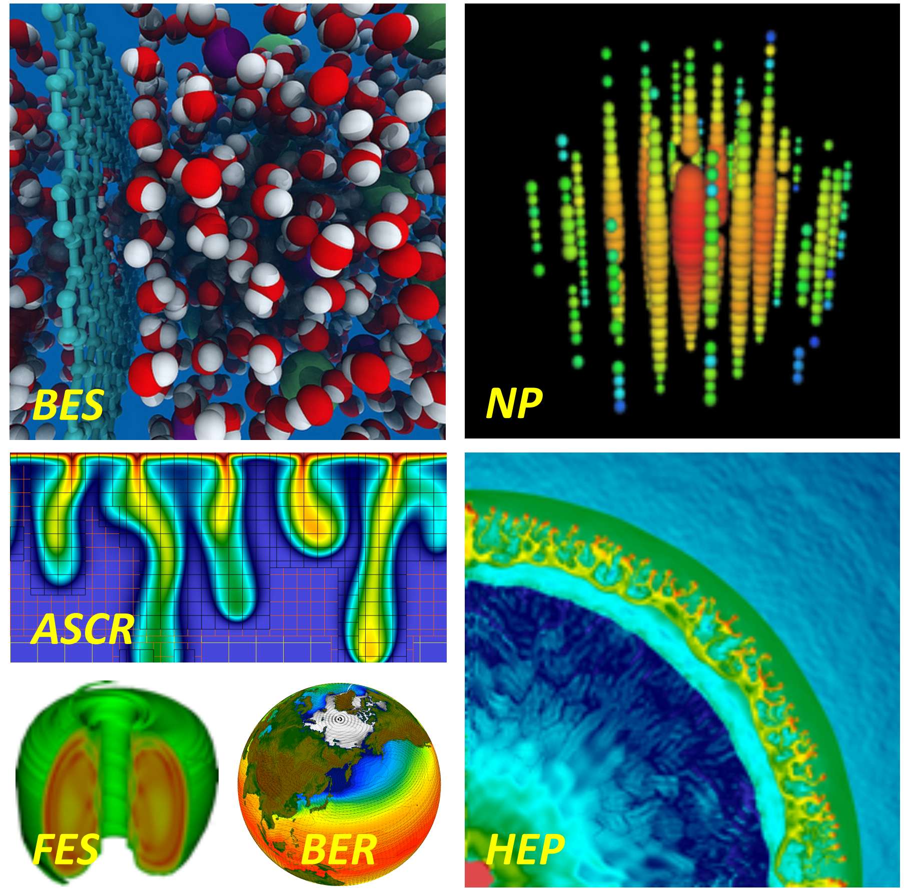
NERSC Science Highlights



NERSC 40 YEARS at the FOREFRONT 1974-2014

Selected User Accomplishments

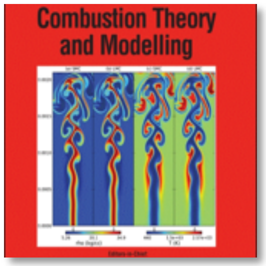
December 2014

U.S. DEPARTMENT OF ENERGY | Office of Science

BERKELEY LAB

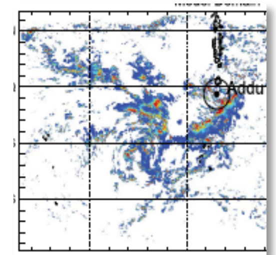
NERSC 40 YEARS at the FOREFRONT 1974-2014

NERSC User Science Highlights

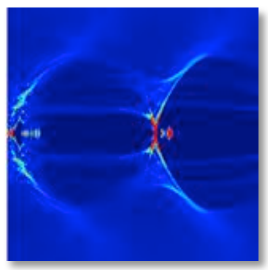


Combustion
New algorithms tested at NERSC boost performance of turbulent combustion simulations
(J. Bell, LBNL)

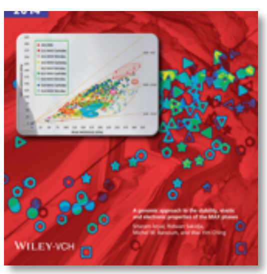
Climate
High-resolution model improves understanding of what has been called the "holy grail" of tropical meteorology.
(S. Hagos, PNNL)



Laser Wakefield
World record for compact 'tabletop' particle accelerator reached due in part to NERSC computation
(**W. Leemans, LBNL)**

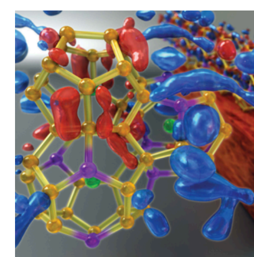


Astrophysics
'CT Scan' of distant Universe at astonishingly large resolution reveals cosmic web in 3D
(K.-G. Lee/Max Planck)



