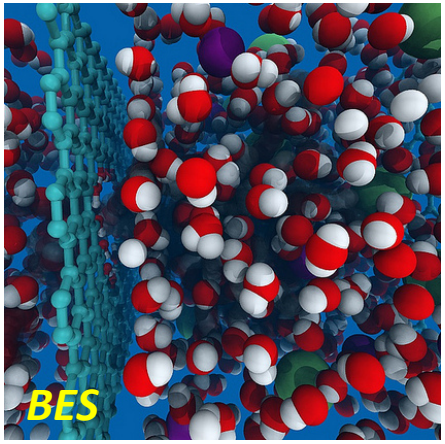
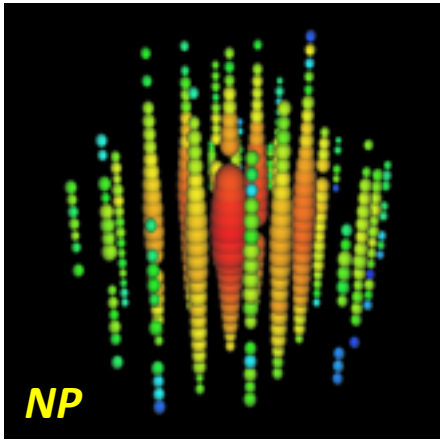
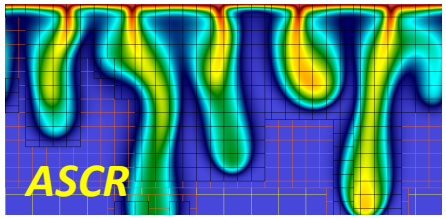
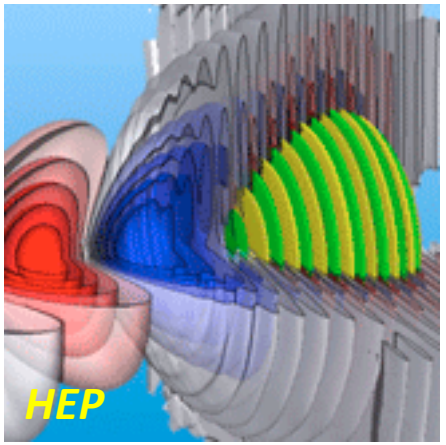
NERSC Science Highlights

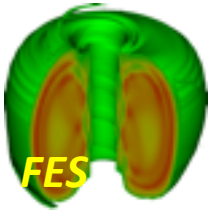
September 2016

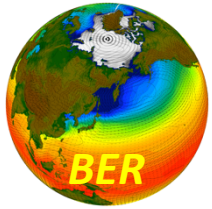












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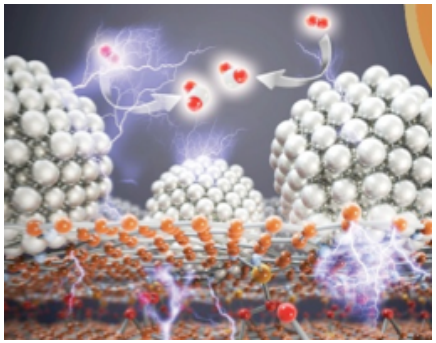
Science Highlights September 2016

Chemical Science

Making polymer electrolyte fuel cells more cost effective.

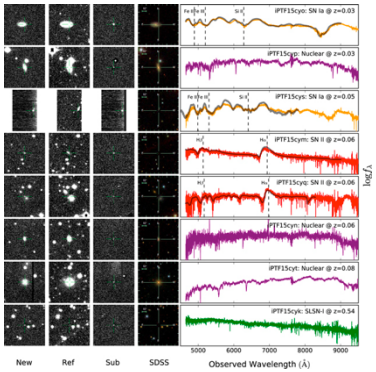
Choi, SABIC, *Journal of Materials Chemistry A*



Biological Science

125,000+ new viral genomes discovered, increasing the number of know viral genes by a factor of 16.

