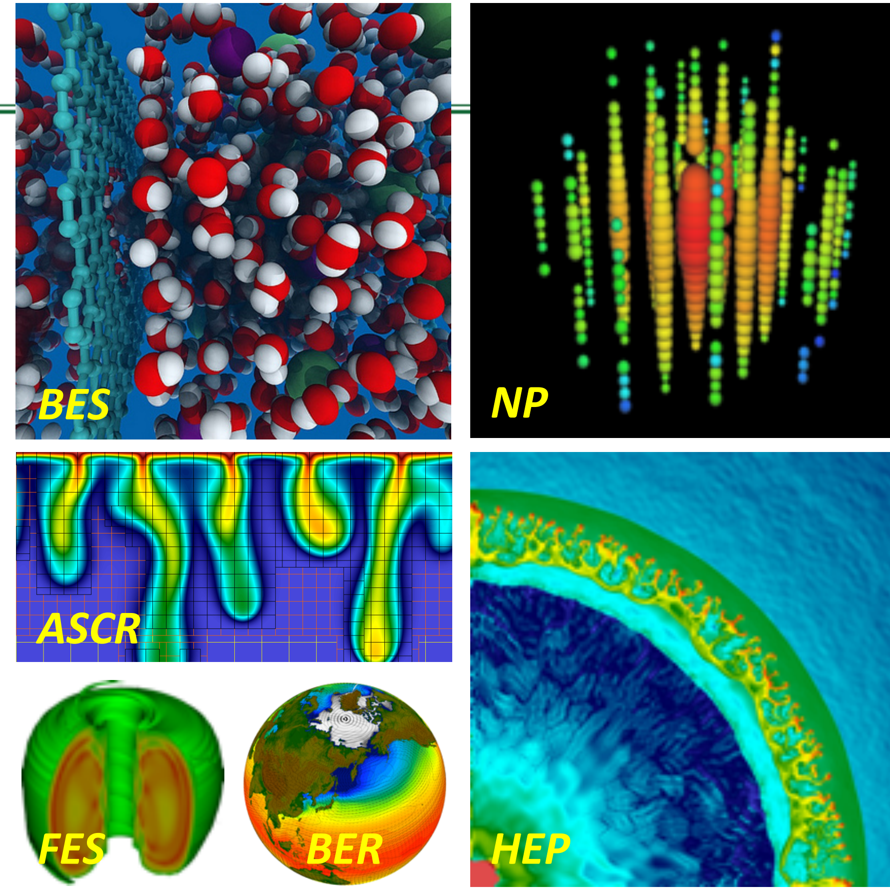
NERSC Science Highlights

December 2016



NERSC

BERKELEY LAB
Lawrence Berkeley National Laboratory

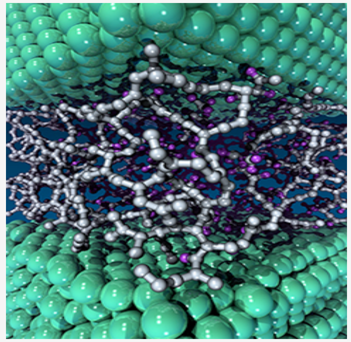
U.S. DEPARTMENT OF ENERGY | Office of Science

Science Highlights December 2016

BES: Materials Science

HPC powers novel approach to understanding lubrication between moving metal interfaces.

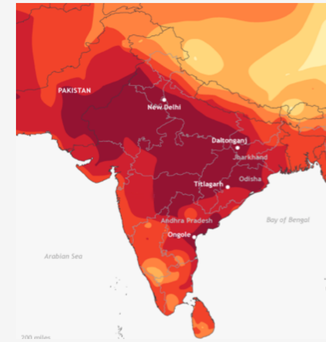
Sankaranarayanan, Argonne, *Nature*

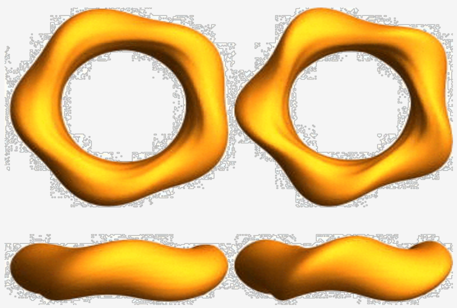


BER: Climate Research

Simulations run at NERSC help confirm observations of rising CO_2 levels on 2015 India/ Pakistan heat waves.

Wehner/O'Brien, LBNL, *Bulletin of American Meteorological Society*

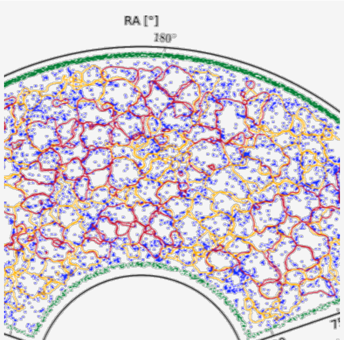




FES: Fusion Energy

Numerical simulations reveal how the sawtooth plasma instability is affected by 3D shaping in certain tokamaks.

