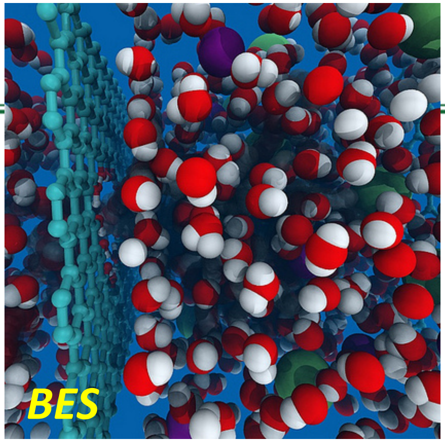
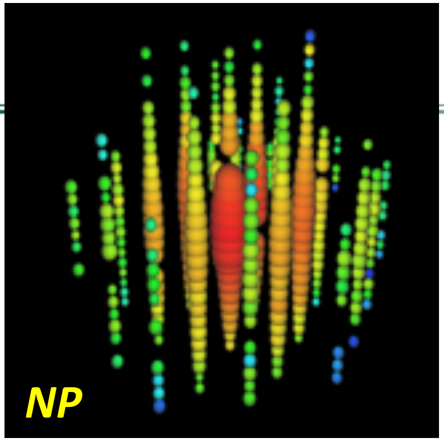
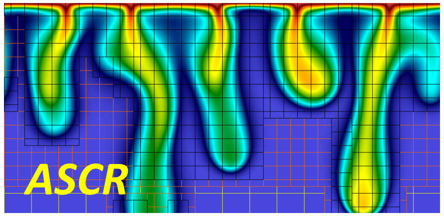
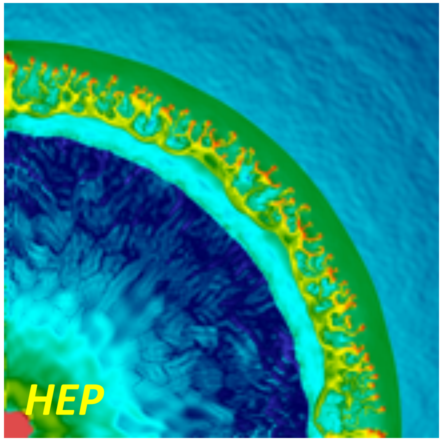
NERSC Science Highlights

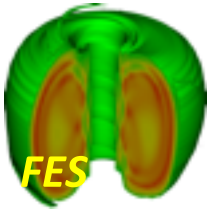
Spring 2017

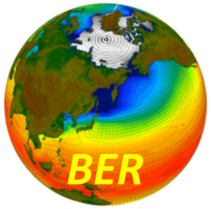












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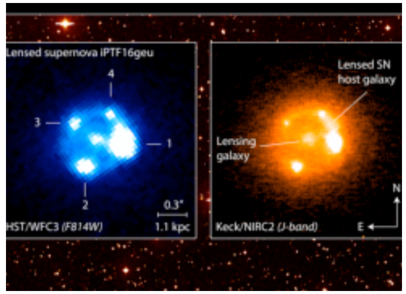
Science Highlights March 2017

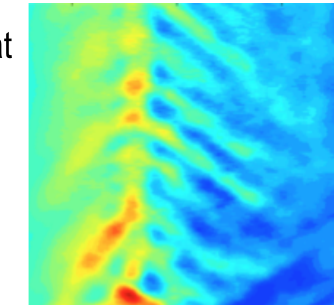
Astrophysics

Using an automated pipeline and NERSC computers astronomers have discovered the first gravitationally lensed Type 1a supernova. PI: Kasliwal, Caltech. *Science*.