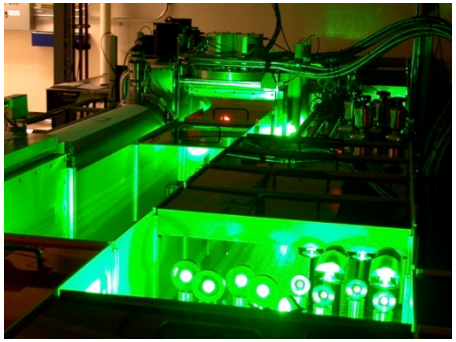
Kyrpides, LBNL, *Nature*



High Energy Physics

The search for an optical counterpart of the first detected gravitational waves.

Kasliwal, Caltech, *Astrophysical Journal Letters*



Accelerator Science

Replacing massive accelerators with table-top devices.

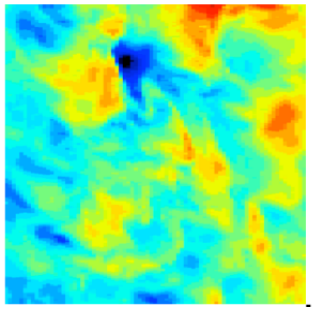
Benedetti/Vay, LBNL, *Nature*; Vay/Rübel, LBNL, *IEEE Computer Graphics and Applications*

Fusion Energy

For possibly the first time, a simulation has quantitatively reproduced experimentally determined H-mode pedestal plasma transport levels.

Hatch, U. Texas, *Nuclear Fusion*

Temperature Fluctuations



Biological Science

Speeding up a bioinformatics application to make biology more predictive.

Luecke, Iowa State, *Intl. Journal of HPC Applications*

Advances in Cost-Effective Fuel Cells

Scientific Achievement

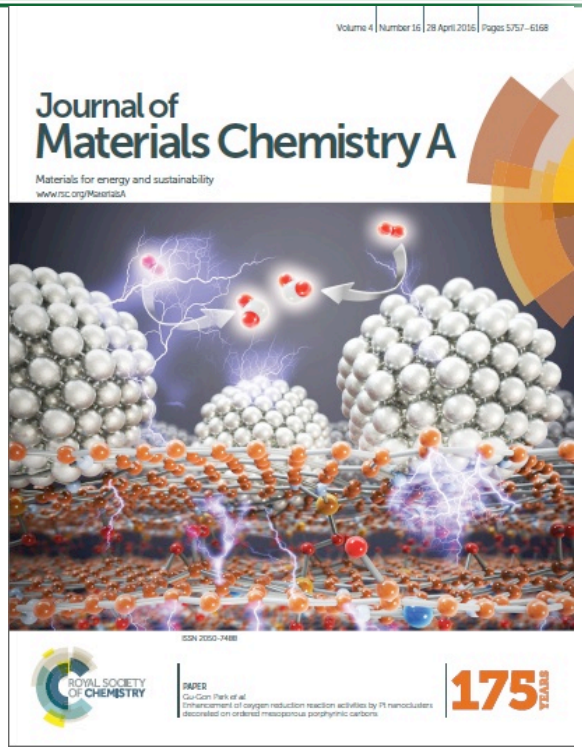
Density functional theory calculations run at NERSC demonstrated how polymer electrolyte fuel cells (PEFCs) can be manufactured more cheaply and run more efficiently by reducing the amount of a single key ingredient: platinum.

Significance and Impact

PEFCs are considered the leading candidate for use in transportation applications and megawatt-scale power generation systems. But producing them commercially is not cost-effective due to the expensive platinum used in the cathode materials. This study showed that it could be possible to use less platinum in the fuel cell electrodes without sacrificing performance.

