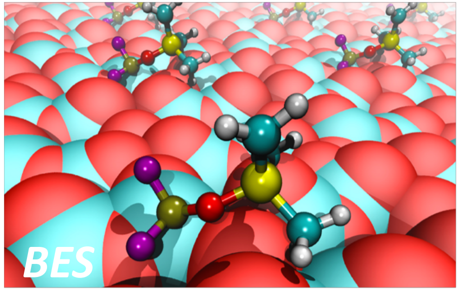
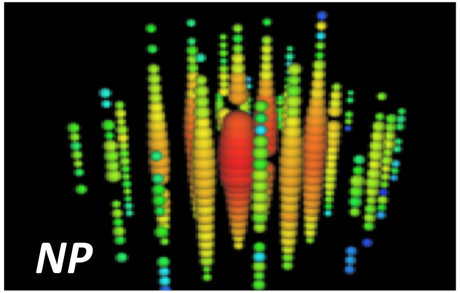
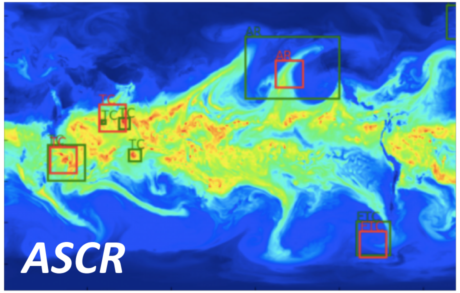
Science Highlights 2018

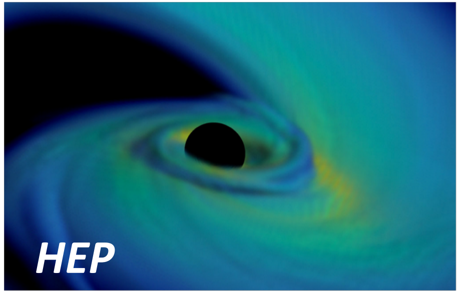
Edition 3

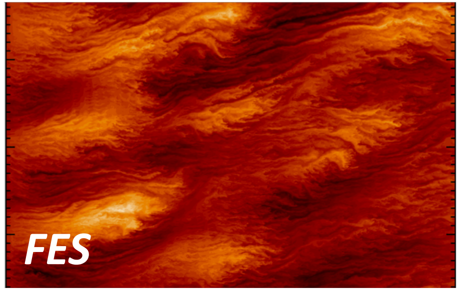
NERSC

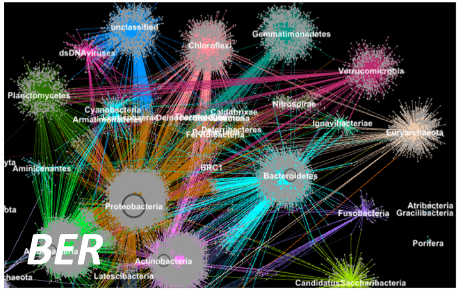








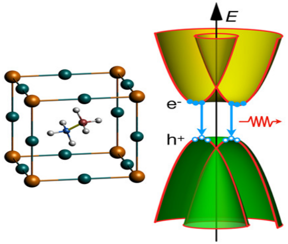




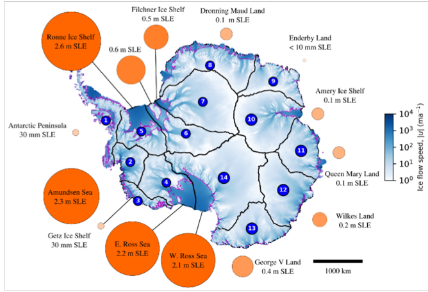
U.S. DEPARTMENT OF ENERGY | Office of Science

Science Highlights 2018 Set 3

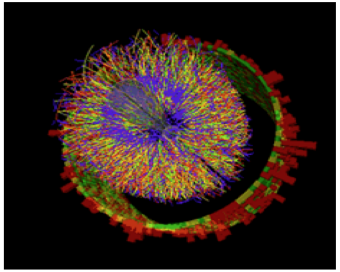
Materials Science
Revealing Reclusive Mechanisms for Solar Cells
NERSC PI: C. Van de Walle, UC Santa Barbara, *ACS Energy Letters*



High Energy Physics
Shedding Light on Luminous Blue Variables
NERSC PI: Yan-Fei Jiang, UC Santa Barbara. *Nature*

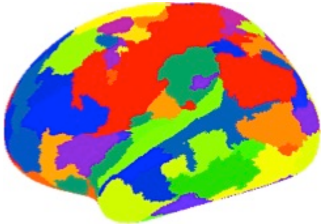


Earth Sciences
Simulations Probe Antarctic Ice Vulnerability
NERSC PIs: D. Martin, Berkeley Lab; E. Ng, Berkeley Lab; S. Price, LANL. *Geophysical Research Letters*

