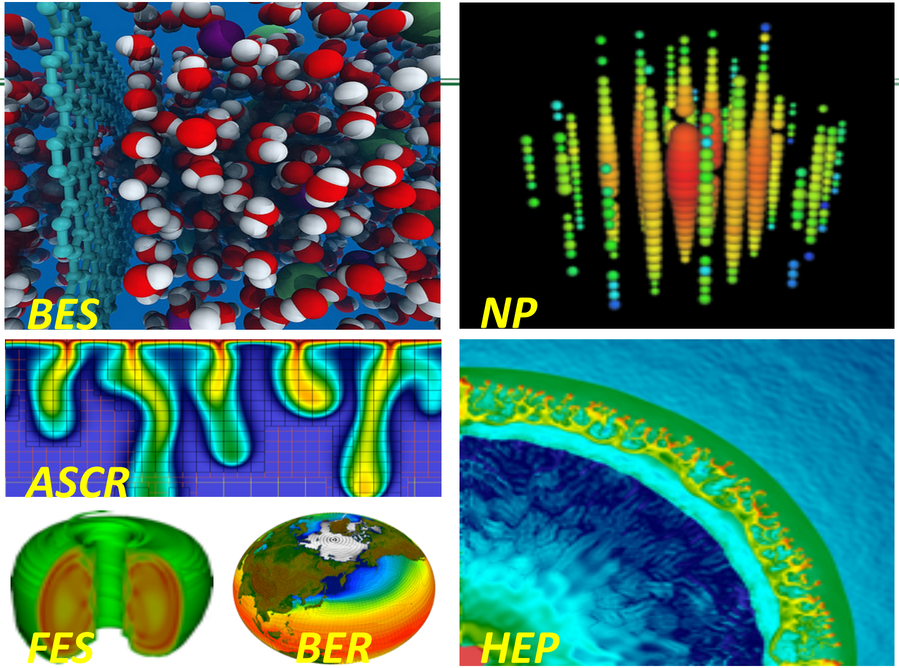
NERSC Science Highlights

December 2017



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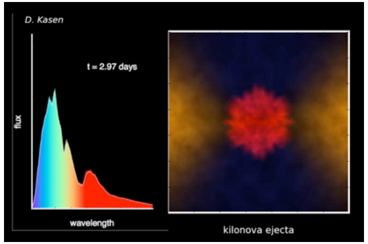
Science Highlights December 2017

NERSC

Astrophysics

Observations + computer models confirm that *kilonovas* produce heavy elements.

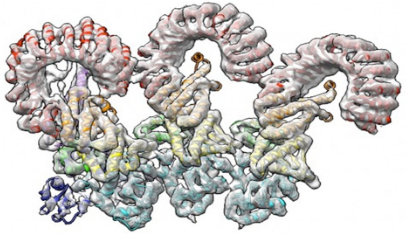
NERSC PI: Kasen, Berkeley Lab. *Nature*

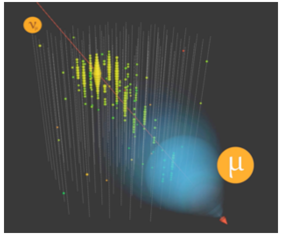


Biological Science

Analyzing cryo-EM images provides insight in immune system function..

NERSC PI: Nogales, UC Berkeley. *Science*

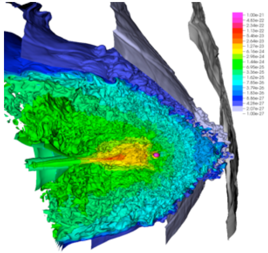




Nuclear Physics

Analysis shows for the first time that the Earth stops high-energy neutrinos.

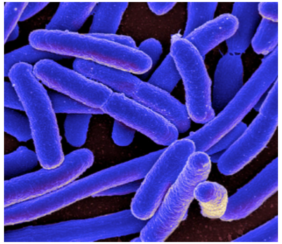
NERSC PI: Palczewski, Berkeley Lab. *Nature*



High Energy Physics

Simulations show how the first supernovae seeded the universe with heavy elements.

