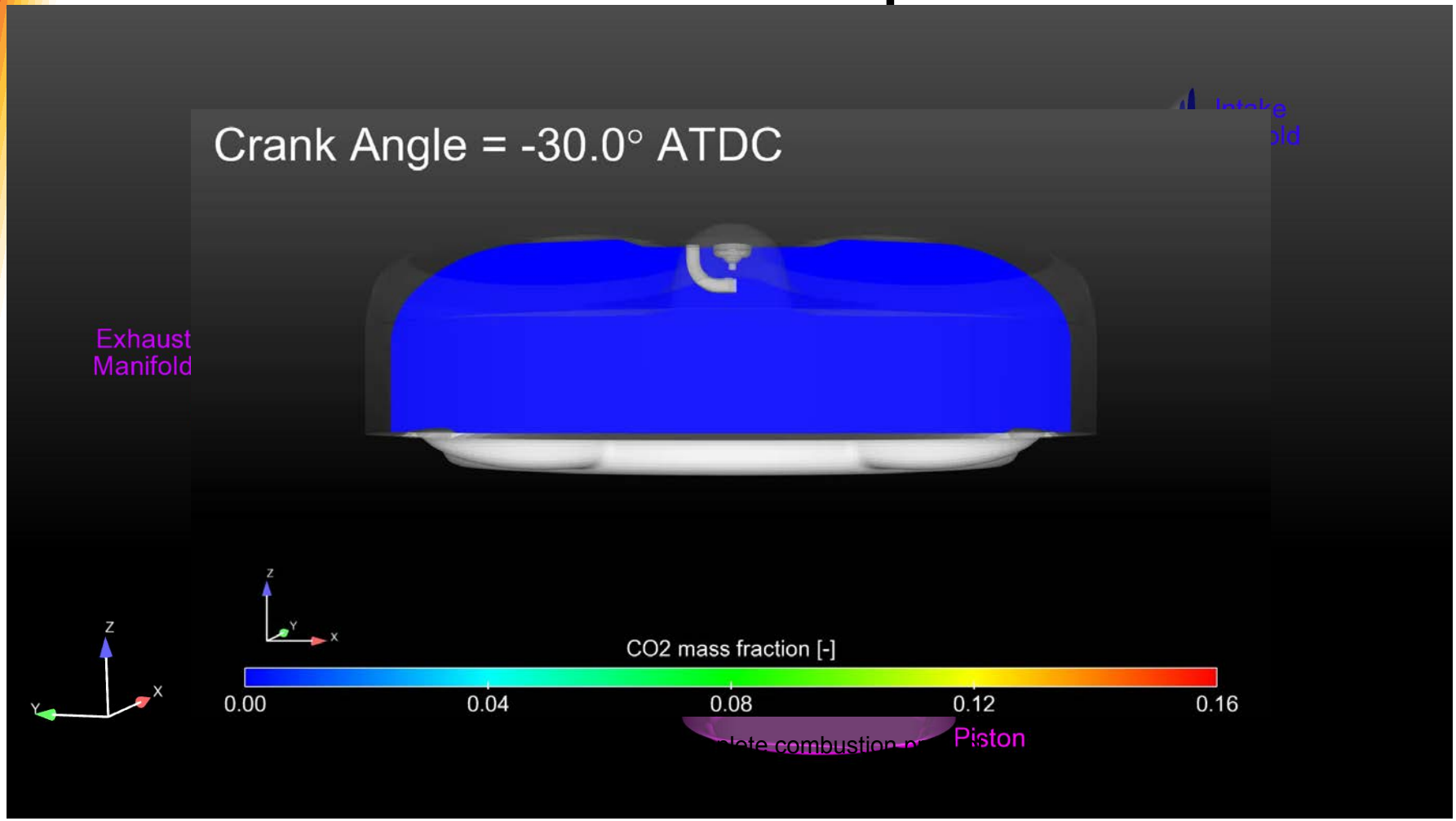
- HPC^{NY} team is investigating the reforming effects on natural gas combustion using new fuels with a focus on Syngas (H_2 + CO).
  - Computational fluid dynamics (CFD) simulations using ConvergeCFD for chemical kinetics and EnSight for visualization.

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





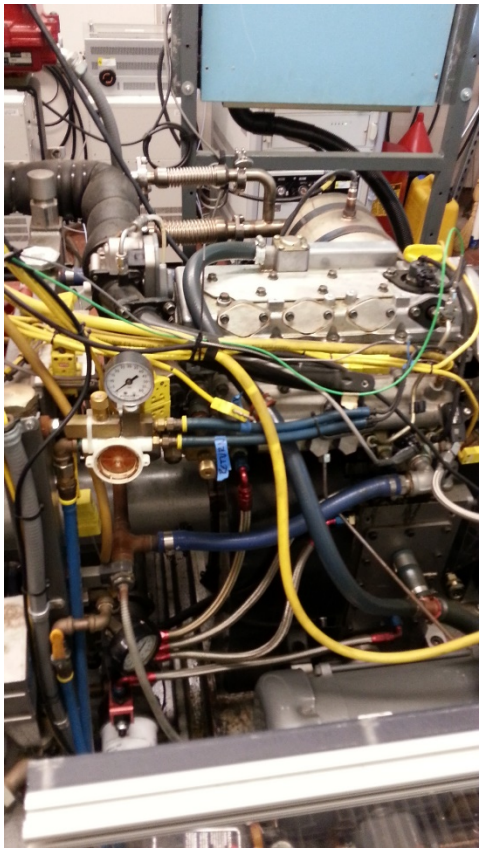
Model Description



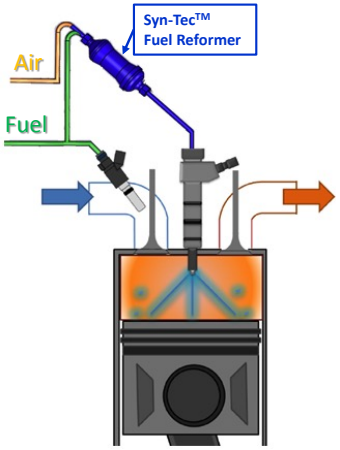
Modeled engine is a light-duty PFI natural gas with CR 12.5:1

Department of Energy Project

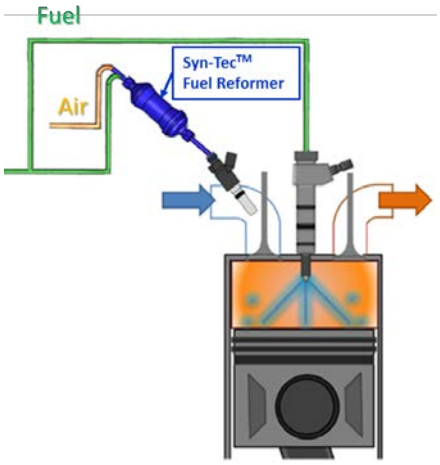
- Recently awarded a $1.1M 3-year project from DOE Vehicle Technologies Office
- Focus: Reactivity Controlled Compression Ignition (RCCI, right) using a single fuel
  - Enabled by an onboard fuel reformer
- Innoveering will work with CCNY to provide and analyze the reformates of gasoline, diesel, and natural gas that are candidate fuels
- Stony Brook will then focus on modeling, simulation and experimental testing of these fuel pairs
  - Cooperative Fuels Research (CFR)
  - Ricardo Hydra diesel engine (right)
- 3 Ph.D. students employed for modeling and experimental work



Ricardo Hydra
Diesel Engine



Version 1



Version 2