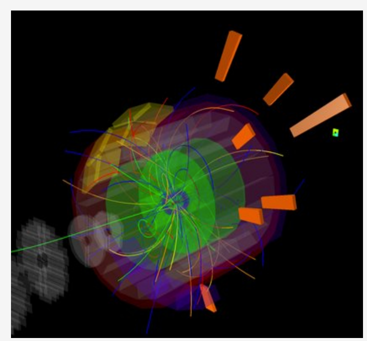
Hanson, Auburn U., *Physics of Plasmas*



HEP: Astrophysics

Largest catalog of cosmic voids tests cosmological models.

Nadathur, U. Portsmouth., *Mon. Notices Royal Astron Soc.*



NP: Nuclear Physics

ALICE data management tool enhances high-energy physics studies at NERSC.

Fasel, LBNL, *Journal of Physics*

New 'Tribofilms' Could Enhance Engine Efficiency

Scientific Achievement

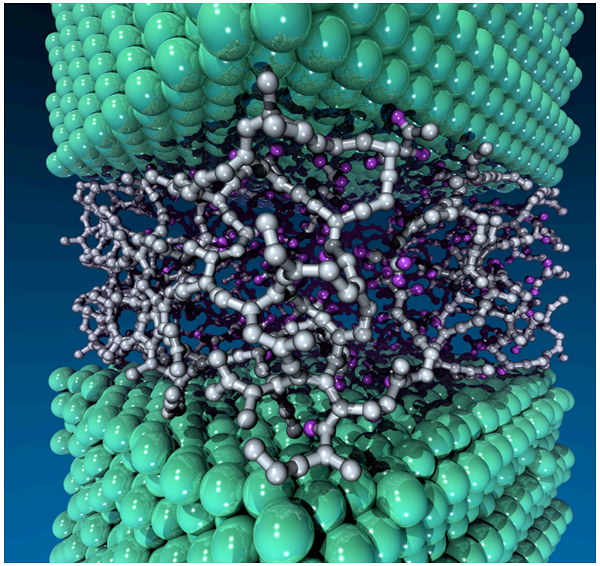
Simulations run on NERSC supercomputers helped Argonne researchers understand how the heat and pressure of an auto engine can generate a newly discovered diamond-like "tribofilm" - a film that forms between moving surfaces.

Significance and Impact

This ultra-durable, self-lubricating tribofilm could enhance the efficiency and durability of future engines and other moving metal parts by allowing them to create self-healing, diamond-like carbon tribofilms. Because the tribofilm develops in the presence of base oil, manufacturers might be able to reduce, or possibly eliminate, some of the modern anti-friction and anti-wear additives in oil.

Research Details

- Through experimentation, the scientists realized the film was developing spontaneously between the sliding surfaces and was replenishing itself, but they didn't understand why and how.
- Molecular dynamics simulations revealed what was happening at the atomic level: that the catalyst metals in nanocomposite coatings were stripping hydrogen atoms from hydrocarbon chains in the lubricating oil, then breaking the chains down into smaller segment that combined under pressure to create the tribofilm.



Supercomputer simulations allowed the researchers to virtually test other potential catalysts (other metals and hydrocarbons in coatings and oils) for their "self-healing" properties in a high-temperature, high-pressure engine environment. Image: Joseph Insley, Argonne National Laboratory

A. Erdemir, G. Ramirez, et al, Nature 536, August 2016, 67–70

NERSC Project PI: S. Sankaranarayanan (Argonne)

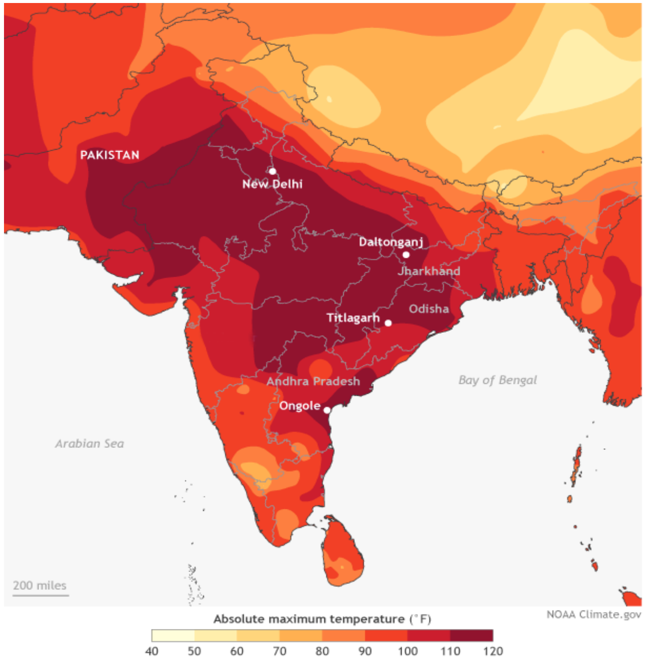
Simulations Confirm Changing Climate Influences Extreme Weather Events

Scientific Achievement

Using supercomputers at NERSC and simulations from the Community Atmospheric Model, an international research team found new evidence that the Earth's changing climate has an effect on extreme weather events such as the 2015 heat waves in India and Pakistan.