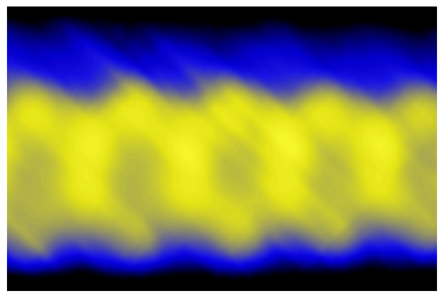
Fusion Energy

Simulations show that pumping heat into a tokomak reactor drives instabilities that create plasma rotation, yielding improved control. PI: Lee, Princeton Plasma Physics Lab. *Physical Review Letters*



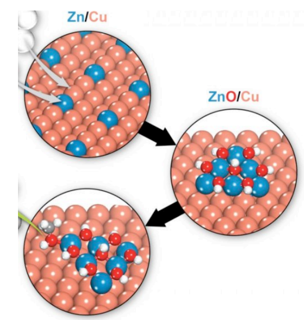
Materials Science

Researchers found a new way to grow narrow ribbons of graphene that will have many applications in electronic devices. NERSC PI: Kent, Oak Ridge, *Nature Communications*



Catalysis

Scientists identified how a Zn/Cu catalyst transforms CO_2 and H to methanol, a useful fuel. NERSC PI: Liu, Brookhaven. *Science*



Computer Science

Researchers used Cori to successfully simulate a 45-qubit quantum circuit, the largest ever simulation of a quantum computer. PI: Haner, ETH Zurich. *arXiv:1704.01127*

Nuclear Physics

The first complex calculations of a subatomic particle called the Sigma were performed at NERSC, providing insights into the nature of the *strong force* of nature. PI: Edwards, Jefferson Lab. *Physical Review Letters*.

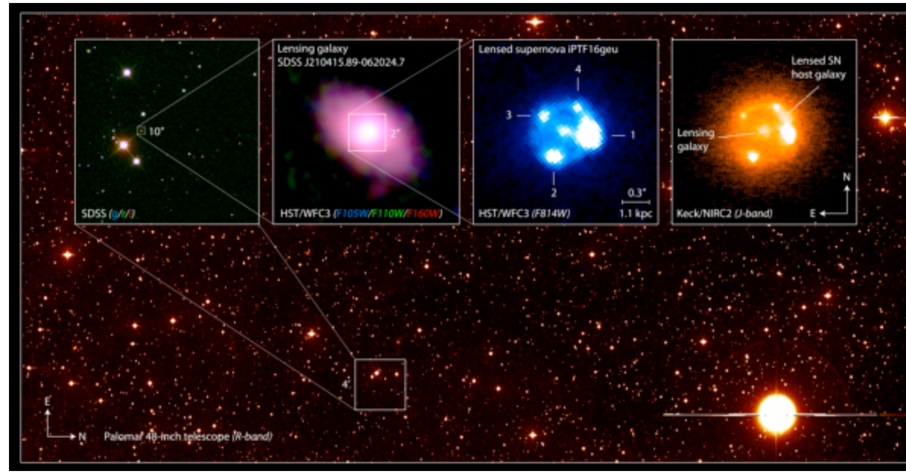
Earth Systems

New simulations are better able to predict extreme waves generated by hurricanes. PI: Wehner, Berkeley Lab. *Geophysical Research Letters*

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.



This composite image shows the gravitationally lensed type Ia supernova iPTF16geu, as seen with different telescopes. Image credit: Joel Johansson, Stockholm University

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.

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.
- iPTF data is also archived at NERSC.

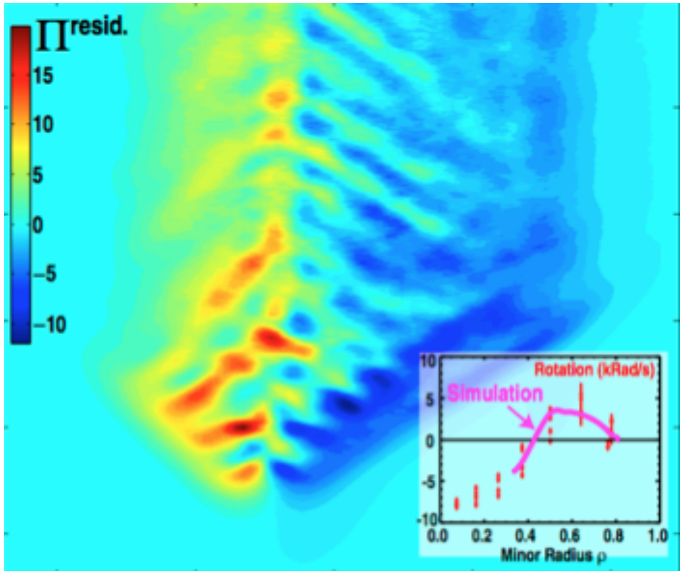
A.Goobar, R. Amanullah, et al, Science 356, 6335, April 2017, 291-295

NERSC Project PI:
M. Kasliwal, CalTech

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.



