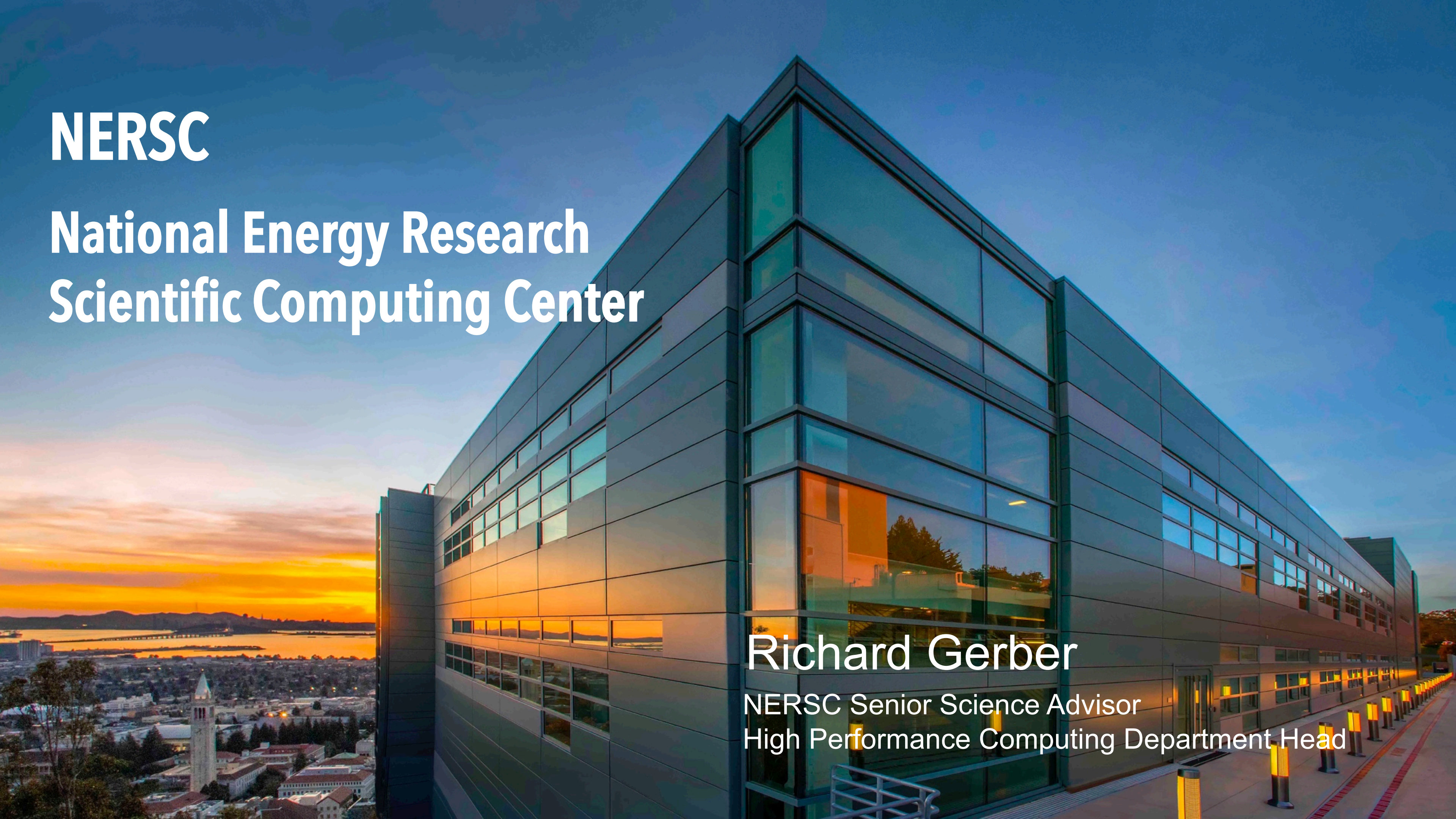


# NERSC

## National Energy Research Scientific Computing Center

Richard Gerber

NERSC Senior Science Advisor

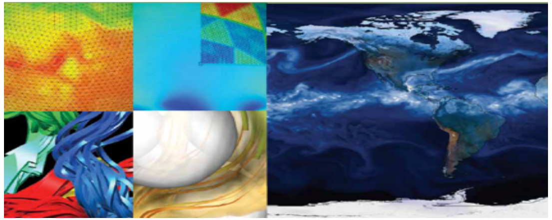
High Performance Computing Department Head

# NERSC: the Mission HPC Facility for DOE Office of Science Research

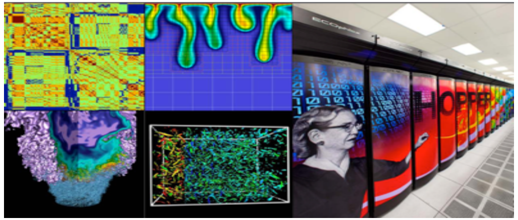
NERSC

U.S. DEPARTMENT OF ENERGY | Office of Science

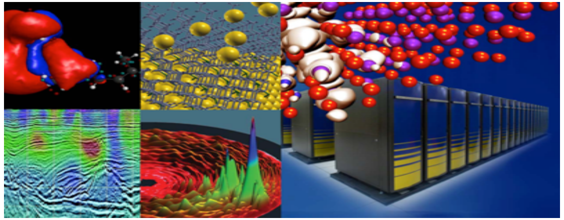
Largest funder of physical science research in the U.S.