Significance and Impact

The researchers examined observational and simulated temperatures and heat indexes, concluding that the heat waves "were exacerbated by anthropogenic climate change." While these countries typically experience severe heat in the summer, the 2015 heat waves—which occurred in late May/early June in India and in late June/early July in Pakistan—have been linked to the deaths of nearly 2,500 people in India and 2,000 in Pakistan.



Hottest daytime temperatures in India during the week of May 24-30, 2015, based on interpolated weather station data provided by the India Meteorological Department. Image: Wikimedia

Research Details

- The experimental design used "factual" simulations of the world and compared them to "counterfactual" simulations of the world that did not include enhanced levels of carbon dioxide in the atmosphere.
- The researchers ran a large number of simulations, which is important for studying a rare event; if it is rare, then you need a large amount of data in order to have it occur frequently enough that you can understand it.

M. Wehner, et al, *Bull. of the American Met. Soc.*, Dec. 2016

NERSC Project PI: M. Wehner, T. O'Brien (LBNL)

Effects of 3D Shaping on Fusion Reactor Plasma Instabilities

Scientific Achievement

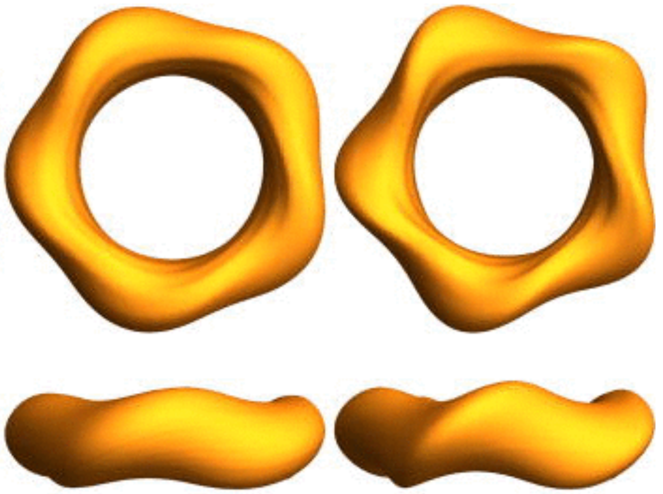
Numerical simulations of sawtoothing in the Compact Toroidal Hybrid (CTH) experiment –a magnetic fusion energy confinement device at Auburn Univ. –helped physicists better understand certain factors that can influence common plasma instabilities in a fusion reactor.

Significance and Impact

In sawtoothing - a common plasma instability seen in fusion reactors – the electrical current flowing through the plasma repeatedly peaks and crashes, causing the plasma to degrade or even terminate during a reaction. Supercomputing simulations can improve our understanding of the sawtooth cycle and the factors that effect it, leading to improved plasma stability. The findings are relevant to disruption avoidance in full-scale fusion reactors such as ITER.

Research Details

- By running magnetohydrodynamic (MHD) models on NERSC's Edison system, the researchers were able to confirm observations that had suggested that 3D shaping from the magnet coil in the CTH experiment affects the properties of the sawtooth instability.
- The researchers used the NIMROD code to evolve a set of extended resistive MHD equations in a toroidal geometry, finding that as the helical field strength increases, the period of the instability decreases.



Numerical magnetohydrodynamic simulations were used to gain insight into how the sawtooth instability is affected by 3D shaping from the Compact Toroidal Hybrid stellarator field. As the vacuum function is increased, the plasma become helically deformed. Image: N.A. Roberds, et al

N.A. Roberds, et al, *Physics of Plasmas*, 23, 092513, 2016

NERSC Project PI: J. Hanson (Auburn U.)

