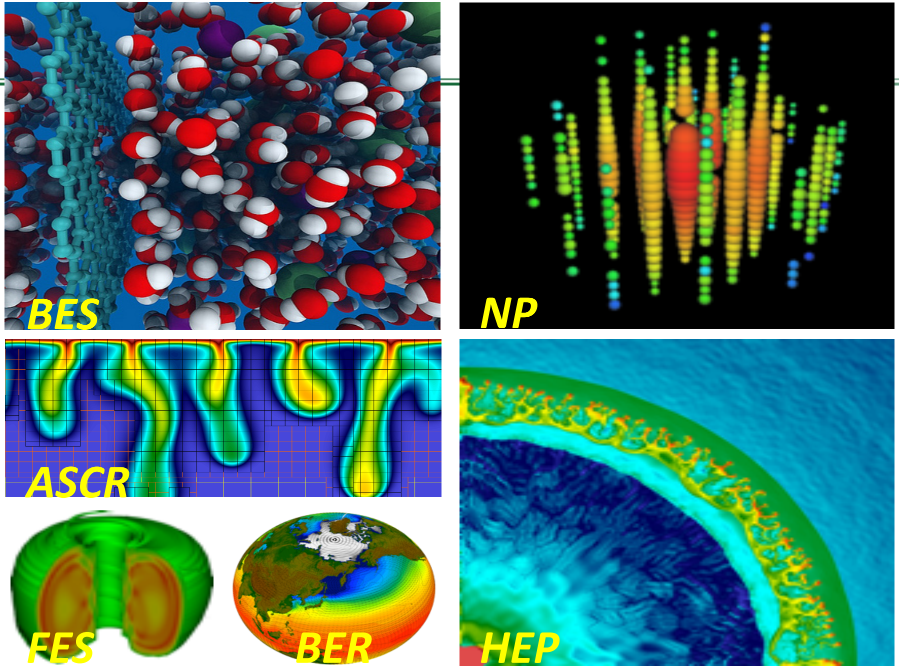
NERSC Science Highlights

September 2017



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Science Highlights September 2017

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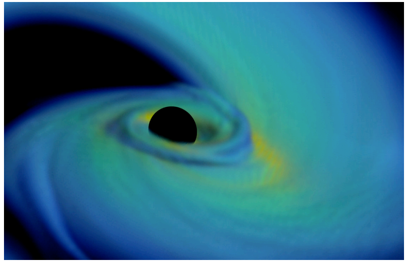
Astrophysics

Simulations reveal dynamics of black hole/neutron star merger.

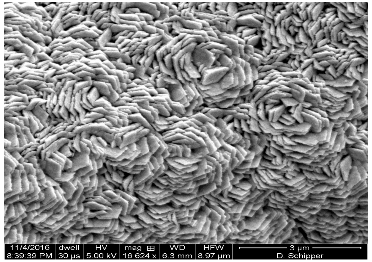
NERSC PI: Foucart, Berkeley Lab. *Classical and Quantum Gravity*

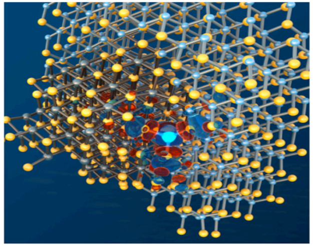


Chemical Science

DFT calculations help identify new catalyst for clean energy.

NERSC PI: Grabow, Univ. of Houston. *Nano Energy*

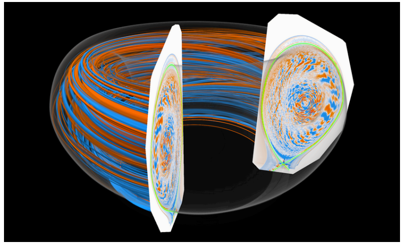




Materials Science

Computations help predict defect-free nanomaterials used in many optoelectronic devices.

NERSC PI: Vörös, Argonne. *Nanoletters*



Fusion Energy

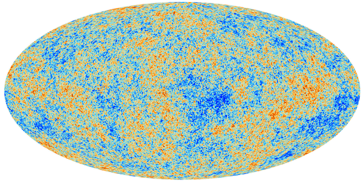
Recycled neutral atoms increase plasma turbulence in tokamak reactors.