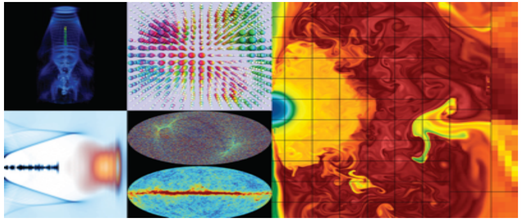
Bio Energy, Environment



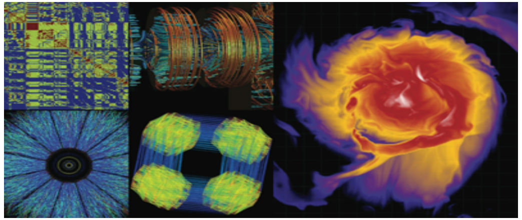
Computing



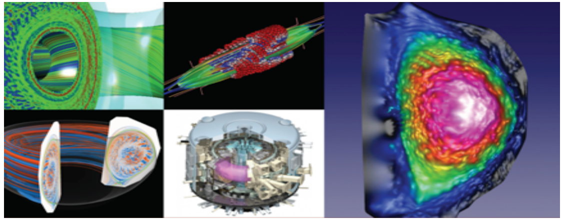
Materials, Chemistry, Geophysics



Particle Physics, Astrophysics



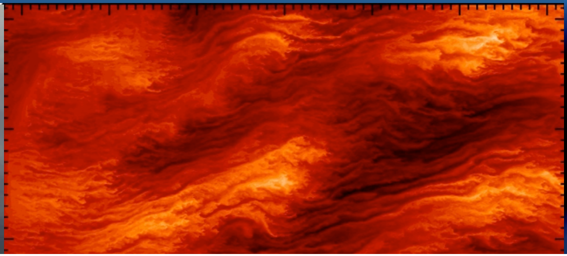
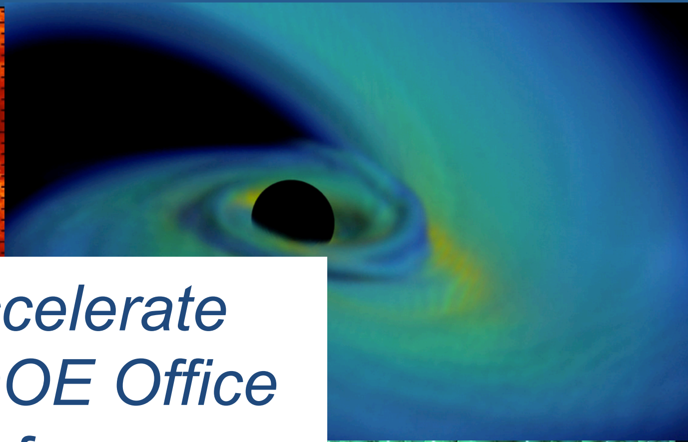
Nuclear Physics



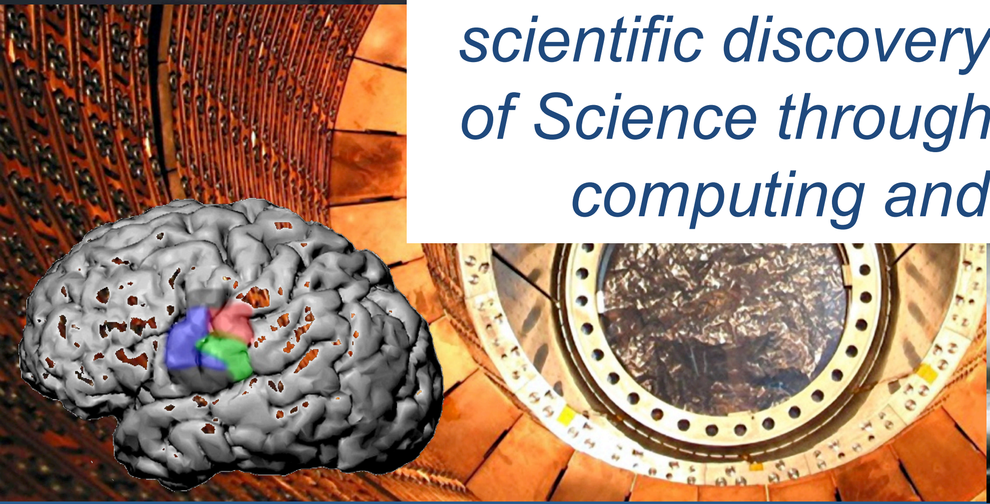
Fusion Energy, Plasma Physics

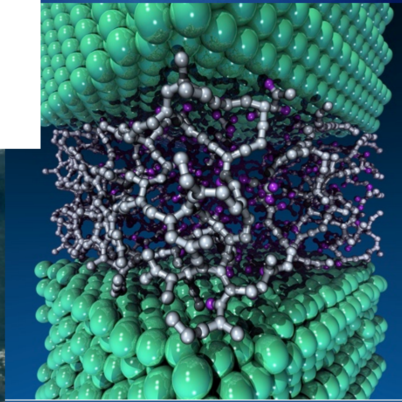
6,000 users, 700 projects, 700 codes, 48 states, 40 countries, universities & national labs