Research Details

- The research team ran DFT calculations on NERSC's Edison system to test a non-precious-metal-based cathode material containing only a small amount of platinum.
- Their calculations, which used approximately 300,000 core hours at NERSC confirmed that platinum nanoclusters on metal–nitrogen doped ordered mesoporous porphyrinic carbon significantly enhance the oxygen-reduction reaction activity in the catalyst.



The researchers synthesized a new class of electrocatalysts consisting of a trace amount of platinum nanoclusters on metal-nitrogen doped ordered mesoporous porphyrinic carbon to enhance the intrinsic catalytic activity.

S. Hwang, Y. Choi, et al,
Journal of Materials Chemistry A, 2016, 4, 5869-5876

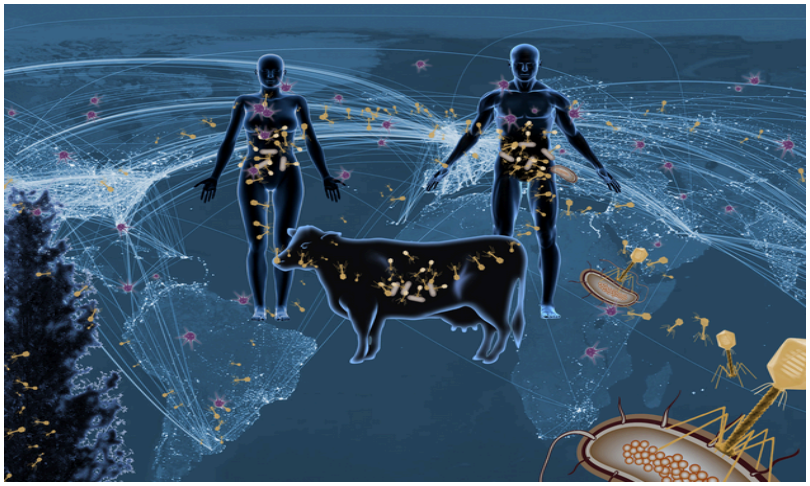
Earth's Viral Diversity Unveiled

Scientific Achievement

In a study published in *Nature*, researchers at the Joint Genome Institute (JGI) used the largest collection of assembled metagenomic datasets from around the world to uncover over 125,000 partial and complete viral genomes, the majority of them infecting microbes.

Significance and Impact

This effort, which leveraged the strong collaboration between NERSC and JGI, increases the number of known viral genes by a factor of 16 and provides researchers with a unique resource of viral sequence information. Given the role that viruses play in host metabolism, gene flow, and microbial communities, it is critical to capture viral linkages with their hosts.



DOE JGI researchers utilized the largest collection of assembled metagenomic datasets from around the world to uncover over 125,000 partial and complete viral genomes, the majority of them infecting microbes.

Research Details

- The researchers used non-targeted metagenomics, referencing both isolate viruses and manually curated viral protein models, and the largest and most diverse dataset to date. The team analyzed over 5 trillion bases of sequences available in JGI's Integrated Microbial Genomes with Microbiome Samples system collected from 3,042 samples around the world from 10 different habitat types. Their efforts to sift through the veritable haystack of datasets yielded over 125,000 viral sequences encoding 2.79 million proteins.
- It took about 10 million core-hours for all the computations against 4,000 metagenomes and around 50,000 isolate genomes.

Paez-Espino, Eloe-Fadrosh, Pavlopoulos, et al, Nature, 536, 425–430, Aug. 25, 2016