NERSC PI: Chang, PPPL. *Nuclear Fusion*

Experimental Cosmology

Full-scale Cori simulations help prepare for next-generation cosmic background measurements.

PI: Borrill, LBNL.



Earth Science

'Hindcasting' shows climate change role in severe Colorado flooding.

NERSC PI: Wehner, Berkeley Lab. *Weather & Climate Extremes*

When Neutron Stars and Black Holes Merge

Scientific Achievement

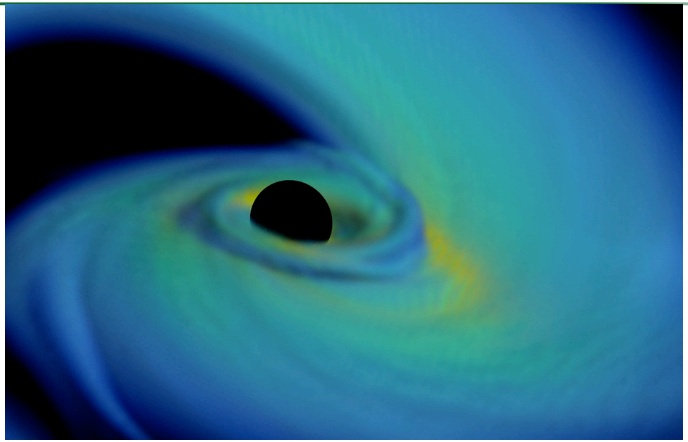
An international team of researchers used the Edison supercomputer at NERSC to make state-of-the-art calculations of a merger between a black hole and a neutron star.

Significance and Impact

This simulation of an object known as a *kilonova* is important to interpreting observations of black hole-neutron star mergers detected in gravitational waves and optical telescopes. The details shed light on how neutron stars rip apart and how these events seed the universe with heavy elements.

Research Details

The simulations were featured in the journal *Classical and Quantum Gravity*. The team modeled nuclear reactions that take place in a tidal tail and disk that forms around the merged object, showing how heavy elements are formed in the process and calculating how the event should appear to observers on Earth.



This simulation shows the formation of an inner disk of matter and a wide, hot disk of matter 5.5 ms after merger of a neutron star and a black hole. (Credit: Classical and Quantum Gravity)

R. Fernandez, et al, Classical and Quantum Gravity, 34, 2017, 154001

NERSC Project PI: F. Foucart, Berkeley Lab

Predicting Defect-free Nanomaterials

Scientific Achievement

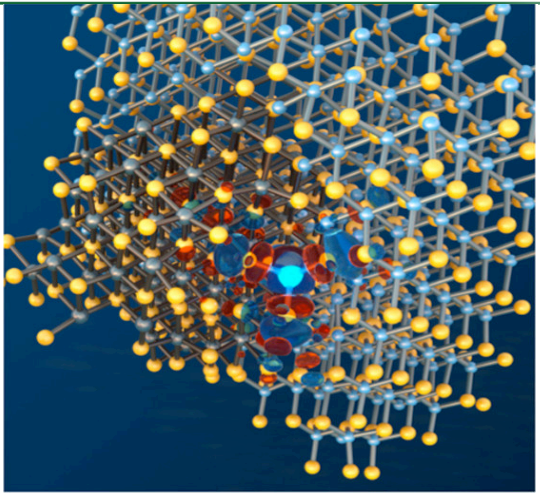
Heterogeneous nanostructured materials are used in various optoelectronic devices, including solar cells. But the interfaces contain structural defects that can affect device performance. Using calculations run at NERSC, researchers from Argonne National Lab and the University of Chicago found the root cause of the defects in two materials and provided design rules to avoid them.

Significance and Impact

The team focused on heterostructured nanoparticles, developing a computational strategy to investigate at the atomic level the effect of the structure of the interfaces on the materials' optoelectronic properties, identifying certain atomic "trap states." They then used the model to predict a new material that does not have these trap states and should perform better in solar cells.

