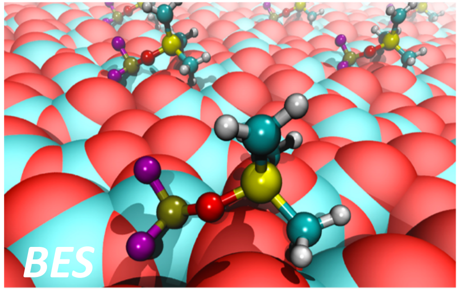
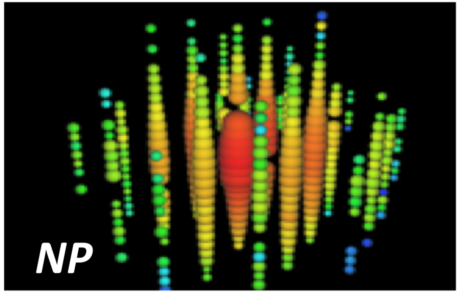
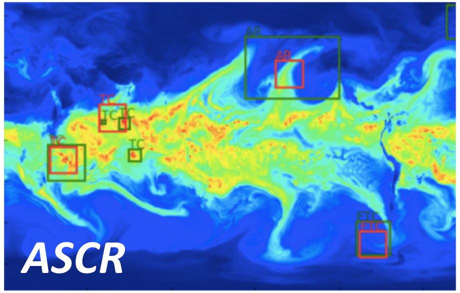
NERSC Science Highlights

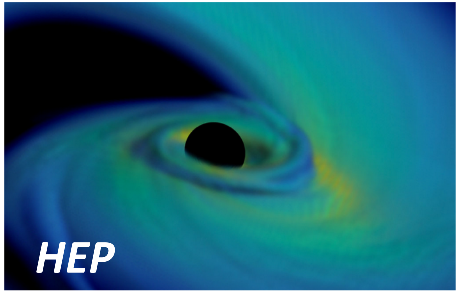
March 2018

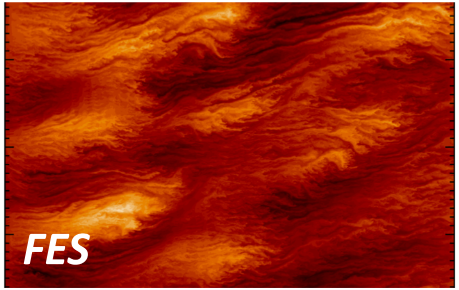
NERSC

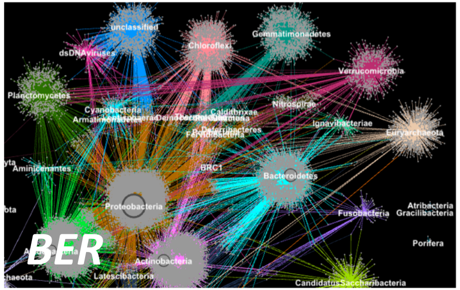












Science Highlights March 2018

Fusion Energy

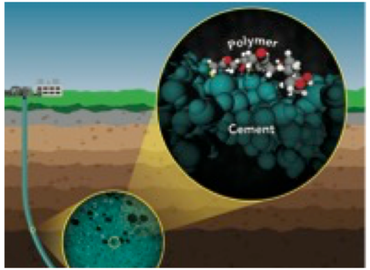
"Disruptive" Magnetic Islands Confine Fusion Plasmas

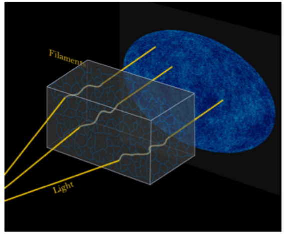
NERSC PI: Chang, Princeton Plasma Physics Lab, *Physics of Plasmas*

Chemical Science

Simulations Shed Light on Self-Healing Cement

NERSC PI: Glezakou, Pacific Northwest National Laboratory. *ACS Applied Materials and Interfaces*