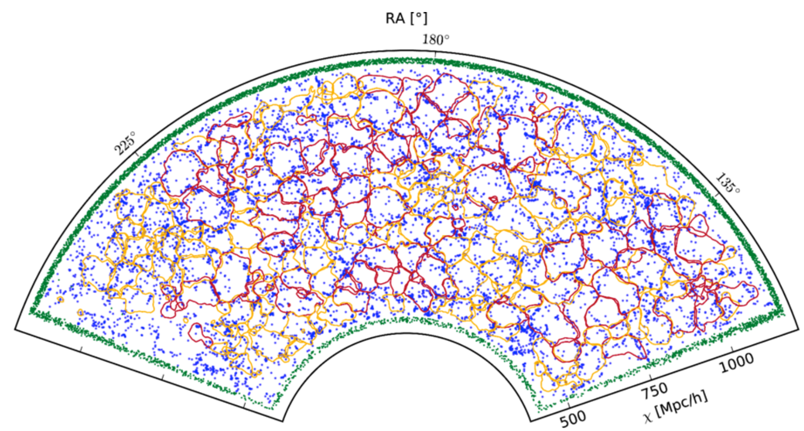
Testing Cosmology with a New 'Catalogue of Voids'

Scientific Achievement

Researchers developed a new public catalog of cosmic voids using data from the Baryon Oscillation Spectroscopic Survey (BOSS) and CMASS galaxy surveys. The catalog contains information on the location, sizes, densities, shapes and bounding surfaces of nearly 9,000 voids – the largest public void catalog to date.

Significance and Impact

Cosmic voids are vast spaces between filaments (the largest-scale structures in the Universe), which contain very few or no galaxies. The void size distribution is a sensitive probe to test theories that deviate from the standard "ΛCDM" (Lambda Cold Dark Matter) cosmology. A first analysis shows that the void size distribution is in excellent agreement with ΛCDM. However, the standard ΛCDM model cannot explain the void density distribution, which could offer early evidence that unknown physics is required.



The cross-section of voids in the LOWZ survey, colored according to whether the average galaxy density within the void is negative (red) or positive (yellow). Galaxy positions are overlaid in blue, and buffer mock catalog galaxies around the survey edges in green. (Nadathur & Hotchkiss, MNRAS 454 889)

Research Details

- simulations are required to validate the techniques and algorithms used to identify the voids and test the ability to differentiate between standard ΛCDM and alternative models.
- The researchers used supercomputers at NERSC and other sites to create the needed mock catalogs.

S. Nadathur, *Monthly Notices of the Royal Astronomical Society,* 461 (2016) 358

NERSC Project PI: J. Borrill, LBNL

New Workflow Software Streamlines High-Energy Nuclear Physics Data Analysis

Scientific Achievement

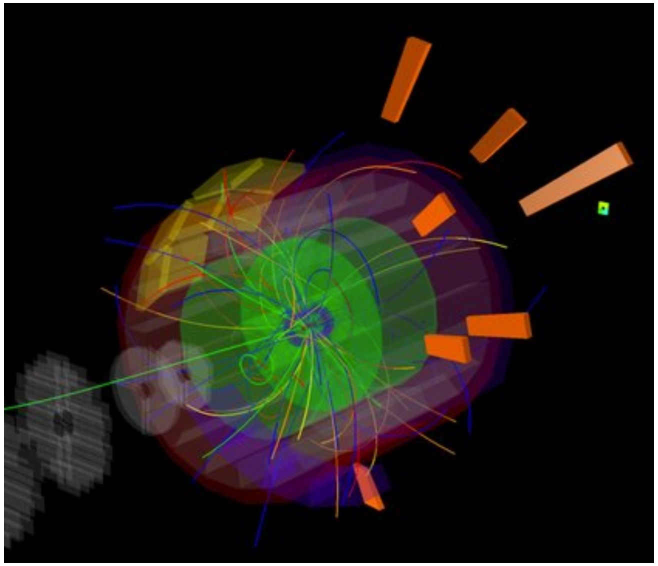
Berkeley Lab researchers working with the ALICE Collaboration have developed a data analysis tool to simplify workflows for high-energy nuclear physics studies by handling common tasks such as job submission, software management and local data management in a framework that can be adapted to multiple HPC environments.

Significance and Impact

The processing and analysis of event-based data from high energy nuclear physics experiments is well suited for commodity computing hardware. ANALISA (A NERSC ALICE Submitter Agent) is a new software tool for running serial ALICE jobs on HPC systems designed for parallel processing.

Research Details

- ALICE is an experiment developed to study dense QCD matter, achieved through the collision of heavy ions at the very high energies achieved at the Large Hadron Collider (LHC) at CERN.
- Simulations and data analyses processed on NERSC systems are critical to producing important measurements of particle collisions at the LHC.
- The ANALISA tool, initially designed to process standalone ALICE simulations for detector and software development, has been successfully deployed on several NERSC supercomputers and configured for and tested on NERSC's Cori system.



A computerized representation of a proton-proton collision captured by the ALICE detector at CERN, the most powerful particle accelerator in the world. Image: CERN

M. Fasel, *Journal of Physics*, 762, 2016, 012031

NERSC Project PI: J. Porter, ALICE Collaboration, LBNL

NERSC

National Energy Research Scientific Computing Center