Simulation of plasma turbulence generating positive (red) and negative (blue) residual stress that drives rotation shear. (inset) Comparison between measured and simulated rotation profile. Image credit: W. X. Wang

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.

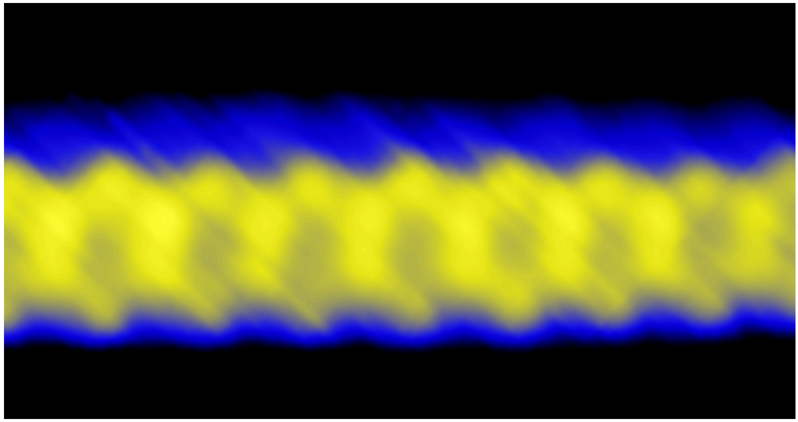
A. Grierson et al, *Physical Review Letters,* 118, 015002, January 2017

NERSC Project PI: Wei-Li Lee, PPPL

A Better Way to Grow Graphene

Scientific Achievement

Researchers from Oak Ridge National Laboratory found a new way to grow narrow ribbons of graphene, a lightweight and strong structure of single-atom-thick carbon atoms linked into hexagons, that may address a shortcoming that has prevented the material from achieving its full potential in electronic applications.



This graphene nanoribbon was made bottom-up from a molecular precursor. Nanoribbon width and edge effects influence electronic behavior. Image credit: Oak Ridge National Laboratory; scanning tunneling microscopy by Chuanxu Ma and An-Ping Li

Significance and Impact

The researchers established how the bottom-up synthesis of a graphene nanoribbon can be controlled by charge injections from a scanning tunneling microscopy (STM) tip. At selected sites, this new technique can create interfaces between materials with different electronic properties. Such interfaces are the basis of many semiconductor electronic devices, including integrated circuits, transistors, LEDs and solar cells

C. Ma, Z. Xiao, et al, *Nature Communications*, 8, 14815, March 2017

Research Details

Through experiments and first-principles calculations using the Quantum Espresso code at NERSC and ORNL, the researchers found that the hole injections from an STM tip can trigger a cooperative domino-like cyclodehydrogenation even when the polymers are quasi-freestanding with suppressed substrate effect.

NERSC Project PI: P. Kent, ORNL

Converting CO_2 into Methanol

Scientific Achievement

Using supercomputers at NERSC and experiments, Brookhaven scientists identified how a zinc/copper catalyst transforms carbon dioxide and hydrogen to methanol, a useful fuel.