# NERSC's Mission

*NERSC's mission is to accelerate scientific discovery at the DOE Office of Science through high performance computing and data analysis.*

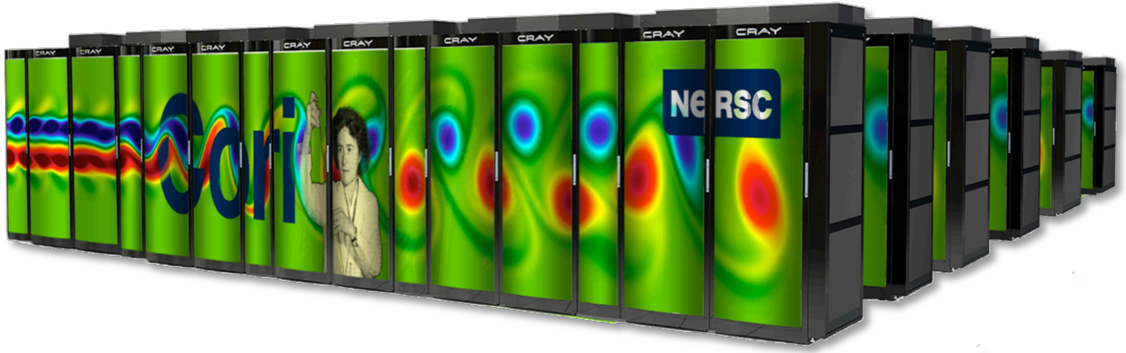




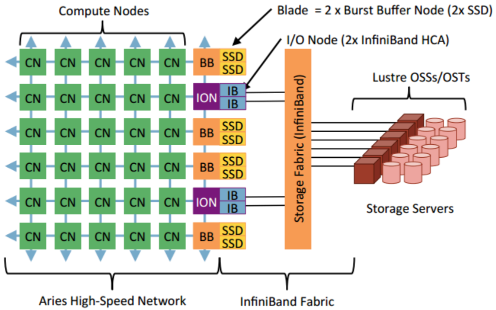
# Fulfilling Our Mission

NERSC provides first-of-their-kind computational and data systems

The center is widely recognized as a world leader for enabling user productivity.




Cori: #6 on world list of Top 500 supercomputers




THENEXTPLATFORM

**FIRST BURST BUFFER USE AT SCALE BOLSTERS APPLICATION PERFORMANCE**

May 16, 2016 Nicole Hemsoth

# National Energy Research Scientific Computing Center

- We're very proud of the science produced by our users
- It energizes our staff
- It's why we can compete with Facebook, Google, Apple, …

1 » 2 » 3 » 4 » 5

**RARE SUPERNOVA DISCOVERY USHERS IN NEW ERA FOR COSMOLOGY**

Discovered! The first ever multiply-imaged gravitationally-lensed Type Ia supernova. With more of these events, researchers could measure the universe's expansion rate within four percent accuracy. Berkeley researchers do have a method for finding more.

» Read More

# How Can We Measure Scientific Productivity?

- Should we measure productivity in the number of publications, citations, and patents, or should we use an indicator like Hirsch's h index?
- Publications?
  - People can easily publish their work in smaller pieces to get more papers out of one project.
  - Citations? people can cite themselves and pad papers with unnecessary numbers of references.
  - Field dependency: some science areas publish smaller studies more frequently
- Hirsch's h index
  - Suffers from problems like field dependency and misuse of references, as well.
- AAAS: With all this uncertainty, it might not be a bad idea for the federal science agencies to fund research, or thoroughly conduct their own investigations, that will determine how to best measure scientific productivity.
- So, although there is not a good solution, we look at publications and their impact through citations.

# NERSC's Users are Highly Productive Scientifically

- NERSC users produce more scientific publications than any other center in the world*; ~2K/year
- 838 citations via Web of Science in 2017 so far (not perfect!)

| Journal | Articles |
|---|---|
| Journal of Physical Chemistry Chemical Physics | 45 |
| Physical Review B (condensed matter and materials) | 42 |
| Astrophysical Journal | 30 |
| Physical Review Letters | 29 |
| Journal of Chemical Physics | 28 |
| Nature Communications | 27 |