Research Details

This study—which included studies of atomic and electronic structures—used four million supercomputing hours at NERSC. Most of the atomic structure calculations were run on Cori, NERSC's 30-petaflop system, with the rest being run on Edison.



Cross section of the interface between a lead chalcogenide nanoparticle and its embedding cadmium chalcogenide matrix. Credit: Peter Allen, Univ. of Chicago

F. Giberti, et al, Nanoletters, 17 (4), 2547-2553, March 2017

NERSC Project PI: M. Vörös, Argonne

Splitting Water into Hydrogen and Oxygen

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Scientific Achievement

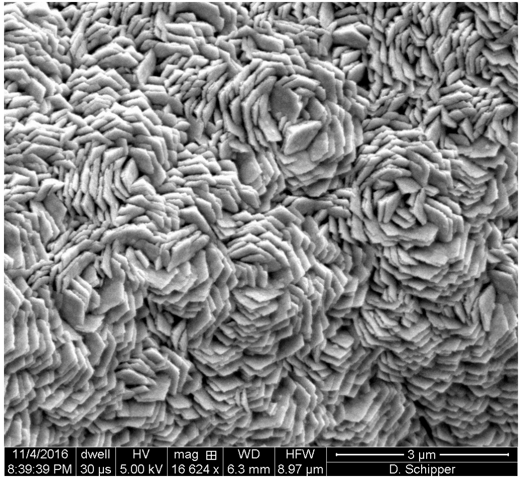
Scientists at Rice and the University of Houston have developed a new catalyst—an electrolytic film comprising nickel, graphene and a compound of iron, manganese and phosphorus—that can split water into hydrogen and oxygen to produce clean energy.

Significance and Impact

Catalysts enable the practical production of many environmentally friendly fuels and make chemical processes cheaper and less toxic. However, catalysts are often made of expensive materials like platinum and palladium. Cheaper and more efficient catalysts are key to the production of clean energy.

Research Details

- The researchers ran a series of density functional theory calculations at NERSC to identify the atomic structure of active catalytic sites and how to control the catalytic material for better selectivity.
- NERSC's supercomputers allowed them to run simulations with larger and more realistic representations of the catalytic material than they were able to achieve on their local cluster.



A catalyst developed by Rice University and the University of Houston splits water into hydrogen and oxygen without the need for expensive metals like platinum. Image: Desmond Schipper

Z. Zhao, et al, Nano Energy 39, Sept. 2017, pp 444-453

NERSC PI: L. Grabow, Univ. of Houston

Preparing for Next-Generation CMB Experiments

Scientific Achievement

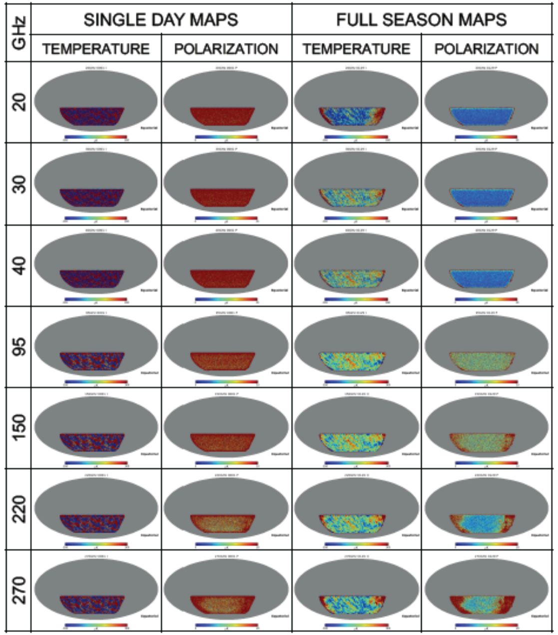
Berkeley Lab cosmologists achieved a critical milestone while preparing for upcoming Cosmic Microwave Background experiments: scaling their data simulation and reduction framework TOAST (Time Ordered Astrophysics Scalable Tools) to run on 600,000+ Intel Xeon Phi processors on NERSC's Cori supercomputer.