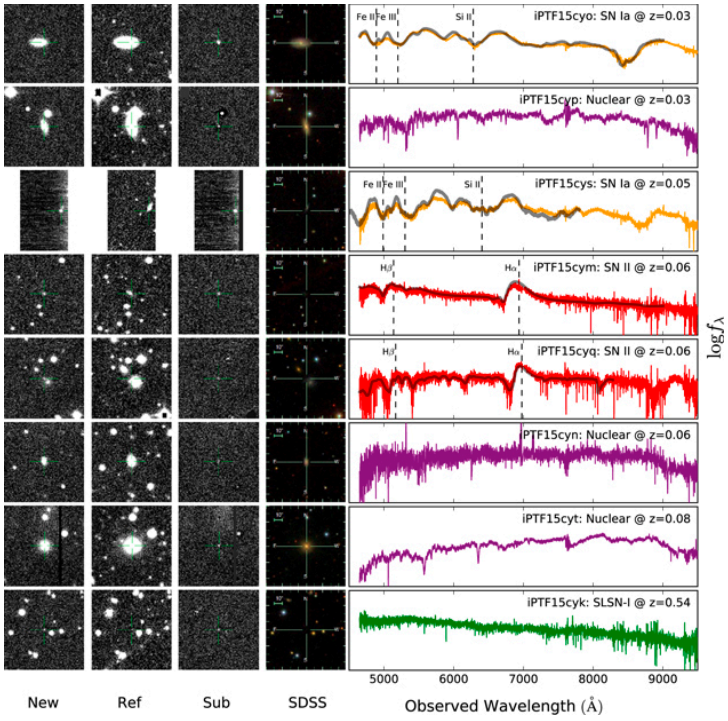
The Search for a Visible Gravitational Wave Source

Scientific Achievement

Upon the first detection of a gravitational wave event, the intermediate Palomar Transient Factory (iPTF) autonomously responded with a search for an optical counterpart. Initially eight transient candidates were identified; within two hours all eight were spectroscopically classified by the Keck II telescope.

Significance and Impact

The direct detection of gravitational waves marks the dawn of a new era in astronomy. The detection and study of the anticipated electromagnetic counterpart would provide a wealth of information about the objects that produce gravitational waves. Even though none of the candidates in this study appear to be associated with the event, this end-to-end discovery and follow-up campaign bodes well for future searches in the post-detection era of gravitational waves.



Keck II/DEIMOS classification spectra of eight iPTF candidates obtained within two hours of discovery.

Research Details

- Within minutes of obtaining the data, the iPTF automated real-time image subtraction pipeline at NERC began loading optical counterpart candidates into the iPTF database. More than 127,000 candidates were loaded into the NERSC database.
- The automated machine-learning-aided filtering algorithms rejected the moving objects in the solar system, variable stars in the Milky Way and subtraction artifacts.

M. Kasliwal, et al, The *Astrophysical Journal Letters*, Vol. 824, No. 2, June 17, 2016

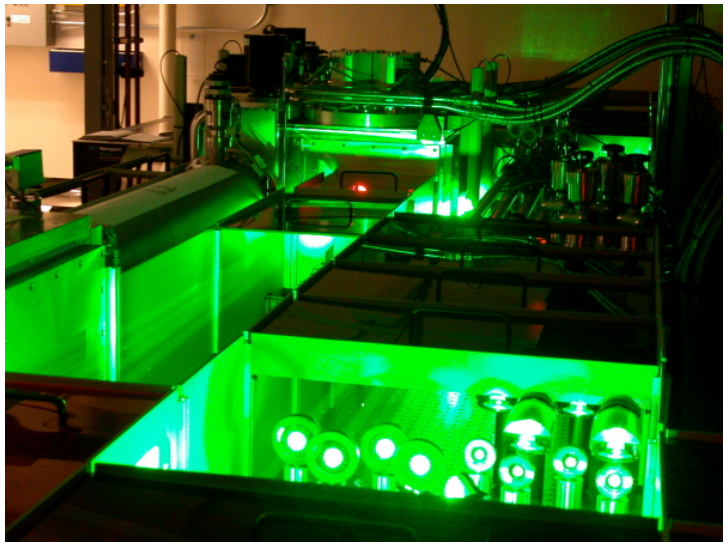
Advanced Simulations Support Breakthrough Coupling of Two Plasma Accelerator Stages.

Scientific Achievement

A team ledby Berkeley Lab researchers has demonstrated that an electron beam accelerated by a laser-driven plasma wave can be further accelerated by a second plasma wave — a fundamental breakthrough in advanced accelerator science.