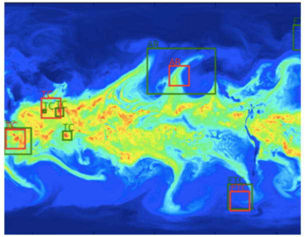




Cosmology

Mapping the Filamentary Structure of the Universe

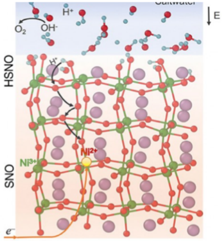
NERSC PI: Bailey, Berkeley Lab. *Nature Astronomy*



Computer Science

Deep Learning at 15 PF

NERSC PI: Prabhat, Berkeley Lab. *SC 17 Proceedings*



Materials

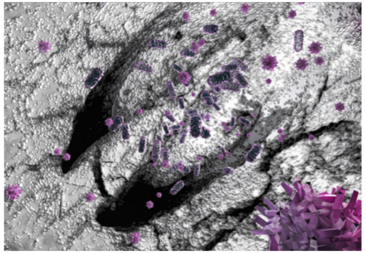
Sensors for Extreme Environments

NERSC PI: Sankaranarayanan, Argonne National Lab. *Nature*

Biology & Environment

Deeper Understanding of Livestock Greenhouse Gas Emission

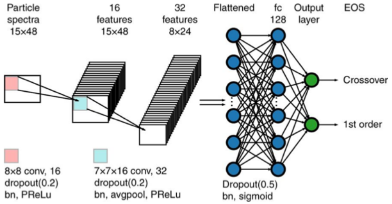
NERSC PI: Fagnan, Joint Genome Institute. *Nature Biotechnology*



Nuclear Physics

Deep Learning Probes Mysteries of Nuclear Matter.

NERSC PI: Chan, Berkeley Lab. *Nature Communications*



"Disruptive" Magnetic Islands Confine Fusion Plasmas

Scientific Achievement

The multiscale kinetic interaction of magnetic islands – bubble-like structures that form in fusion plasmas – with high-temperature background plasma has been simulated in the realistic geometry of a tokamak fusion energy device for the first time.

Significance and Impact

Researchers from Princeton Plasma Physics Laboratory (PPPL) found that, unlike in previous simplified simulations and analytic studies that assumed flattening of plasma pressure, the islands can allow particles to orbit across them, drive 3D plasma flows that suppress turbulence and keep the plasma pressure from being flat, which is required to achieve sustained energy generation in the presence of unavoidable islands.

Details of the simulated fluctuation, flow and confinement are consistent with experimental observations from the KSTAR tokamak in South Korea. These findings could significantly influence our understanding of plasma disruption precursion events and how to suppress them.

J.M. Kwon, et al, Physics of Plasmas 25, 052506 2018, doi: 10.1063/1.5027622
NERSC Project PI: C.S. Chang, PPPL

Korean Superconducting Tokamak Advanced Research facility (KSTAR). Image: Korean National Fusion Research Institute

Research Details

Working with the XGC code developed at PPPL, the team modeled magnetic islands using plasma conditions from KSTAR. The plasma structure around the islands proved markedly different from standard assumptions, as did their impact on plasma flow, turbulence and plasma confinement, agreeing with experiments. This study used 6.2 M hours on Cori. XGC receives optimization support from the NERSC Exascale Scientific Applications Program (NESAP).

Simulations Shed Light on Self-Healing Cement

Scientific Achievement

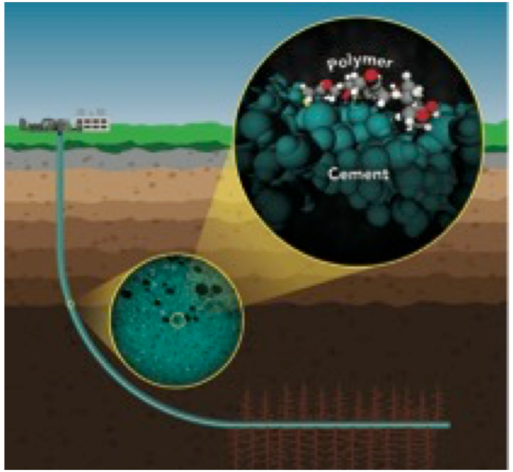
Pacific Northwest National Laboratory (PNNL) researchers developed a unique 'self-healing' cement—a composite of cement and a polymer— that can repair itself in as little as a few hours. And thanks to ground-breaking simulations run on NERSC supercomputers, the team was able to understand how the process works so they can identify weakness and improve the cement's durability.