Significance and Impact

Next-generation experiments like CMB Stage-4 will probe the Big Bang with unprecedented sensitivity, gathering orders of magnitude more data than previous experiments. The full Cori system – and its successors – will be needed to design the experiments, build and validate their analysis pipelines, reduce the experimental data, and deliver the reduced data to the scientific community.

Research Details

The team worked with NERSC, Intel and Cray via NERSC's NESAP for Data program. The simulated data included the sky signal plus realistic instrumental noise and atmospheric fluctuations. The optimized TOAST code was deployed in a Docker container and the application was run with the NERSC-developed Shifter container-for-HPC software, enabling a start-up time of <90 sec.



Cumulative daily maps of sky temperature and polarization at each frequency showing how the atmosphere and noise integrate down over time. Simulations: Julian Borrill, LBNL

Recycled Atoms Boost Plasma Turbulence

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Scientific Achievement

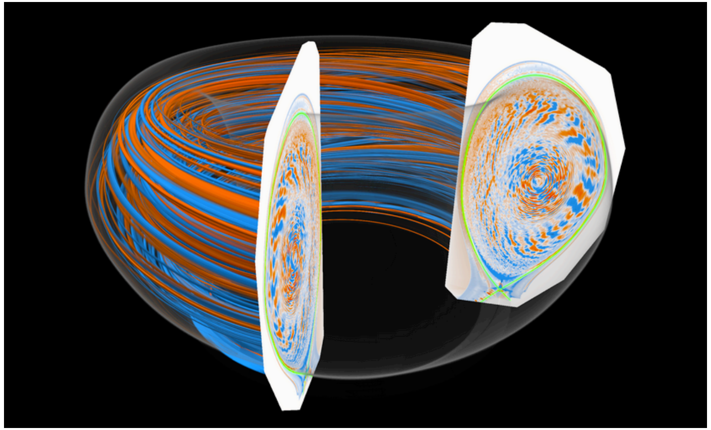
Using NERSC supercomputers, physicists at Princeton Plasma Physics Laboratory modeled how recycled neutral atoms, which arise when hot plasma strikes a tokamak reactor's walls, increase plasma turbulence driven by what are called the "ion temperature gradient" modes.

Significance and Impact

Findings from this research are expected to improve understanding of the transition of plasmas from low to high confinement (H-mode), the mode in which future tokamaks are expected to operate. It may also lead to a better understanding of fusion performance in ITER, the large experimental fusion research facility being built in France.

Research Details

The PPPL team used the XGC1 code—an extreme scale edge gyrokinetic particle code, with turbulence, background plasma and neutral particle dynamics solved together —to achieve the simulation. The study began on Titan at the Oak Ridge Leadership Computing Facility and then completed at NERSC.



Plasma density fluctuation in a tokamak plasma turbulence driven by ion temperature gradient. The green line shows the magnetic separatrix surface that contains the edge plasma pedestal within a few centimeters from it. Credit: S. Ku, PPPL

D.P. Stotler, et al, Nuclear Fusion, 57, 086028, July 4, 2017

NERSC Project PI: C.S. Chang, PPPL

‘Hindcasting’ Extreme Weather Events

Scientific Achievement

Researchers have been able to “hindcast” the conditions that led to the Sept. 9-16, 2013 flooding around Boulder, CO and found that climate change made the storm much more severe.

Significance and Impact

Hindcasting is a way of testing a mathematical model; researchers enter known or closely estimated inputs for past events into the model to see how well the output matches the known results. By running simulations using various climate scenarios, researchers were able to determine that the storm was more severe in today’s climate than it would have been in one without climate change.

Research Details

The storm was so strong that even today’s largest supercomputers couldn’t resolve critical features using global climate models. So the researchers used the “WRF” regional model to “hindcast” conditions that led to the flooding, allowing them to study the problem in greater detail, breaking the area into 12-km squares. They used NERSC supercomputers to run 101 hindcasts.

Sept. 16, 2013: U.S. Highway 34 in Greeley is breached by the South Platte River in flood stage. (Credit: US Environmental Protection Agency)

P. Pall, et al, Weather and Climate Extremes, July 2017, doi: 10.106/ j.wace.2017.03.004

NERSC Project PI: M. Wehner, Berkeley Lab

National Energy Research Scientific Computing Center