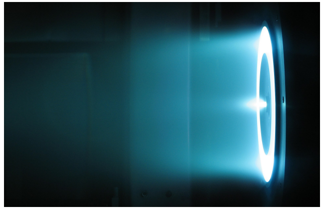


Nuclear Physics
Enabling Science Discovery for STAR
NERSC PI: J. Porter, Berkeley Lab. *J. Phys.: Conference Series*

Advanced Computing
Scalable Machine Learning in HPC
NERSC PI: L. Oliker, Berkeley Lab, *21st International Conference on AI and Statistics*



Plasma Physics
Plasma Propulsion Systems for Satellites
NERSC PI: I. Kaganovich, Princeton Plasma Physics Lab, *Physics of Plasmas*



Revealing Reclusive Mechanisms for Solar Cells

NERSC

Scientific Achievement

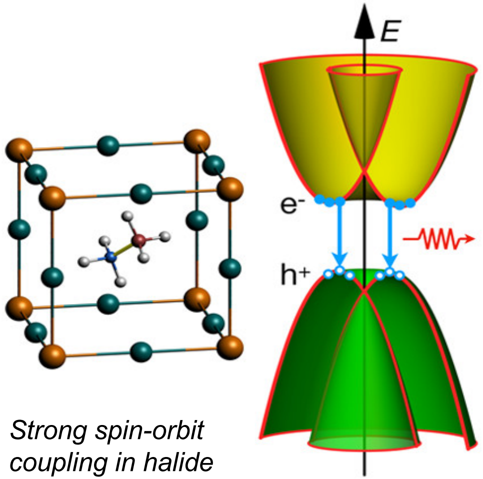
Researchers from the University of California, Santa Barbara used NERSC supercomputers to better understand the solar conversion efficiencies of hybrid perovskites and produce critical insights into how they work.

Significance and Impact

Hybrid perovskites are spectacularly efficient materials for photovoltaics. Just a few years after the first perovskite solar cells were fabricated, they have already achieved solar conversion efficiencies greater than 22 percent. Interestingly, the fundamental mechanisms that are responsible for this high efficiency are still being vigorously debated. The results of this study showed that a frequently cited explanation, based on low radiative rates, was not viable. This now provides a sound basis for future accurate modeling and design.

Research Details

Using more than 1,000 nodes on NERSC's Cori supercomputer, the team not only disproved one explanation for high solar cell efficiencies, but also studied how the materials could be used in light emitting diodes (LEDs). "These calculations are extremely demanding, and the compute power provided by NERSC has been instrumental in obtaining these results," commented lead researcher Chris Van de Walle.



Strong spin-orbit coupling in halide perovskites induces splitting of the band edges, which could affect recombination rates.
Image credit: X. Zhang and J.-X. Shen.

*X. Zhang, J.-X. Shen, W. Wang, and C. G. Van de Walle, "First-Principles Analysis of Radiative Recombination in Lead-Halide Perovskites"; ACS Energy Letters **3**, 2329 (2018). 10.1021/acsenergylett.8b01297*

Shedding Light on Luminous Blue Variables

Scientific Achievement

3D simulations run at NERSC, the Argonne Leadership Computing Facility, & NASA provided new insights into unique objects known as Luminous Blue Variables (LBV) – rare, massive, stars that can shine up to a million times brighter than the Sun. The team found that helium plays a major role in triggering the outbursts and their simulations predicted yet unseen short-term variability.

Significance and Impact

Astrophysicists are intrigued by LBVs because their luminosity and size dramatically fluctuate on a timescale of months. LBVs also periodically undergo giant eruptions, violently ejecting gases into space. Although scientists have long observed LBVs, the physical processes causing their behavior are still largely unknown, and traditional 1-D models are inadequate.

Research Details

Researchers from UC Santa Barbara, UC Berkeley, and Princeton University ran 3D simulations to study three different LBV configurations. The team used millions of computing hours on NERSC's Cori system, at ALCF, and at NASA. NERSC consultants provided assistance, including helping debug and optimize I/O issues on Cori.

