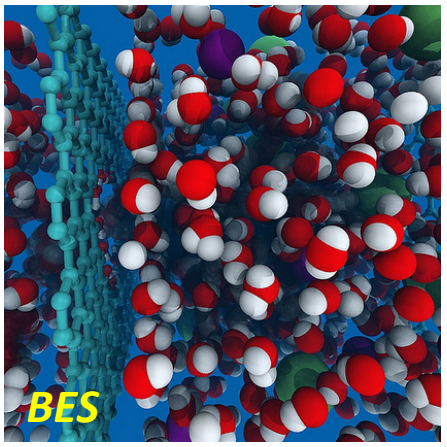
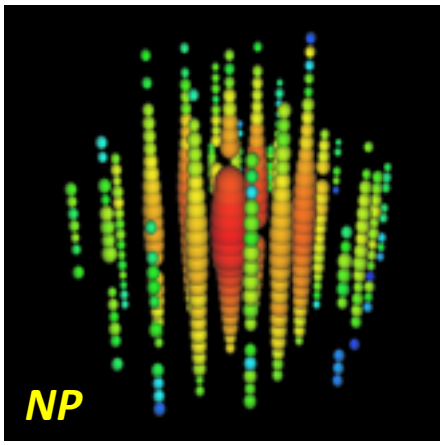
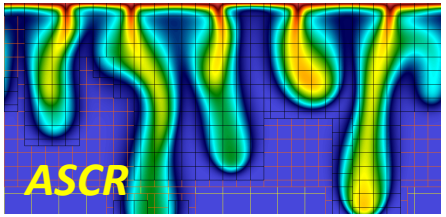
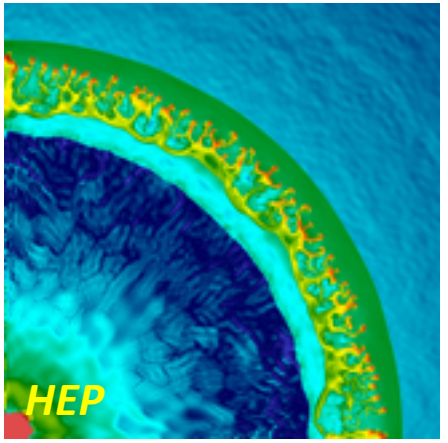
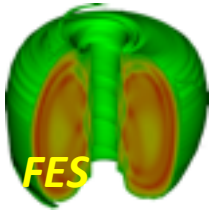
NERSC Science Highlights

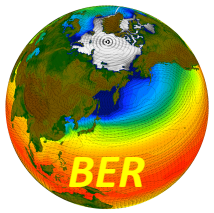












NERSC 40 YEARS at the FOREFRONT 1974-2014

Selected User Accomplishments

September 2014

U.S. DEPARTMENT OF ENERGY | Office of Science

BERKELEY LAB
Lawrence Berkeley National Laboratory

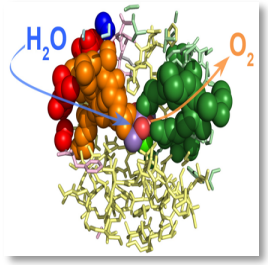
NERSC User Science Highlights

Chemistry

Quantum chemistry simulations yield results that challenge conventional wisdom about how acids behave in water.
(C. Mundy, PNNL)

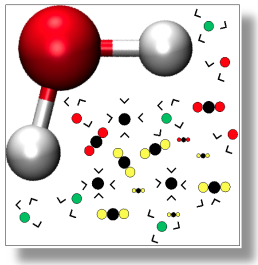
Data Science

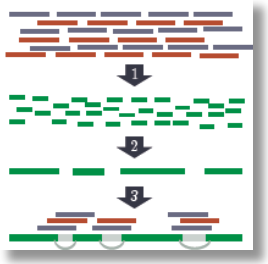
NERSC innovations in data analysis pipelines for DOE beamline facilities yield important science results.



Biochemistry

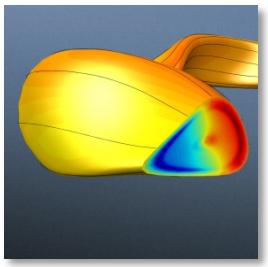
Quantum calculations establish critical basis for understanding environmental fate of a major global pollutant.
(**J. Smith, ORNL**)





Genomics

Novel algorithm running on Edison has resulted in unequaled processing speed for key genomics computations.
(K. Yelick., UC Berkeley)

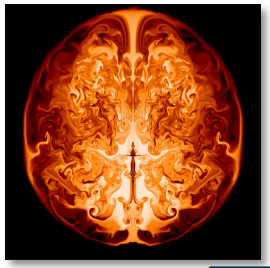


Fusion

New calculations shed light on internally-generated plasma currents that could help reduce fusion reactor costs.
(M. Landreman/W. Dorland (U. of Maryland)