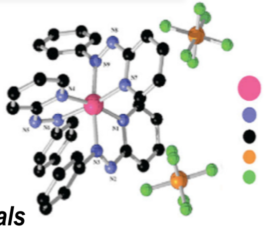
NERSC PI: Chen, EACOA. *The Astrophysical Journal*



Materials Science

Scientists take big step towards making practical next-generation “memristor” memory devices.

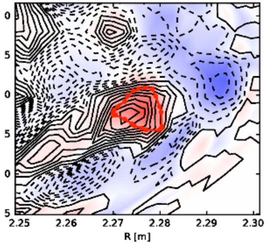
NERSC PI: Batista, Yale Univ. *Nature Materials*



Fusion Science

Analysis show how plasma ‘blobs’ cause problems in fusion reactors.

NERSC PI: Chang, PPPL. *Plasma Physics and Controlled Fusion*



Bioscience

Simulations reveal how bacteria react to environmental stress.

NERSC PI: Palsson, UC San Diego. *Proc Nat. Acad. Sci.*

Origin of Heavy Elements

Scientific Achievement

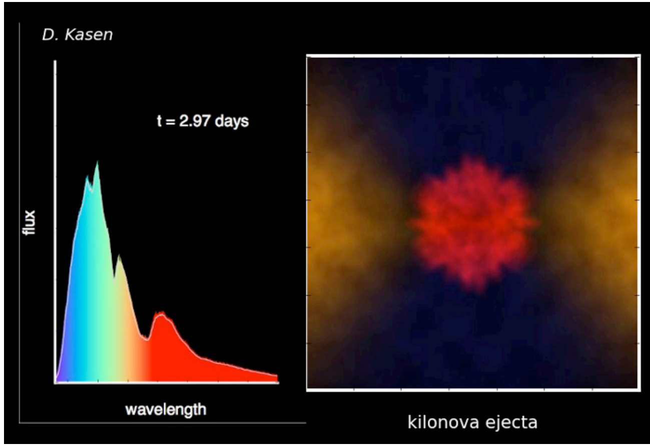
In a study published in *Nature*, optical and infrared signals from a neutron star merger were found to be consistent with computer model predictions of a *kilonova*, an event that is 1,000 times brighter than a classical nova. The observations followed the detection of gravitational waves from the neutron star merger GW170817.

Significance and Impact

Physicists have long discussed how elements heavier than iron could be produced and simulations of neutron star mergers have predicted that kilonovas are prime candidates. The observations in this paper are the first to provide strong evidence to support this theory.

Research Details

The researchers used 4,000 compute cores to run the general relativistic magnetohydrodynamical code HARMPI and the radiation transport code SEDONA to produce highly resolved simulations of the long-term aftermath and observable light from neutron star mergers.



Theoretical calculation of the evolution of the spectrum of light from a kilonova such as that associated with gravitational wave signal GW170817. The right panel shows an illustration of the expanding radioactive debris cloud that produces the observed radiation. Credit: Dan Kasen

Kasen et. al, Nature ***551****, 80–84 (Nov. 2, 2017)*
doi:10.1038/nature24453

NERSC Project PI: D. Kasen, Berkeley Lab

Toward Better Protections from Pathogens

Scientific Achievement

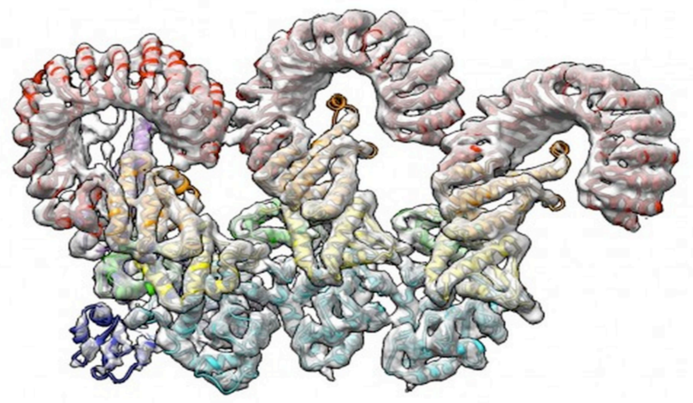
Computational analysis of cryo-electron microscopy (cryo-EM) images helped biologists resolve the structure of a ring of proteins used by the immune system to to detect and respond to a bacterial attack.