4 in Nature
27 in Nature Comm.
60 in 12 journals

4 in Science

8 in PNAS

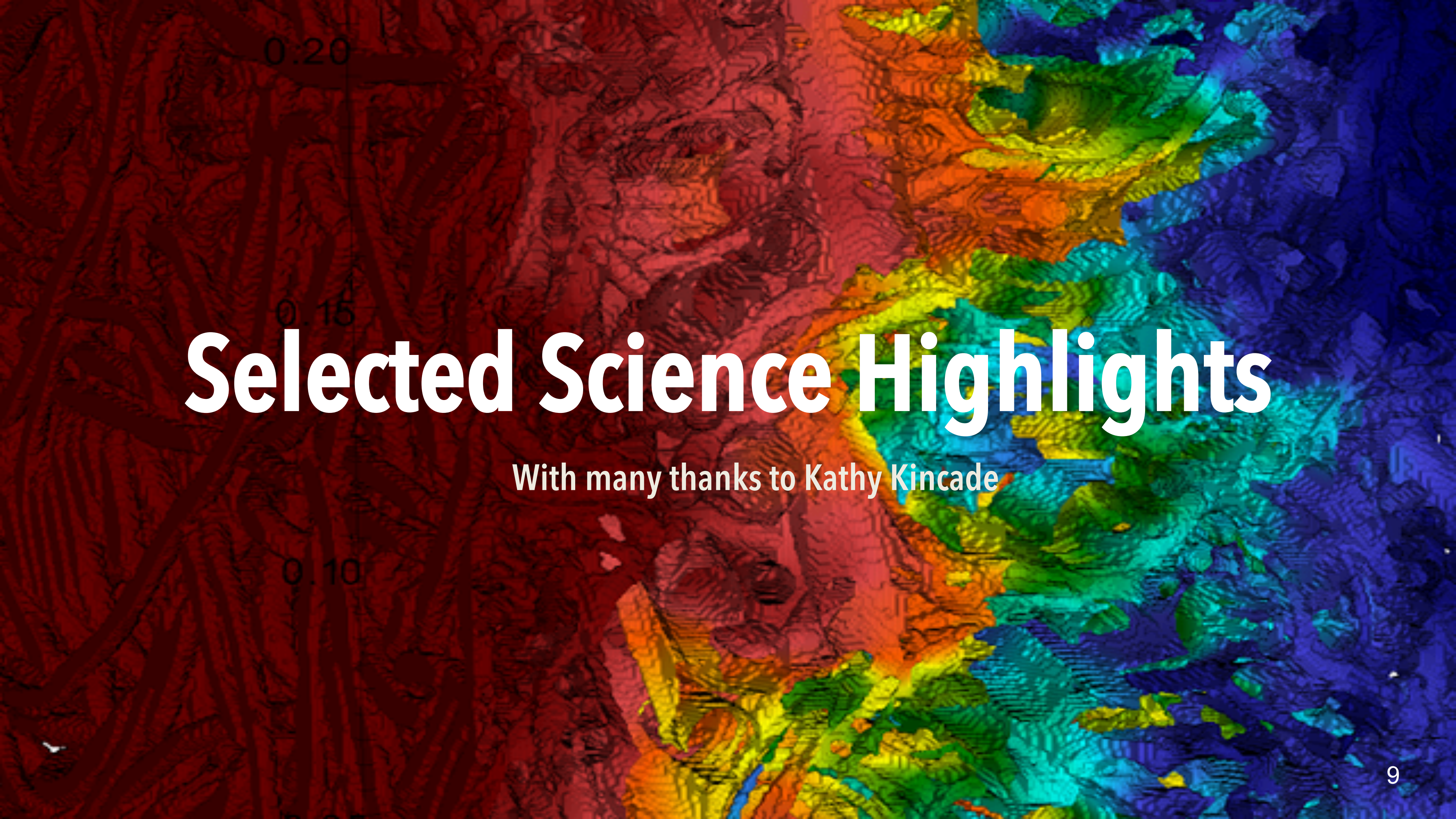


* as far as I can tell

# Top 10 Cited Publications 2012-2017

NERSC

| | | |
|---|---|---|
| Structure, function and diversity of the healthy human microbiome | Huttenhower, Curtis; Gevers, Dirk; Knight, Rob; et al. | Nature, 486, 7402, 202, 2012 |
| Highly Crystalline Multimetallic Nanoframes with Three-Dimensional Electrocatalytic Surfaces | Chen, Chen; Kang, Yijin; Huo, Ziyang; et al. | Science, 343, 6177, 1339, 2014 |
| The Materials Project: A materials genome approach to accelerating materials innovation | Jain, Anubhav; Shyue Ping Ong; Hautier, Geoffroy; et al. | APL Materials, 1, 1, 011002, 2013 |
| Water Desalination across Nanoporous Graphene | Cohen-Tanugi, David; Grossman, Jeffrey C. | Nano Letters, 12, 7, 3602, 2012 |
| A framework for human microbiome research | Methe, Barbara A.; Nelson, Karen E.; Pop, Mihai; et al. | Nature, 486, 7402, 215, 2012 |
| Unusual defect physics in CH3NH3PbI3 perovskite solar cell absorber | Yin, Wan-Jian; Shi, Tingting; Yan, Yanfa | Applied Physics Letters, 104, 6, 063903, 2014 |
| Extraordinary Sunlight Absorption and One Nanometer Thick Photovoltaics Using Two-Dimensional Monolayer Materials | Bernardi, Marco; Palummo, Maurizia; Grossman, Jeffrey C. | Nano Letters, 13, 8, 3364, 2013 |
| Vertical and in-plane heterostructures from WS2/MoS2 monolayers | Gong, Yongji; Lin, Junhao; Wang, Xingli; et al. | Nature Materials, 13, 12, 1135, 2014 |
| The clustering of galaxies in the SDSS-III Baryon Oscillation Spectroscopic Survey: baryon acoustic … | Anderson, Lauren; Aubourg, Eric; Bailey, Stephen; et al. | MNRAS, 441, 24, 2014 |
| IMG: the integrated microbial genomes database and comparative analysis system | Markowitz, Victor M.; Chen, I-Min A.; Palaniappan, Krishna; et al. | Nucleic Acids Research, 40, 115, 2012 |




# Selected Science Highlights

With many thanks to Kathy Kincade

# Design and Discovery of Ferroelectric Materials

## Scientific Achievement

Chemists from the University of Pennsylvania demonstrated a multi-scale simulation, run at NERSC, of lead titanate oxide that provides new understanding about what it takes for polarization within ferroelectric materials to switch.