Astrophysics

Rad-hydro simulation of primordial star suggests a totally new pathway to highly energetic thermonuclear supernova explosion.
(K. Chen/S. Woosley (U. Minnesota/UC Santa Cruz)



Relearning Acid-Base Fundamentals

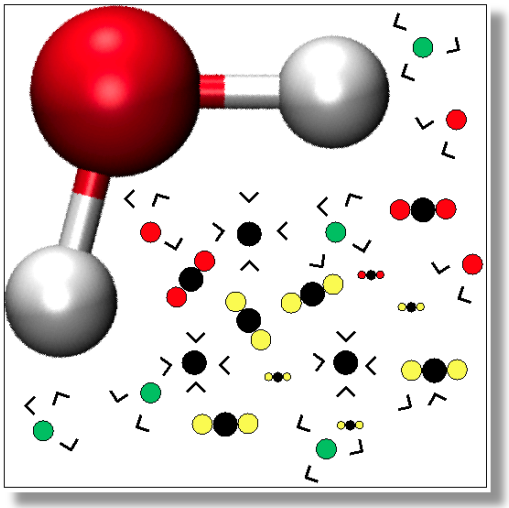
- Quantum chemistry simulations done at NERSC have produced results that challenge conventional wisdom about how acids behave in water.
- The extent to which acids dissociate (move apart) is important in a great many chemical reactions, such as in batteries and in metal corrosion.
- Key finding is that positively and negatively charged ions don't separate quite as much as had been commonly thought.
- Key enabling technologies were the use of HPC to allow simulation of longer-range effects and comparison of molecular dynamics results with independent experimental measurements.

On the Cover: It may be necessary to recast acid/base concepts in freshman chemistry texts based on improved understanding gained simulation results from NERSC. Researchers found that hydrochloric acid (HCl) does not dissociate as expected, but that the hydronium ion (H_3O+) and chloride ion (Cl^-) are paired across a range of concentrations.

The Journal of Physical Chemistry B 118(26):7211-7220.
DOI: 10.1021/jp501091h

Probing Mercury's Partnering Preferences

- **In aquatic conditions, mercury is frequently bound to sulfur-containing molecules. A quantum mechanical study at NERSC has explained, for the first time, why mercury prefers sulfur over other similar atoms such as oxygen.**
  - The reason is related to the strength of an interaction between mercury and water molecules; requires a machine like Edison to compute the longer-range interactions with water.
- **Establishes a basis for the fundamental chemistry of mercury that is not possible from experimentation alone.**
- **Results are critical for understanding toxicity, transport, and environmental fate of this major global pollutant.**



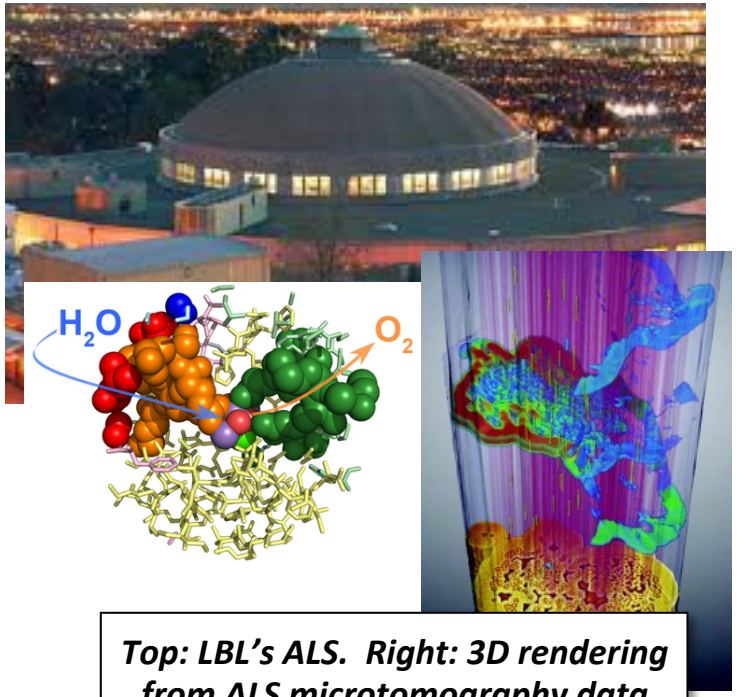
That mercury (red and black in the artist's conception above) prefers to chemically bond to sulfur has been known for over 50 years but now, quantum chemistry studies at NERSC finally explain why. The results are a key first step toward understanding critical factors in alleviating damaging effects on the environment and on human health.