Significance and Impact

The study, led by Berkeley Lab and UC Berkeley researchers, used cryo-EM to capture high-resolution images of a protein ring called an “inflammasome” as it was bound to flagellin, a protein from the whiplike tail used by bacteria to propel themselves. This approach provides new insight into potential strategies for protection from bacterial infections.

Research Details

Using NERSC resources, the researchers were able to scale up their structure-determination pipeline and quickly determine atomic structures of macromolecular complexes with a wide range of functions in microbes and plants. They also mined the structural information to understand how genomic data is translated into functional capabilities and are using this database as a pipeline for modeling biological function.



Using cryo-electron microscopy, researchers have revealed the structure of a multi-protein complex called the NAIP5-NLRC4 inflammasome, which helps identify invading bacteria. Credit: Nicole Haloupek, UC Berkeley/Howard Hughes Medical Institute

J. Tenthorey, et al, Science Nov. 17 2017, Vol. 358, Issue 6365
doi:10.1126/science.aao1140

NERSC Project PI: E. Nogales, Berkeley Lab

Stopping Neutrinos In Their Tracks

Scientific Achievement

The IceCube Collaboration showed for the first time that high-energy neutrinos are absorbed by Earth as predicted by the Standard Model of particle physics. Neutrinos interact rarely with normal matter, but the Earth is large enough to stop some of them, and IceCube was able to measure that effect.

Significance and Impact

The results not only support the Standard Model, but are inconsistent with some more speculative theories. A detailed understanding of how high-energy neutrinos interact with Earth's matter will also allow researchers to probe the composition of Earth's core and mantel.

Research Details

- Simulations to support the analysis were run at NERSC; the IceCube project uses NERSC's Cori, Edison & PDSF systems for data analysis and simulations.
- Historical data is archived at NERSC.

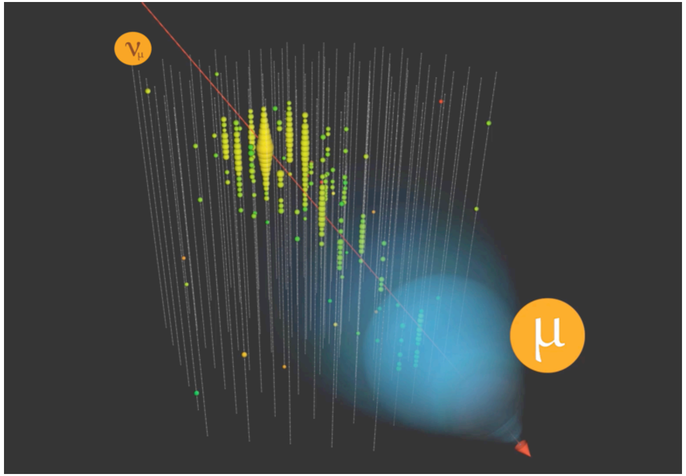


Illustration of how a muon interacts in the IceCube detector array. Credit: IceCube Collaboration

The IceCube Collaboration, Nature 551, 596–600 (Nov. 2017) doi:10.1038/nature24459