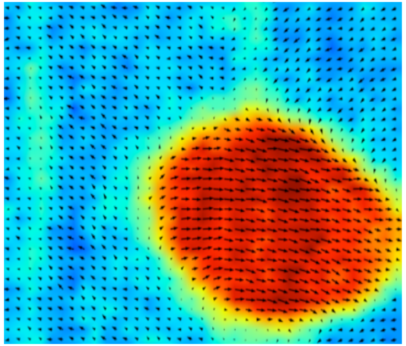
## Significance and Impact

Ferroelectric materials are useful because their spontaneous electric polarization can be reversed by an external electric field. They are crucial "smart materials" for sensors, such as ultrasound machines and probe-based microscopes.

Despite proliferation in commercial applications, however, there are many gaps in the theoretical principles that explain the behavior of ferroelectric materials. This new mathematical model is expected to aid efforts to find and design new ferroelectric materials.

## Research Details

- The ferroelectric material simulated on NERSC's Edison system features titanium ions inside six-pointed octahedral "cages" of oxygen ions. The polarization of a given domain is determined by which points of the cages the titanium ions move toward.
- This study is the first to show that math models calibrated to quantum mechanics can accurately relate the strength of the electric field to the speed at which domain walls move.



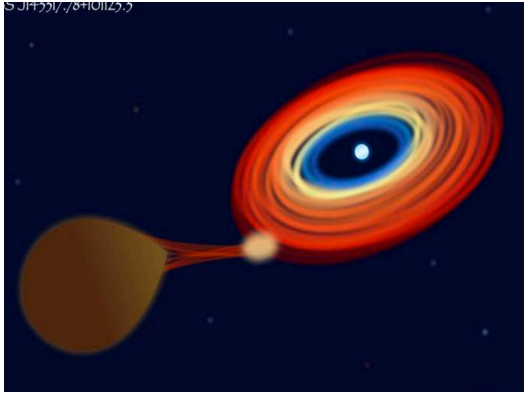
S. Liu, I. Grinberg, A.M. Rappe, *Nature* 534, 360–363, , June 16, 2016

PI: A. Rappe
(Univ. of Pennsylvania)

# Brown Dwarf Companion to Accreting White Dwarf

## Scientific Achievement

In a recent Nature paper an international research team used spectroscopic observations and theoretical predictions to confirm the existence of an irradiated brown-dwarf companion to an accreting white dwarf.



J.V. Hernandez Santisteban, et al, *Nature* 533, May 2016, 366–368

PI: E. Baron (Univ. of Oklahoma)

## Significance and Impact

Astronomers want to better understand how planetary and star systems beyond our own were formed, live, and die. One of the more interesting situations occurs when a compact “white dwarf” star accretes material from a nearby “brown dwarf,” an object that is too small to be a star, yet too large to be called a planet. To date, only a single brown-dwarf donor to an accreting white dwarf has been detected, and no empirical information is available regarding the effect of irradiation on the atmosphere of the donor.

## Research Details

- This work employed PHOENIX, a general-purpose stellar and planetary atmosphere code that can calculate atmospheres and spectra of stars, including white dwarfs and brown dwarfs; and ICARUS, a binary light-curve synthesis code.
- The computations, run NERSC’s Edison supercomputer, allowed the team to model and characterize the signature of the brown dwarf atmosphere.

# How Climate Fluctuations Influence Sea Ice Expansion

NERSC

## Scientific Achievement

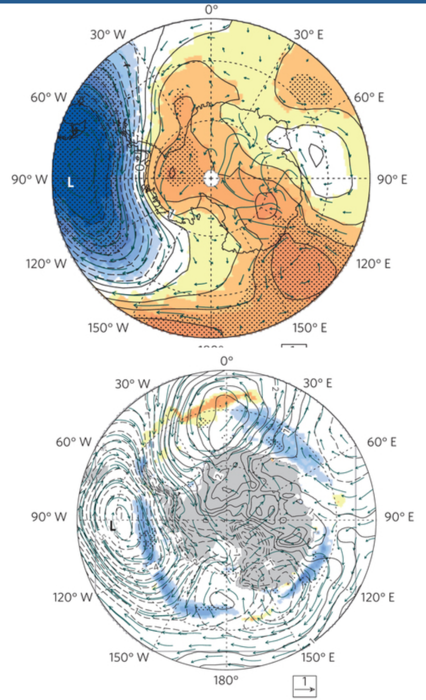
Observations indicate that the Antarctic sea ice been expanding since 2000, while the average findings of all climate models shows a decline. A new study, led by the National Center for Atmospheric Research (NCAR), found that the expansion can be explained by natural climate fluctuation.