Significance and Impact

Laser-driven plasmas can accelerate electrons to very high energies over short distances. This research shows that accelerators can be built by coupling multiple stages of acceleration, which could lead to table-top devices capable of energy gains equivalent to those achieved in large accelerators. Such accelerators could be used for medical and other applications.



The TREX laser at Berkeley Lab's BELLA Center was used in a two-stage laser-plasma acceleration experiment. (Berkeley Lab)

Research Details

- Detailed modeling of the staging experiment was performed at NERSC on Edison with the code INF&RNO (INtegrated Fluid & paRticle simulatioN cOde), a reduced code specifically designed to model laser-plasma accelerators.
- Extensive modeling allowed the researchers to reproduce and interpret the results obtained in several experimental campaigns, and contributed to the optimization of the experiment itself.
- The highly efficient INF&RNO code and access to time on Edison allowed for the quick production of large parameter scans for detailed comparison with experiments

Steinke, et al., *Nature*, 530, February 2016

New In-situ Analysis Framework Enables Modeling at Scale

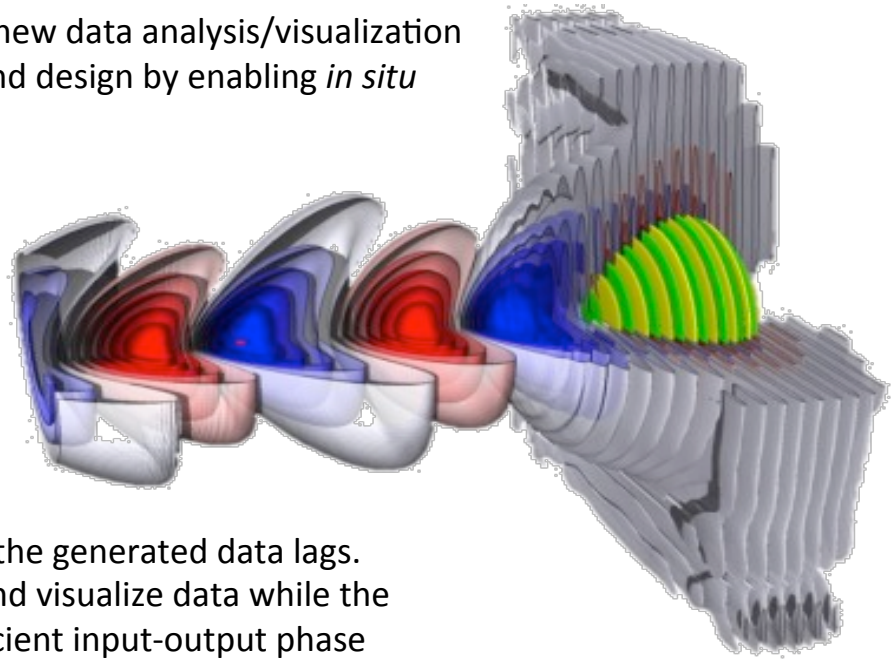
Scientific Achievement

A team of Berkeley Lab researchers has developed WarpIV, a new data analysis/visualization toolkit designed to help speed particle accelerator research and design by enabling *in situ* visualization and analysis of accelerator simulations at scale.

Significance and Impact

Scientists have already made great progress designing what promise to be affordable, compact laser wakefield particle accelerators that would be used for scientific discovery and in applications such as cancer treatment, food sterilization and drug development. However, more large-scale modeling is needed to recognize the full benefit of this technology.

But as the scale of simulations grows, the ability to output all the generated data lags. That's where WarpIV steps in, allowing scientists to analyze and visualize data while the simulation is running, thus bypassing the expensive and inefficient input-output phase of the simulation.



A rendering of plasma laser-driven acceleration, taken from 3D Warp simulations.