Intense light from the star's core pushes against helium-rich pockets in the star's exterior, launching material outward in spectacular geyser-like eruptions. The solid colors denote radiation intensity, with bluer colors representing regions of larger intensity. The translucent purplish colors represent the gas density, with lighter colors denoting denser regions. Image: Joseph Insley, Argonne Leadership Computing Facility

Jiang, Yan-Fei; Cantiello, Matteo; Bildsten, Lars; Quataert, Eliot; Blaes, Omer; Stone, James; Nature, 561:498+; 2018 SEP 27, 10.1038/s41586-018-0525-0

Simulations Probe Antarctic Ice Vulnerability

Scientific Achievement

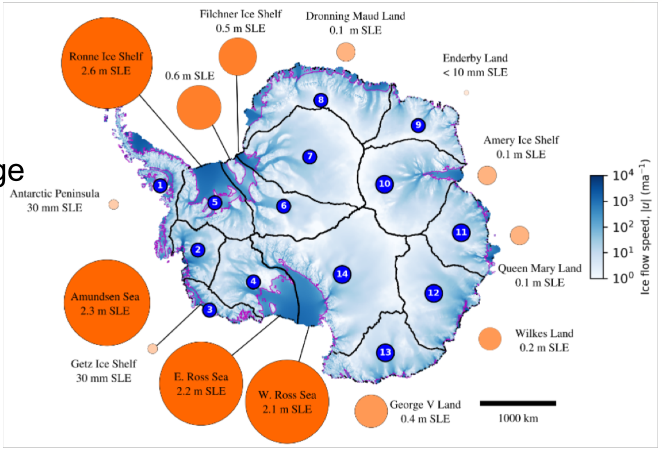
Researchers from Berkeley Lab, Swansea University, and the University of Bristol used a highly-resolved model of the Antarctic Ice Sheet to systematically examine vulnerability to regional collapse of its floating ice shelves and the potential for large contributions to sea level rise (SLR).

Significance and Impact

The biggest uncertainty in near-future SLR comes from the Antarctic Ice Sheet, in which ice flows in relatively fast-moving ice streams. At the ocean, ice flows into enormous floating shelves which push back on their feeder streams, buttressing them and slowing their flow. Melting and loss of ice shelves can result in faster-flowing, thinning and retreating ice leading to accelerated rates of global sea level rise.

Research Details

- To learn where Antarctica is vulnerable to ice-shelf loss, the team divided it into 14 sectors, applied extreme melting to each sector's floating ice shelves in turn, then ran the ice flow model 1,000 years into the future. The greatest vulnerability came from the ice shelves connected to West Antarctica, where much of the ice sits on bedrock lying below sea level.
- The combination of scalable AMR and NERSC computing resources enabled this work, entailing 35,000 years of Antarctic simulation. Former NERSC NESAP postdoc Andrey Ovsyannikov helped optimize the Chombo AMR framework to run on Cori.



Antarctic vulnerability to localized ice shelf collapse. Initial modeled flow speed is shown in shaded blue. Magenta lines indicate initial grounding-line locations. Contribution to sea level rise, after 1000 years of extreme, sustained ice shelf thinning originating in the numbered sectors is illustrated by the adjacent circle area. Image: Dan Martin, LBNL

Martin, Cornford, and Payne (2019). *Geophysical Research Letters*, DOI 10.1029/2018GL081229.

Enabling Science Discovery for STAR

Scientific Achievement

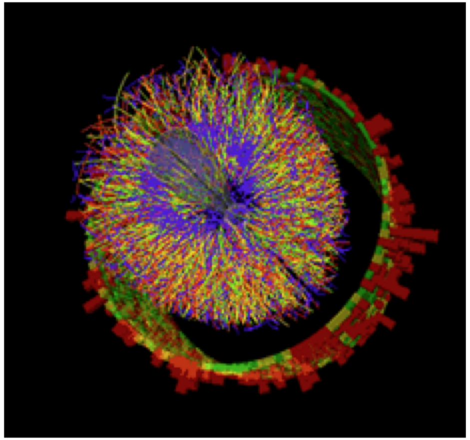
Physicists from Brookhaven National Laboratory (BNL) and Berkeley Lab used Cori to reconstruct data collected from the STAR nuclear physics experiment, an advance that dramatically reduces the time it takes to make detailed data available for scientific discoveries.

Significance and Impact

The researchers reconstructed multiple datasets collected by the STAR (Solenoidal Tracker at RHIC) detector during particle collisions at the Relativistic Heavy Ion Collider (RHIC) at BNL. By running multiple computing jobs in parallel, the team transformed petabytes of raw data into “physics-ready” data in a fraction of the months it would have taken using local resources.

Research Details

Technologies developed at NERSC allowed STAR to build a scalable highly fault-tolerant, multi-step data-processing pipeline. For example, NERSC’s Shifter HPC container system includes a disk caching feature that dramatically improves performance, allowing the team to scale up to 25,600 cores. Staff at LBNL, including Damian Hazen of NERSC and Eli Dart of ESnet—helped identify hardware issues and optimize the required data transfers and the end-to-end workflow.