## Significance and Impact

Surface wind changes that have expanded Antarctic sea ice are mainly driven by sea surface temperature and precipitation anomalies from the naturally occurring Interdecadal Pacific Oscillation (IPO) in the equatorial eastern Pacific, and climate models can simulate these processes.

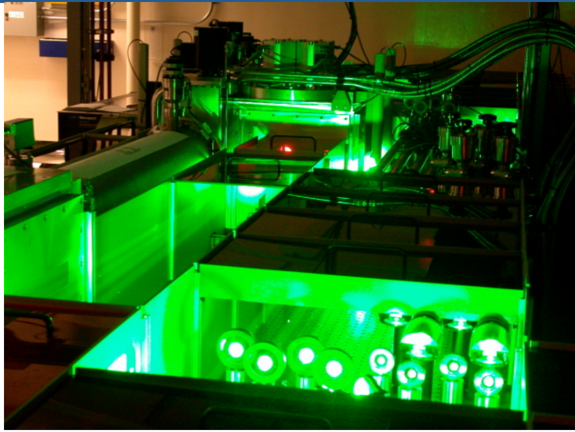
## Research Details

- By comparing physical observations with climate model simulations run at NERSC, NCAR researchers were able to demonstrate a direct connection between Antarctic sea-ice expansion and the IPO.
- The study offers evidence that the negative phase of the IPO, which is characterized by cooler-than-average sea surface temps in the tropical eastern Pacific, has created favorable conditions for the sea ice growth since 2000.




G.A. Meehl, et al, *Nature Geoscience*, July 4, 2016, doi:10.1038/ngeo2751

# Advanced Simulations Support Breakthrough Coupling of Two Plasma Accelerator Stages



## Scientific Achievement

A team led by Berkeley Lab researchers has demonstrated that an electron beam accelerated by a laser-driven plasma wave can be further accelerated by a second plasma wave — a fundamental breakthrough in advanced accelerator science.

## Significance and Impact

Laser-driven plasmas can accelerate electrons to very high energies over short distances. This research shows that accelerators can be built by coupling multiple stages of acceleration, which could lead to table-top devices capable of energy gains equivalent to those achieved in large accelerators. Such accelerators could be used for medical and other applications.

Steinke, et al., *Nature*, 530, February 2016

## Research Details

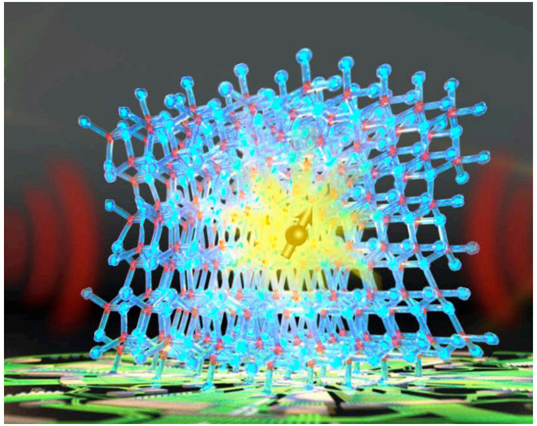
- Detailed modeling of the staging experiment was performed at NERSC on Edison with the code INF&RNO (INtegrated Fluid & paRticle simulatioN cOde), a reduced code specifically designed to model laser-plasma accelerators.
- Extensive modeling allowed the researchers to reproduce and interpret the results obtained in several experimental campaigns, and contributed to the optimization of the experiment itself.
- The highly efficient INF&RNO code and access to time on Edison allowed for the quick production of large parameter scans for detailed comparison with experiments

PIs: C. Benedetti, J-L Vay, LBNL

# Better Materials for Quantum Computing

## Scientific Achievement

One of the leading methods for creating quantum bits (qubits) involves exploiting the structural atomic defects in diamond. However, using diamond is both technically challenging and expensive. Now researchers from the University of Chicago and Argonne National Laboratory have found a way to engineer an analogue defect in aluminum nitride, which could reduce the cost of manufacturing quantum computers.



## Significance and Impact

Quantum computers have potential to break common cryptography techniques, search huge datasets and simulate quantum systems in a fraction of the time it takes today's computers. But engineers first need to be able to control the properties of qubits.

## Research Details

- Using NERSC's Edison supercomputer, the researchers found that by applying strain to aluminum nitride, structural defects can be created in the material that may be harnessed as qubits similar to those seen in diamond.
- Their calculations were performed using different levels of theory and the WEST code, developed at the University of Chicago, which allowed them to accurately predict the position of the defect levels in the band-gap of semiconductors.