Fusion Simulation Could Reduce Costs

- New calculations shed light on internally-generated plasma currents that could help reduce fusion reactor costs by supplying a lot of the current needed to sustain the hot plasma in a device called a "stellerator" (pictured in the inset).
- Colors in the image represent calculated self-generated plasma current intensity in the W7-X stellarator along the magnetic field.
- Using NERSC's Edison system enabled the SFINCS code to solve the "real" four-dimensional drift-kinetic equations for a nonaxisymmetric plasma, such as the type in a stellerator, without using previously common approximations.

NERSC Projects Put Data in the Fast Lane

- Two collaborative efforts underscore NERSC's commitment to accelerating science discovery in big data.
- Collaboration between NERSC, SLAC National Accelerator Laboratory, and the LBL Computational Research Division resulted in a key breakthrough in artificial photosynthesis research.
- NERSC has also helped create a "Science Superhighway" with the SPOT Suite for analyzing Advanced Light Source (ALS) x-ray imaging data.
- Both experiments emphasize near real-time data analysis, helping to sustain DOE's investment in, and increase productivity of, major scientific user facilities.

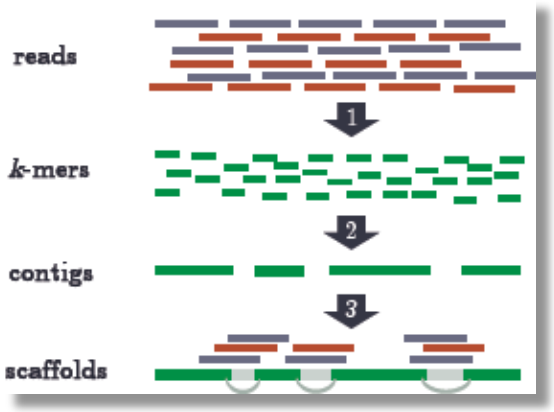


Top: LBL's ALS. Right: 3D rendering from ALS microtomography data showing cracks and individual fiber breaks in a ceramic composite specimen at 1,750 °C. Left: Structure of the light harvesting system in plants showing the reaction center, where light energy is converted to chemical energy.

Nature Comm. 9 July 2014
J. Phys. Chem. Lett., 2013, 4 (14), 2317

Meraculous Genomics Performance

- Computer science research carried out using Edison has resulted in unequaled processing speed for key genomics computations.
- A highly-parallel implementation of a production, whole-genome assembly algorithm called "Meraculous" shows unprecedented performance and scalability to several thousand processor cores.
- This allows reconstruction of the human genome from raw sequencing data in just minutes and vastly reduces processing time for the much more complicated, grand-challenge wheat genome.
- May significantly advance our ability to deal with the deluge of genomic data that is transforming energy and medical science.