Significance and Impact

Wellbore cement – cement that surrounds pipes that bring oil and gas from deep wells to the surface – has a lifespan of about 30-40 years. When it cracks, repairs can top $1.5 million per well. With thousands of subsurface wells running annually, this technology could have a dramatic impact on the cost of energy production.

Research Details

The researchers constructed a first-of-its-kind model based on a method called density functional theory that allowed them to study what happens when bonds break and form inside the cement/polymer system. The simulations modeled about 900 atoms over a month's worth of computing, involving ~500,000 CPU hours.



Large scale simulations were used to determine the fundamental interactions between polymer and cement in self-healing cement composites. Image: Vassiliki-Alexandra Glezakou and Cortland Johnson, PNNL

Nguyen et al., ACS Applied Materials and Interfaces 2018, 10, 30011-3019,
doi: 10.1021/acsami.7b13309

NERSC Project PI: Vassiliki-Alexandra Glezakou, PNNL

Mapping the Filamentary Structure of the Universe

Scientific Achievement

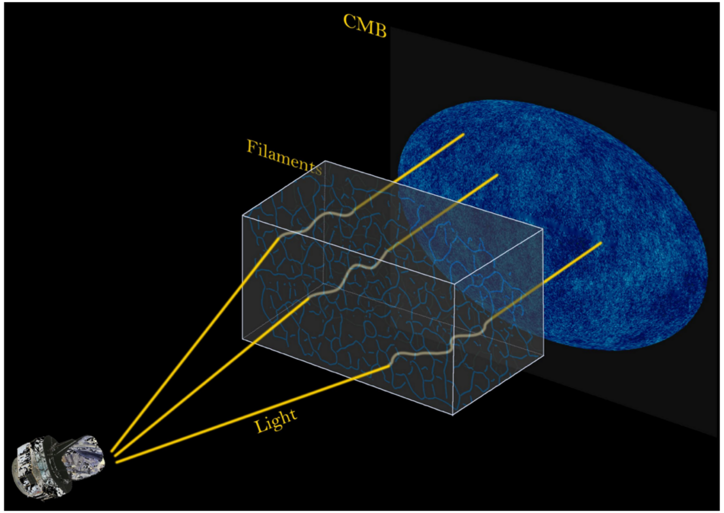
A team of scientists that included researchers from Berkeley Lab decoded faint distortions in the patterns of the universe's earliest light to map filaments – huge tube-like structures invisible to our eyes – that connect dense hubs of galaxy clusters. The team detected the filaments by studying the way their gravity affected observations of the microwave background radiation.

Significance and Impact

Detailed exploration of filaments will help researchers better understand the formation and evolution of the large-scale structure of the universe, including dark matter and dark energy – the poorly understood primary constituents of the universe.

Research Details

Researchers used data from the Baryon Oscillation Spectroscopic Survey and statistical techniques to study the universe's distribution of matter. They also relied on space-based measurements of the cosmic microwave background, computer algorithms to identify filaments from distortions in the CMB, and large cosmological simulations at NERSC to validate their techniques.



This image shows how filaments distort the pattern of radiation from the cosmic microwave background (CMD). The area in the animation spans 7,500 square degrees on the sky. Image: Siyu He, Shadab Alam and Wei Chen.

He, Siyu; Alam, Shadab; Ferraro, Simone; Chen, Yen-Chi; Ho, Shirley, Nature Astronomy, April 9, 2018, Vol 2, 401–406, doi: 10.1038/s41550-018-0426-z

NERSC Project: DESI. DESI is a member of the NERSC NESAP for Data partnership.