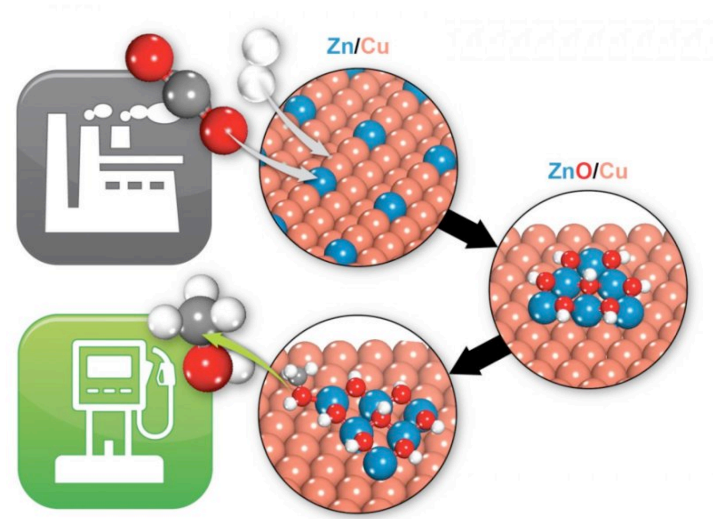
Significance and Impact

Reacting carbon dioxide (CO_2) with Hydrogen (H_2) can produce methanol. But the reaction will not take place on its own; a catalyst is needed to make the process go. In industrial applications, catalysts made from copper (Cu) and zinc oxide (ZnO) on alumina supports are often used, but the process itself is not well understood and has been the subject of much debate.

Research Details

The researchers used computational resources at NERSC to model how two types of model catalysts - one made of zinc nanoparticles supported on a copper surface, and another with zinc oxide nanoparticles on copper - would engage in the CO_2-to-methanol transformations.

These theoretical studies used calculations that took into account the basic principles of breaking and making chemical bonds, including the energy required, the electronic states of the atoms, and the reaction conditions, allowing scientists to derive the reaction rates and determine which catalyst will give the best rate of conversion.



Brookhaven scientists identified how a zinc/copper (Zn/Cu) catalyst transforms carbon dioxide (two red and one grey balls) and hydrogen (two white balls) to methanol (one grey, one red, and four white balls), a potential fuel.

S. Kattel, et al, *Science*, 2017; 355 (6331): 1296

NERSC Project PI:
P. Liu, Brookhaven

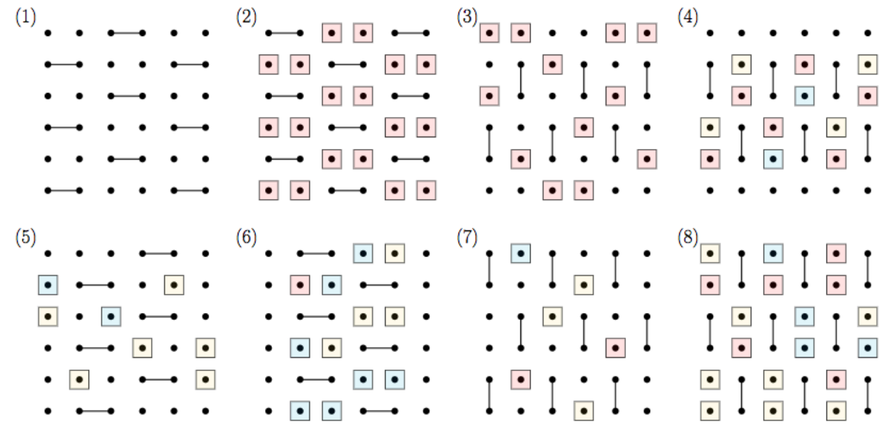
A Record Quantum Circuit Simulation

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.



Low-depth random quantum circuit proposed by Google to show quantum supremacy.

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

Research Details

- In addition to the 45-qubit simulation, which used 0.5 petabytes of memory on Cori and achieved a performance of 0.428 petaflops, 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.

First Complex Calculations of Sigma Particle

Scientific Achievement

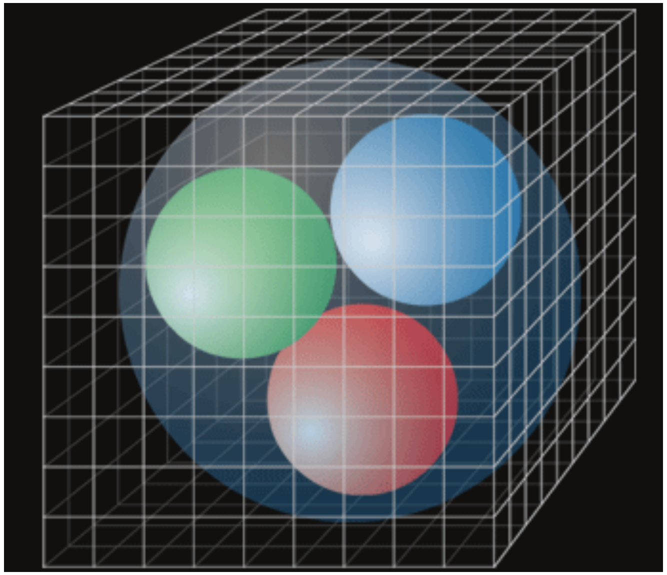
Supercomputing resources at NERSC helped an international team of researchers, representing the Hadron Spectrum Collaboration, achieve the first complex calculations of a subatomic particle called the Sigma.