*Seo, Govoni, Galli, Nature Scientific Reports, Vol. 6, Article No. 20803, Feb. 16, 2016*

PI: M. Govoni, G. Galli (Univ. of Chicago)

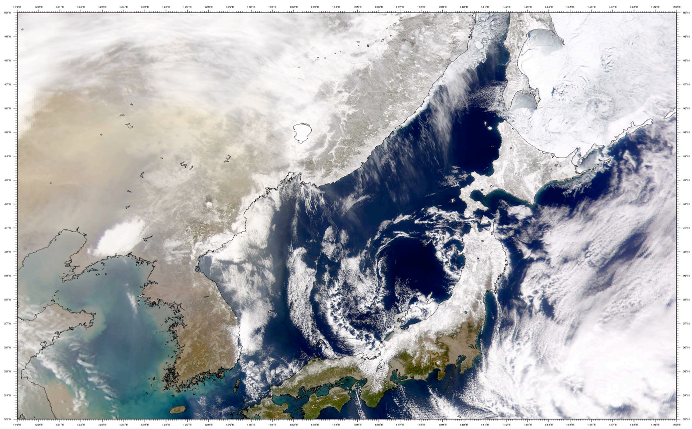
# More Dust, Better Air Quality

## Scientific Achievement

Man-made pollution in eastern China worsens when less dust blows in from the Gobi Desert, according to researchers from Pacific Northwest National Lab, Scripps Institution of Oceanography and UC San Diego.

## Significance and Impact

Dust plays an important role in determining air temperatures and thereby promoting winds to blow away man-made pollution. Less dust means air stagnates, with pollution becoming more concentrated and sticking around longer.



## Research Details

- Using computer models run at NERSC, together with historical data, the team found that reduced natural dust transported from the Gobi Desert translates to increased air pollution in highly populated eastern China.
- The results match observational data from dozen of sites in eastern China. The team found that two to three days after winds had brought dust into the region from western China, the air was cleaner than before the dust arrived.

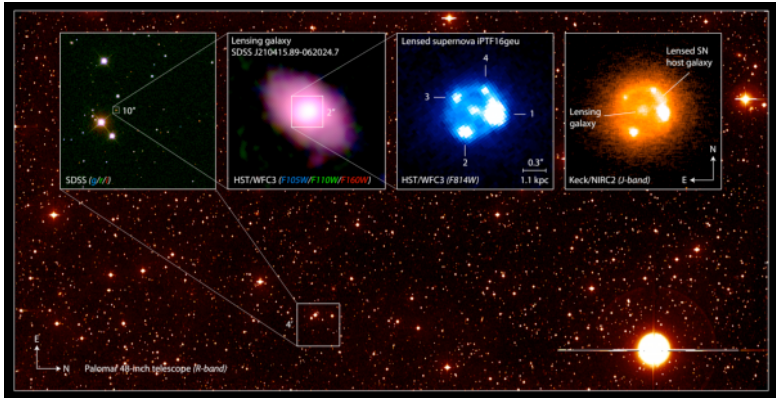
*Y. Yang, et al, Nature Communications 8, 15333, May 2017*

NERSC Project PI: S. Ghan, PNNL

# A Super Rare Supernova Discovery

## Scientific Achievement

With the help of the Intermediate Palomar Transient Factory (iPTF) and a galaxy 2 billion light years away from Earth that's acting as a "magnifying glass,'' astronomers captured multiple images of a Type Ia supernova (iPTF16geu) appearing in four different locations on the sky - the only Type Ia so far discovered that has exhibited this "gravitational lensing" effect.




## Significance and Impact

Astrophysicists believe that if they can find more of these magnified Type Ia's, they may be able to measure the rate of the universe's expansion to unprecedented accuracy and shed some light on the distribution of matter in the cosmos.

*A.Goobar, R. Amanullah, et al, Science 356, 6335, April 2017, 291-295*

NERSC Project PI:
M. Kasliwal, CalTech

## Research Details

- The iPTF, located at the Palomar Observatory in Southern California, comprises a wide-field camera mounted on the robotic Samuel Oschin Telescope that scans the sky nightly.
- As soon as observations are taken, the data travel more than 400 miles to NERSC, where machine learning algorithms running on NERSC's supercomputers sift through the data in real time and identify candidates, such as the iPTF16geu supernova, for further study.

# Shedding Light on Mysterious Plasma Flows

## Scientific Achievement

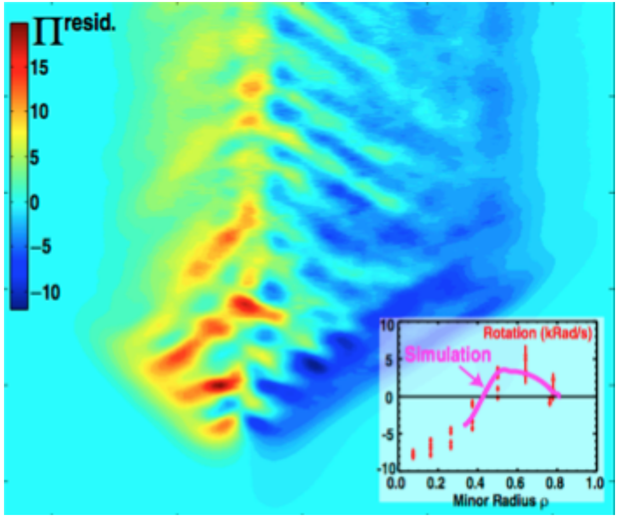
Researchers at Princeton Plasma Physics Laboratory (PPPL) and General Atomics used NERSC supercomputers to simulate a mysterious self-organized flow of the superhot plasma that fuels fusion reactions. The findings show that pumping more heat into the core of the plasma can drive instabilities that create plasma rotation inside the doughnut-shaped tokamak reactor that houses the hot charged gas.