NERSC PI: T. Palczewski, Berkeley Lab

How 1st Supernovae Altered Early Star Formation

Scientific Achievement

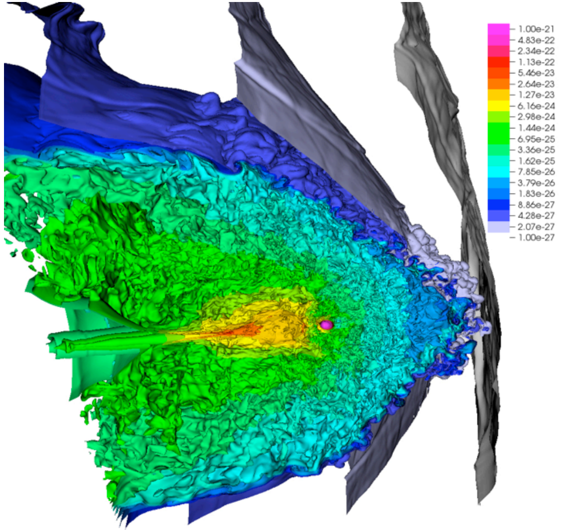
An international team of astronomers and cosmologists ran multi-scale, multi-physics 2D and 3D simulations at NERSC to show how elements expelled from the first supernovae helped populations of stars in the early universe start to evolve from extremely massive and hot objects towards one like those seen in our galaxy today.

Significance and Impact

This study demonstrated a new methodology that combines small, stellar-scale simulations (typical of astrophysics) and large, galactic-scale simulations (typical of cosmology) to provide more insight into the formation of the early universe.

Research Details

The team ran small-scale, high-resolution simulations of the chemical enrichment of a dark matter halos with elements produced in a nearby supernova explosion. They used NERSC computers to produce a series of 2D and 3D simulations that helped them examine the role of dark matter halo photoevaporation in the early formation of stars and the assembly of later galaxies.



This simulation shows the turbulent gas when a supernova collides with a nearby star-forming halo. Credit: Ken Chen, EACOA

K. Chen, et al, The Astrophysical Journal, 844:111, August 2017, doi: 10.3847/1538-4357/aa7b34

NERSC Project PI: K. Chen, EACOA

HPC for Better Computer Memory Technologies

Scientific Achievement

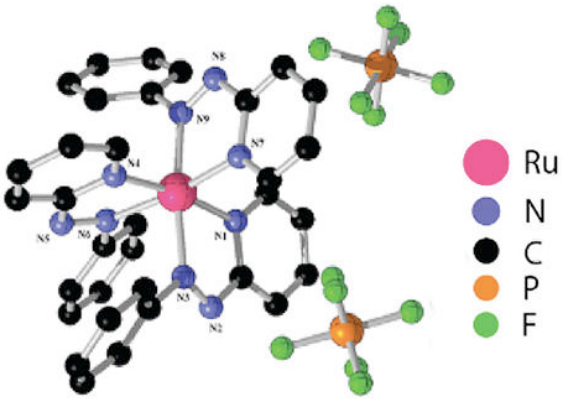
In a recent *Nature Materials* article researchers describe a new robust "memristor" device and theoretical insights into why it has the size, stability, reproducibility, and endurance to supplant flash memory technologies in future generations of digital devices.

Significance and Impact

The team performed calculations at NERSC to gain an understanding of why their device, based on a spin-coated active layer of a transition metal complex, performs so well. The insight may accelerate the deployment of organic resistive memory devices and the findings have wider applicability for other semiconductor materials, particularly those used in neuromorphic and logic circuits.

Research Details

The researchers used a computational methodology that combines large-scale density functional theory molecular dynamics and simulations of electronic relaxation to accurately describe the electronic relaxation processes in functionalized titanium-dioxide surfaces.



An international team of researchers has developed thin, molecular films that can store information, with potential applications in the computer industry. Credit: Yale University

S. Goswami, et al, Nature Materials, Oct. 23, 2017,
doi: 10.1038/NMAT5009

NERSC Project PI: Victor Batista, Yale Univ.