Research Details

To create WarpIV, the team combined two software tools already widely used in high energy physics: Warp, an advanced particle-in-cell simulation framework, and VisIt, a 3D scientific visualization application. Together, they give users the ability to perform *in situ* visualization and analysis of their particle accelerator simulations at scale while reducing memory usage and saving computer time.

O. Rübel, et al, *IEEE Computer Graphics and Applications,* 36, May-June 2016

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HEP/ASCR

PIs: J-L Vay, O. Rübel (LBNL)

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Speeding Up a Bioinformatics Application

Scientific Achievement

A team of computer scientists and geneticists from Iowa State University, the University of Maryland and the University of Arkansas have demonstrated significant speedups of the epiSNP bioinformatics program using the Edison supercomputer at NERSC.

Significance and Impact

Gaining a better understanding of how pieces of an individual's genome affects its traits can make biology more predictive. In humans, this can help determine predisposition to disease. In crops like wheat, it could lead to greater production using less land or water.

The research team studied beneficial fatty acids in angus-sired beef cattle to inform breeding decisions that could make meat healthier.

Research Details

- The team used the epiSNP bioinformatics program to perform pairwise comparisons of genotypes and how they affect traits such as height, weight or makeup of body tissues.
- Such pairwise comparisons are typically "computationally expensive." The more combinations that are calculated, the higher the computational cost. Finding out how to speed up the computation lowers these costs.
- To achieve their results, the scientists used Coarray Fortran, which allowed them to use a Partitioned Global Address Space programming model.

N.T. Weeks, et al, *International journal of High Performance Computing Applications*, July 12, 2016, doi: 10.1177/1094342016658110

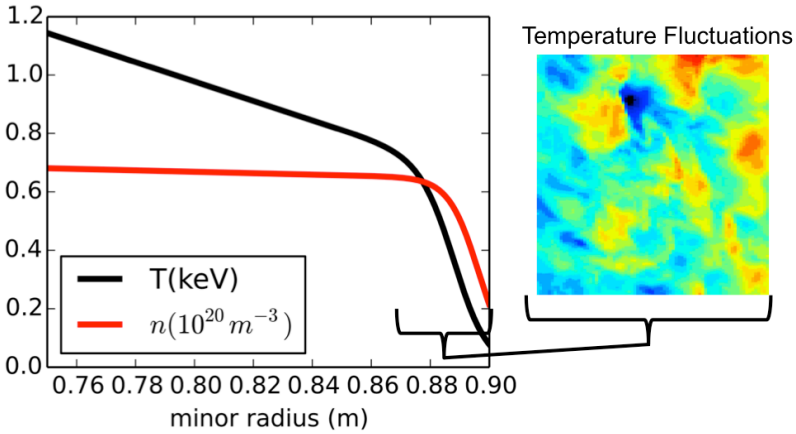
Advances in a Theoretical Understanding of Fusion Edge Plasma Transport

Scientific Achievement

For possibly the first time, a simulation has quantitatively reproduced the H-mode pedestal plasma transport observed experimentally at the JET fusion device. Understanding this process is key to developing sustained fusion reactions as a cost-effective source of clean energy.

Significance and Impact

The tokamak fusion reactor H-mode is defined by a narrow insulating region—the pedestal—at the edge of a fusion plasma, where turbulence is suppressed and sharp pressure gradients develop. The pedestal is at the center of the most pressing issues facing fusion energy research.



Understanding and controlling complex effects and structures at the plasma edge are key to containing the burning plasma and reducing damage to wall components.

Research Details

- Using Edison, the researchers demonstrated, through simulations using the code *GENE* that an instability known as the microtearing mode (MTM) is the dominant instability in the pedestal of a representative JET discharge.
- The simulations show that MTM-driven turbulence, in combination with other known effects, produces transport levels closely matching experimental power balance across most of the pedestal, demonstrating the capacity of these mechanisms to limit pedestal evolution.

D. Hatch et al., *Nuclear Fusion*, 56, August2016,

National Energy Research Scientific Computing Center