## Significance and Impact

The findings could lead to improve control of fusion reactions in ITER, the international experiment under construction in France to demonstrate the feasibility of fusion power, and other fusion devices.

## Research Details

The researchers used GTS, a first principles kinetic code, to simulate the physics of turbulent plasma transport by modeling the behavior of plasma particles as they cycled around magnetic fields. The simulation predicted the rotation profile by modeling the intrinsic torque of the turbulence and the diffusion of its momentum. The predicted rotation agreed well, in shape and magnitude, with the rotation observed in DIII-D experiments.




A. Grierson et al, *Physical Review Letters,* 118, 015002, January 2017

NERSC Project PI: Wei-Li Lee, PPPL

# A Record Quantum Circuit Simulation

## Scientific Achievement

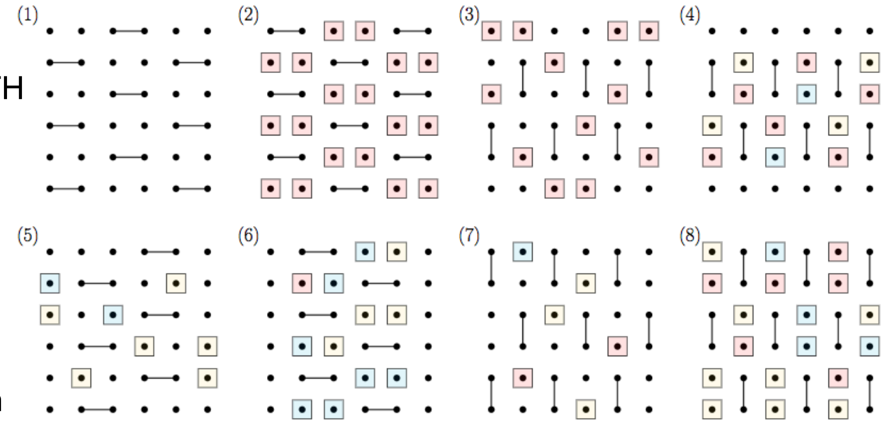
Researchers from the Swiss Federal Institute of Technology (ETH Zurich) used NERSC's 30-petaflop supercomputer, Cori, to successfully simulate a 45-qubit (quantum bit) quantum circuit, the largest simulation of a quantum computer achieved to date.

## Significance and Impact

The current consensus is that a quantum computer capable of handling 49 qubits will offer the computing power of the most powerful supercomputers in the world. This new simulation is an important step in achieving "quantum supremacy"— the point at which quantum computers finally become more powerful than ordinary computers.

## Research Details

- In addition to the 45-qubit simulation, the researchers also simulated 30-, 36- and 42-qubit quantum circuits.
- For the 45-bit simulation, they used 8,192 of 9,688 Intel Xeon Phi processors and 0.5 petabytes of memory.




Thomas Häner, Damian S. Steiger, 0.5 Petabyte Simulation of a 45-Qubit Quantum Circuit, arXiv:1704.01127 [quant-ph]

NERSC PI: T. Haner, ETH Zurich

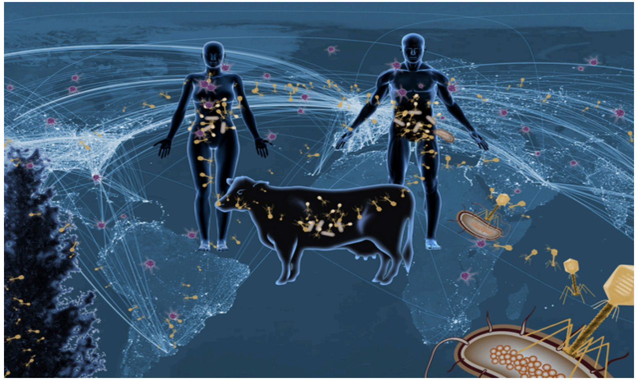
# Earth’s Viral Diversity Unveiled

## Scientific Achievement

In a study published in *Nature*, researchers at the Joint Genome Institute (JGI) used the largest collection of assembled metagenomic datasets from around the world to uncover over 125,000 partial and complete viral genomes, the majority of them infecting microbes.

## Significance and Impact

This effort, which leveraged the strong collaboration between NERSC and JGI, increases the number of known viral genes by a factor of 16 and provides researchers with a unique resource of viral sequence information. Given the role that viruses play in host metabolism, gene flow, and microbial communities, it is critical to capture viral linkages with their hosts.



*Paez-Espino, Eloe-Fadrosh, Pavlopoulos, et al, Nature,* 536, 425–430, Aug. 25, 2016

PI: N. Kyrpides (LBNL)

## Research Details

- The researchers used non-targeted metagenomics, referencing both isolate viruses and manually curated viral protein models, and the largest and most diverse dataset to date. The team analyzed over 5 trillion bases of sequences available in JGI’s Integrated Microbial Genomes with Microbiome Samples system collected from 3,042 samples around the world from 10 different habitat types. Their efforts to sift through the veritable haystack of datasets yielded over 125,000 viral sequences encoding 2.79 million proteins.
- It took about 10 million core-hours for all the computations against 4,000 metagenomes and around 50,000 isolate genomes.