Significance and Impact

After decades of catching only brief glimpses of the Sigma's existence from experimental data that showed its effects on other subatomic particles, this calculation gives scientists a new way to study the sigma and gain new insights about the "strong force" that exists inside all matter.

Research Details

- This study is part of a larger effort to investigate quantum chromodynamics (QCD), the fundamental theory of strong interactions. Understanding QCD is important to gain a deeper understanding of the fundamental laws of physics.
- The researchers used the Chroma lattice field theory code for their calculations, used for lattice QCD calculations.
- Supercomputers at NERSC, ORNL and the University of Illinois at Urbana-Champaign were used to generate the gauge configurations: snapshots of the environment of subatomic particles (the vacuum of space described by QCD).



Quantum chromodynamics is the fundamental theory of strong interactions (the mechanism responsible for the strong nuclear force) and one of the four known fundamental interactions in physics.

R. Briceno, et al, *Physical Review Letters, 118, 022002, January 2017*

NERSC Project PI:
R. Edwards, Jefferson Lab

Catching Extreme Waves with High-Resolution Modeling

Scientific Achievement

Using decades of global climate data generated at a spatial resolution of about 25 kilometers, researchers were able to identify the formation of tropical cyclones, also referred to as hurricanes and typhoons, and the extreme waves that they generate.

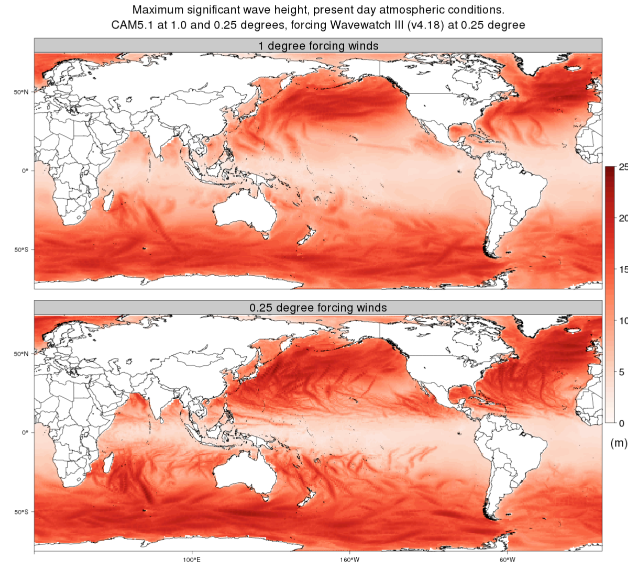
Significance and Impact

The findings demonstrate the importance of running climate models at higher resolution. Better predictions of how often extreme waves will hit are important for coastal cities, the military and industries that rely upon shipping and offshore oil platforms. The majority of existing models used to study the global climate are run at resolutions that are insufficient to predict tropical cyclones. The simulations in this study are the first long-duration global data sets to use a resolution of 25 kilometers.

Research Details

The researchers ran the Community Atmosphere Model version 5 (CAM5) climate model at NERSC with data collected in three-hour increments at a low resolution of 100 kilometers and a high resolution of 25 kilometers. They found that the high-resolution simulations included tropical cyclones while the low-resolution ones did not.

To see if the cyclones had an effect on waves, they ran global wave models at both resolutions. They saw extreme waves in the high-resolution model that did not appear in the low-resolution ones.



The maximum wave height in the time series above show differences in storm characteristics, including the presence or absence of tropical cyclones, when different resolutions are used. Image credit: Ben Timmermans, Berkeley Lab

B. Timmermans, et al, *Geophysical Research Letters, 44, 3, February 2017*

NERSC Project PI: M. Wehner, Berkeley Lab

National Energy Research Scientific Computing Center