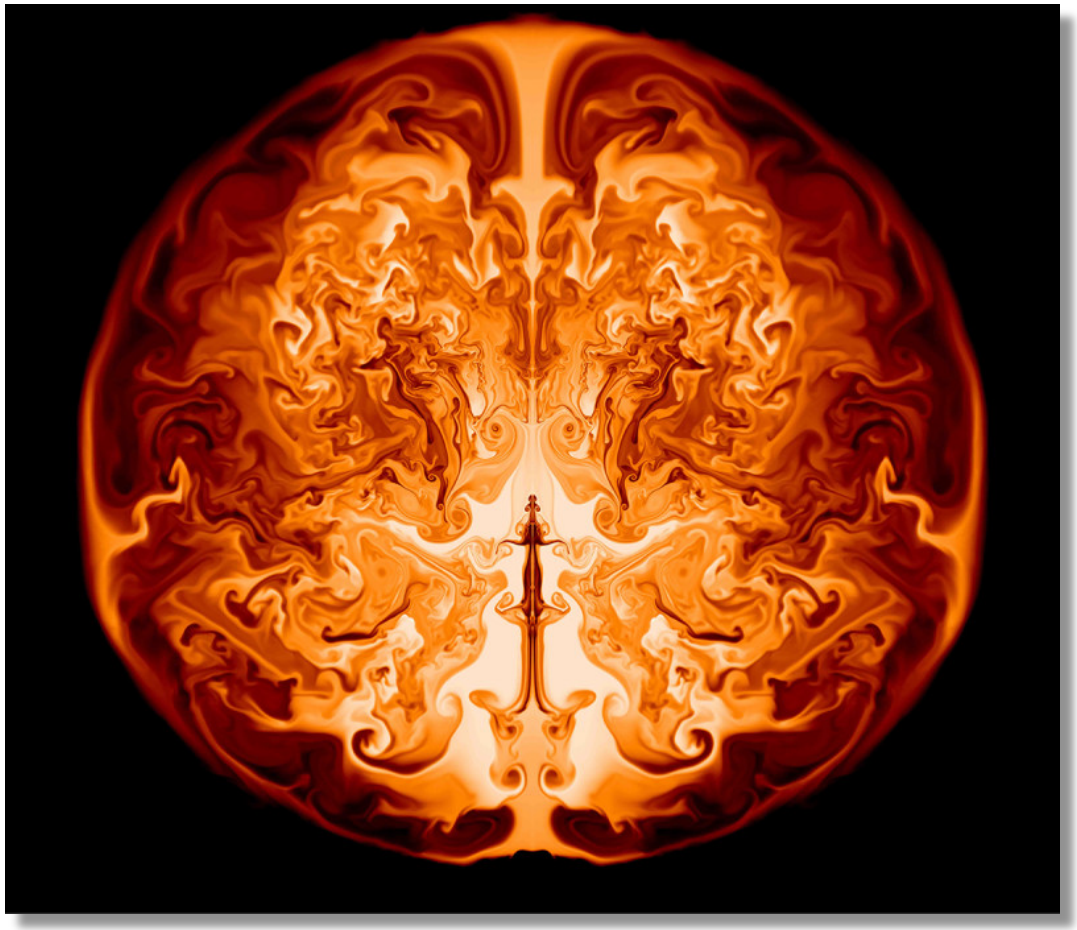


A visualization of some of the steps involved in Meraculous, a state-of-the-art de novo *genome assembler, the performance and scalability of which was optimized using a novel one-sided communication algorithm that facilitates fine-grained parallelism and results in performance improvement from* days *to* seconds.

Proc. IEEE SC14 Conference

Unusual Demise for Some Ancient Stars

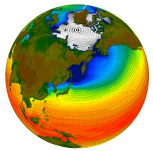
- The image shows a snapshot from a CASTRO rad-hydro simulation of a primordial star's demise due to a highly energetic thermonuclear supernovae explosion powered by helium burning.
- The star's weight is about 55,000 times that of our sun; its diameter is slightly larger than that of the orbit of the Earth around the sun.
- Primordial stars are important because they produced all chemical elements heavier than hydrogen and helium.
- No simulations had ever suggested that stars of this type could explode in this way; prevailing thought had been that they would become a supermassive black hole without exploding.



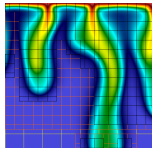
The Astrophysical Journal Volume 790 Number 2 July 2014

About the Title Slide Images

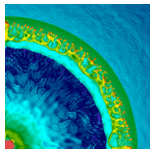
Evolution of electrical current density, parallel to magnetic field, in the Pegasus Toroidal Experiment; provided by John O'Bryan and Carl Sovinec, University of Wisconsin-Madison; Sponsored by Office of Fusion Energy Sciences



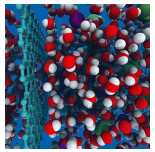
A single month from a simulation of the 20th century by the CCSM capturing wind directions, ocean surface temperatures, and sea ice concentrations. Image courtesy Gary Strand (NCAR) and copyright University Corporation for Atmospheric Research. Sponsored by Office of Biological and Environmental Research



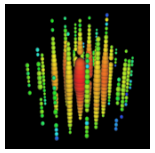
Simulation of density-driven flow for CO_2 storage in saline aquifers. Shown is a snapshot of the CO_2 concentration after onset of convection overlayed on the AMR grid. Image courtesy of George Pau and John Bell (LBNL). Sponsored by Office of Advanced Scientific Computing Research.



Collision between two shells of matter ejected by a massive star in two pair-instability supernova eruptions, only years apart, just before the star dies, showing a slice through a corner of the event. Shell radius (red knots) is about 500 times the Earth-Sun distance. Colors represent gas density (red is highest, dark blue is lowest). Image courtesy of Ke-Jung Chen, School of Physics and Astronomy, Univ. Minnesota. Sponsored by Office of High Energy Physics.



Snapshot from a Molecular Dynamics simulation showing water molecules (red and white), and sodium, chloride ions (green and purple) in saltwater, encountering a sheet of graphene (pale blue, center) perforated by holes of the right size, with water passing through (left side), but sodium and chloride being blocked. Provided by D. Cohen-Tanugi and J. C. Grossman, MIT; Sponsored by Office of Basic Energy Sciences



Observation of a PeV-energy neutrino. Each sphere represents a digital optical module sensor in the IceCube detector. Sphere size is a measure of the recorded number of photoelectrons. Colors represent arrival times of photons (red, early; blue, late). Sponsored by Office of Nuclear Physics

National Energy Research Scientific Computing Center