This image shows collision events at STAR – thousands of particle tracks and the signals registered as some of those particles strike various detector components. Image: Brookhaven National Laboratory

M. Mustafa et al, J. Phys.: Conf. Ser., 898, 082023

Scalable Machine Learning in HPC

NERSC

Scientific Achievement

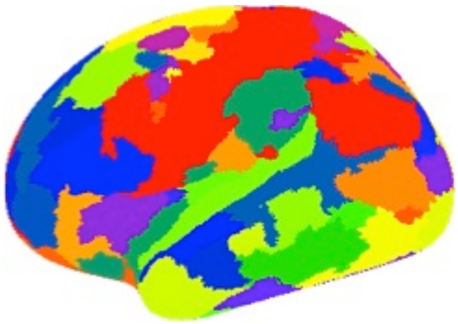
Researchers from UC Berkeley, Carnegie Mellon, UC Santa Barbara and Berkeley Lab used NERSC supercomputers to demonstrate that a powerful machine learning algorithm called CONCORD can be applied to huge data sets beyond the what could be done previously.

Significance and Impact

Some of the most challenging problems in science involve understanding the interactions between thousands or even millions of variables: how a disease may be caused by a subset of the 20 thousands of human genes, or agricultural production improved by a combination of microbial species among millions in the environment. The problem is to discover the most significant relationships between all of these variables, while separating the accidental relationships or confounding effects. These new results will allow application of machine learning techniques to problems previously out of reach.

Research Details

The researchers ran their algorithm on an enormous data set from the Human Connectome Project, which computed estimates for about 4 billion parameters, and conducted a demonstration problem with over 800 billion parameters. The team also showed it could use fMRI data to estimate the underlying conditional dependency structure of the brain.



A human brain parcellation derived from HP-CONCORD's results using a graph clustering algorithm applied to a set of data from the Human Connectome Project.

P. Koanantoakool et al, Proceedings of the 21st International Conference on AI and Statistics 2018, Lazarote, Spain. PMLR: Volume 84.

Plasma Propulsion Systems for Satellites

Scientific Achievement

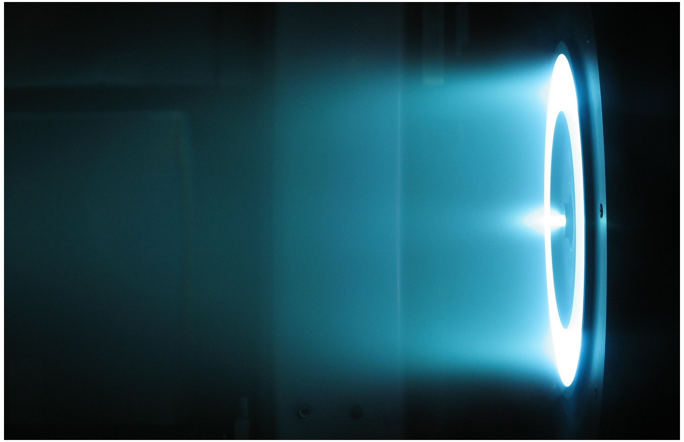
Researchers from Princeton Plasma Physics Laboratory (PPPL) have been uncovering the physics behind plasma propulsion systems that maneuver satellites in space. Using NERSC supercomputers the team was able to accurately model the plasma spokes observed in experiments, providing new insight into this poorly understood phenomenon.

Significance and Impact

The behavior of plasma and its instabilities critically affect device performance, efficiency, and longevity. One instability leads to formation of a “spoke” that is commonly seen in experimental devices like a Hall device, a type of ion propulsion thruster. Being able to accurately model these effects also has application to other plasma devices, like plasma switches that enable efficient long-distance power transmission.

Research Details

Simulations were run using the Large-Scale Plasma code and produced a highly non-linear turbulent rotating structure very similar to that of the rotating spoke observed in experiments. Simulations suggest that the spoke develops in the non-linear regime of what is known as the collisionless Simon-Hoh instability.



6-kW Hall thruster in operation at the NASA Jet Propulsion Laboratory. By JPL- Public Domain, https://commons.wikimedia.org/w/index.php?curid=20155610.

Powis, Andrew T.; Carlsson, Johan A.; Kaganovich, Igor D.; Raitses, Yevgeny; Smolyakov, Andrei, "Scaling of spoke rotation frequency within a Penning discharge"; PHYSICS OF PLASMAS, 25 2018 JUL, 10.1063/1.5038733

National Energy Research Scientific Computing Center