Deep Learning at 15 Petaflops

Scientific Achievement

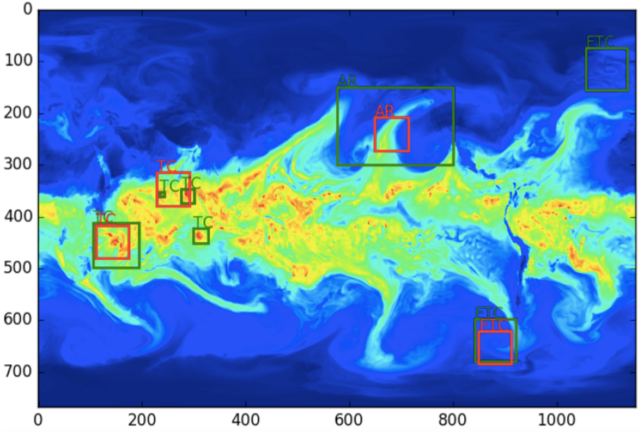
Deep-learning training performance on the Cori supercomputer at NERSC has been enabled at 15 petaflops – 15 million billion calculations per second – giving climate scientists the ability to use machine learning to identify extreme weather events in the output of huge climate simulations.

Significance and Impact

Supercomputers like Cori provide scientists with an extraordinary tool to model climate change significantly faster and far more accurately than was possible on previous generation supercomputers. For example, Cori can model the Earth system 300x to 10,000x faster than real time. This meets the needs of climate scientists who need to run many-century long simulations to evaluate the impact of climate change far into the future. But data produced by the runs are huge, posing a severe challenge for humans trying to analyze the results.

Research Details

Researchers from NERSC, Intel, the Montreal Institute for Learning Algorithms, and Microsoft Research teamed up to create a novel, semi-supervised convolutional deep neural network (DDN). Predictive accuracies ranging from 89.4% to as high as 99.1% showed that DDNs can identify weather fronts, tropical cyclones and atmospheric rivers.



Relation between ground truth (green boxes) and classification plus regression results (red boxes) of the DNN trained to recognize atmospheric phenomena. Image: Prabhat

Kurth et al., SC 17 Proceedings of the International Conference for High Performance Computing, Networking, Storage, and Analysis. doi:10.1145/3126908.3126916

NERSC Project PI: Prabhat, Berkeley Lab

Deeper Understanding of Livestock Greenhouse Gas Emission

Scientific Achievement

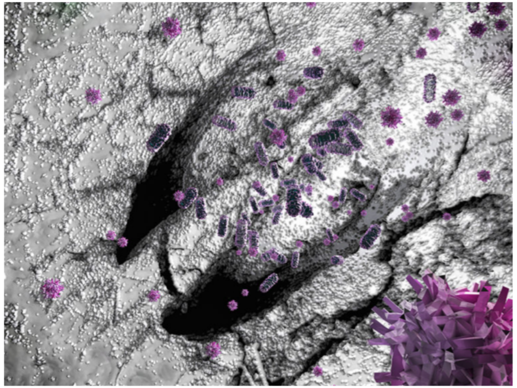
Using supercomputers at NERSC, an international research team that included scientists from the Joint Genome Institute (JGI) generated a catalog of microbial genes found in the guts of ruminants – sheep and cattle – and were able to assign individual microbes to functions that occur in the digestion of plant cells. The study generated 401 genomes, greatly expanding the previous set of only 14.

Significance and Impact

Livestock productivity depends on how microorganisms in the animals' rumen convert undigestible plant material into nutrients used for growth. However, this process produces greenhouse gases, estimated to be the equivalent of 15% of all emissions. Understanding the fermentation process in ruminants can help find a balance between food production and greenhouse gas emissions as well as provide insights into how to develop new biofuels.

Research Details

The samples were drawn from the Hungate collection of rumen microbiota. In additional to providing the genomic sequences, the team searched 1.4 million coding sequences against 1.9 billion sequences collected in the IMG/M database at JGI and found most of the Hungate genomes were indeed present in rumen samples. The team found that almost a third of the species were present in the human gut as well.



Depiction of a rumen microbiome. Rumen microbes play a vital role in allowing ruminant livestock to break down the food they eat and produce milk, meat and wool. Image: Ella Maru studio, www.scientific-illustrations.com

Seshadri R, et al. Nature Biotechnology, March 19, 2018
doi:10.1038/nbt.4110here

NERSC PI: Kjiersten Fagnan, JGI

Sensors for Extreme Environments

Scientific Achievement

Scientists have discovered a new film containing samarium, nickel and oxygen (SNO) that can detect minute changes in electric fields while operating in harsh environments like saltwater.