The Blob that Ate the Tokamak

Scientific Achievement

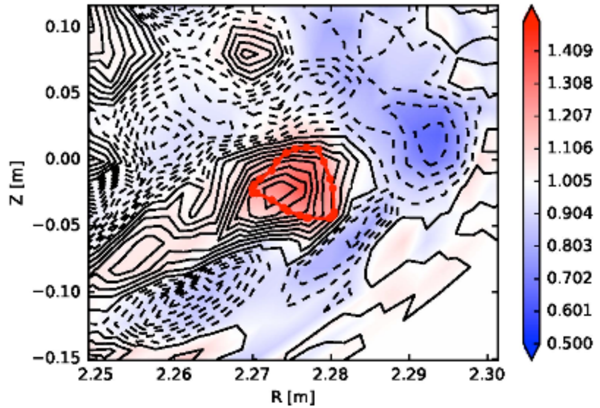
Using NERSC supercomputers, physicists at Princeton Plasma Physics Laboratory have gained new understanding of the turbulent "bubbles" (blobs) that percolate within the plasma edge during a fusion reaction and how they can negatively impact performance.

Significance and Impact

Blobs play an important role in the outward movement of particles in plasma and they could cause 50% of the particle loss at the plasma edge. This study gives fusion scientists a better understanding of how heat moves from plasma to the walls, potentially causing damage.

Research Details

The PPPL team transferred Terabytes of simulation data from Oak Ridge, where it was produced, to NERSC for analysis. The analysis, which was performed on NERSC's Edison supercomputer, used a blob detection and tracking method to reveal how the blobs move to the plasma edge and interact with the walls.



Normalized density contour (red) at a single poloidal plane, with fluctuating potential contour lines overlaid to show positive potential (solid black) and negative potential (dashed black). A detected density blob is outlined in the thick red contour line. Credit: PPPL

R.M. Churchill, et al, Plasma Phys. Control Fusion 59 (2017), 105014 [doi:10.1088/1361-6587/aa7c03](doi:10.1088/1361-6587/aa7c03)

NERSC Project PI: C.S. Chang, PPPL

How Bacteria Adapt to Environmental Stress

Scientific Achievement

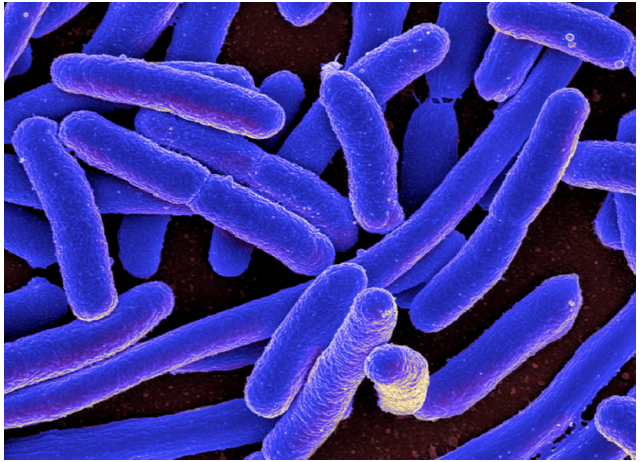
Researchers at the University of California San Diego developed a genome-scale computational model, FoldME, that can accurately predict how E. coli bacteria respond to temperature changes and genetic mutations and then reallocate their resources to stabilize proteins.

Significance and Impact

This work and the FoldME model provide a comprehensive, systems-level understanding of how cells adapt under environmental stress, with statistical descriptions of multiscale cellular response consistent with many datasets. The model could aid in designing engineered organisms for biofuel production and patient-specific treatments for bacterial infections.

Research Details

This steady used computational resources of NERSC to run large-scale simulations with parameter sampling. The supercomputing services provided by NERSC allowed the researchers to either run many of these techniques in parallel for hundreds of proteins, speeding up what would otherwise be week-long simulations of these complex problems.



Researchers at UC San Diego developed a genome-scale model that can accurately predict how E. coli bacteria respond to environmental stress. Credit: NIAID

K. Chen, et al, PNAS, vol. 114 no. 43, 11548–11553, doi: 10.1073/pnas.1705524114

NERSC Project PI: B. Palsson, UCSD

National Energy Research Scientific Computing Center