Significance and Impact

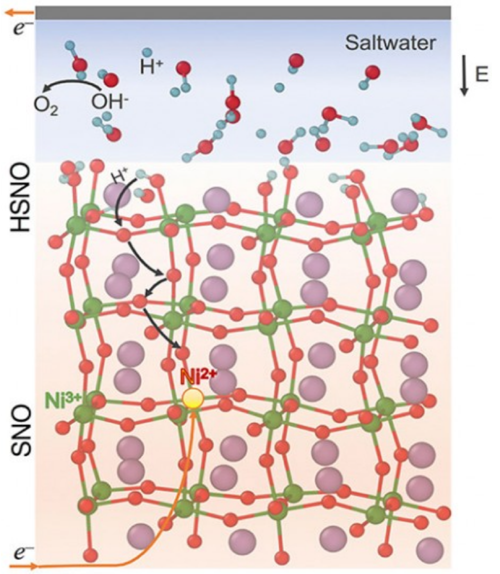
Designing materials for sensors that function in relatively corrosive environments is of interest to many technologies, including energy, ocean monitoring and biological applications. The main challenge to designing such materials is maintaining their chemical makeup and shape. The material designed by the researchers is stable in salt water, does not corrode, and works efficiently at temperatures of interest in the environment. A potential application is to detect electrical signals from maritime vessels and sea creatures.

Research Details

- Ab initio molecular dynamics simulations of the molecular SNO-water interactions run on NERSC's Cori system helped explain the sensing mechanism in detail and helped identify proton transfer in SNO.
- Additional simulations were run at Argonne National Lab.

Zhang et al., Nature 553, 68 (2018). [DOI: 10.1038/nature25008]

NERSC PI: S. Sankaranarayanan, Argonne National Lab



Saltwater helps a reversible phase transition occur in samarium nickelate (SNO) thin films. Here, the samarium, nickel, hydrogen and oxygen atoms are shown as purple, green, blue and red spheres, respectively. Image: Badri Narayanan, Argonne National Lab

Deep Learning Probes Mysteries of Nuclear Matter

Scientific Achievement

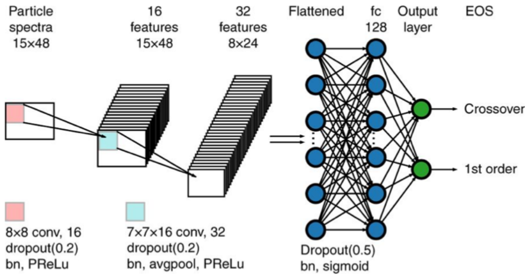
Researchers has demonstrated that deep neural network machine learning techniques can be used to study how the constituents of normal atomic nuclei transition to a plasma of free quarks and gluons under extreme conditions. The methods allows researchers to unveil hidden information from the experimental output of heavy-ion collision experiments.

Significance and Impact

A key open question in nuclear physics surrounds the equation of state of nuclear matter: how quarks and gluons respond to changes in temperature and density. In today's universe quarks and gluons are confined to protons and neutrons in the atomic nucleus, but in the intense conditions following the big bang, they formed a soup of free-roaming particles. These conditions are being replicated in high-energy heavy-ion collisions at facilities like the Relativistic Heavy Ion Collider (RHIC) at Brookhaven Lab. Observables from these experiments do not give equation of state information directly, so that's where deep learning comes in: finding correlations "hidden" in the experimental measurements.

Research Details

Running on supercomputers at NERSC, the researchers applied supervised learning to a deep convolutional neural network to identify high-level correlations of measured particle momentum and angular distribution and thus decipher the nature of the QCD phase transition.



The convolution neural network architecture designed to identify the QCD transition - the transition from normal nuclear matter to a new form of matter due to temperature or density increases. Image: Long-Gang Pang

Pang, L-G, et al, Nature Communications, Volume 9, Article number: 210 (2018) doi: 10.1038/s41467-017-02726-3

NERSC Project PIs:
Chan, Y-D, Wang, X-N,
Berkeley Lab

NERSC

National Energy Research Scientific Computing Center