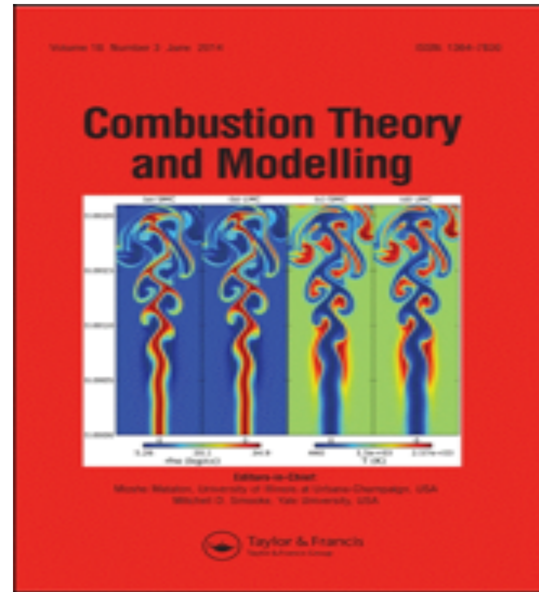
Materials Science
An "omics" approach yields new, potentially useful new materials with unusual properties
(Y.-M. Ching, U. Missouri)

Materials Science
A new inexpensive silicon-based semiconductor for solar energy conversion was discovered via NERSC computation
(G. Galli, U. Chicago)



Boosting Combustion Research

- **Methane flame simulations can run 6x faster using a code with turbulence algorithms developed on NERSC's Hopper.**
- **The new code uses a hybrid OpenMP/MPI parallel programming method designed for next-generation "manycore" architectures such as Cori.**
- **The faster simulations compute more detailed flame chemistry and allow more robust treatment of advection and diffusion of the combustion reactants.**
- **The code scales to approximately 100K cores and shows excellent thread performance on an Intel Xeon Phi coprocessor.**

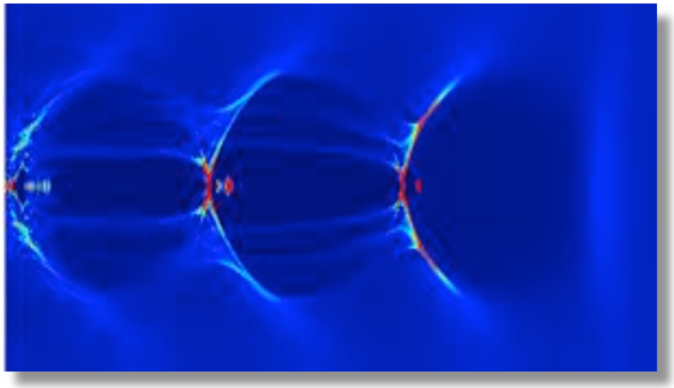


On the Cover: snapshot from a jet fuel combustion simulation performed using a new, faster code that was developed using Hopper. The images show total mass density (left) and temperature (right).

Combustion Theory and Modelling, 18:3, 361-387, DOI: 10.1080/13647830.2014.919410

Power to the Electrons!

- **Simulations at NERSC helped set operation parameters for a system that accelerated subatomic particles to the highest energies ever recorded from a compact accelerator.**
- **The system uses Laser-Plasma Wakefield Acceleration (LPWA), which produces ultra-high gradients that show great promise for reducing cost and size of next-generation accelerators for DOE high energy physics.**
- **Rapid simulations helped evaluate plasma density and allowed for the exquisite control over the laser that is needed because at the energies considered, minor misalignment of the laser beam can cause big damage to the plasma container.**



Simulation of a laser plasma wakefield as it evolves in a 9-cm long tube of plasma. The charge "wake" (three are shown) allows electrons to "ride" the wake to greater and greater speeds and energies. The work was selected as one of ten Best Physics Papers of 2014 by Scientific American.

Physical Review Letters 113, 245002 (2014)

Material Genomics to the MAX

- Layered materials called "MAX" phases containing certain metals plus carbon or nitrogen are important because they have unique characteristics; they conduct heat/electricity like metals but also can be stiff, strong, brittle, and heat-tolerant like ceramics.
- A comprehensive assessment of the elastic and electronic properties of 792 possible MAX phases was carried out at NERSC using *ab initio* methods.
- This allowed an "omics" approach to screening the compounds, identifying electronic characteristics contributing to elastic and thermodynamic stability.
- Materials genome data mining algorithms also helped identify several new thermodynamically stable MAX phases with unusual mechanical parameters that had never been synthesized in the laboratory or theoretically investigated.

On the Cover: Plots showing correlation of two key materials characteristics (bulk modulus, which is resistance to uniform compression, and shear modulus, the response to a cutting-like stress) based on computed data from NERSC.

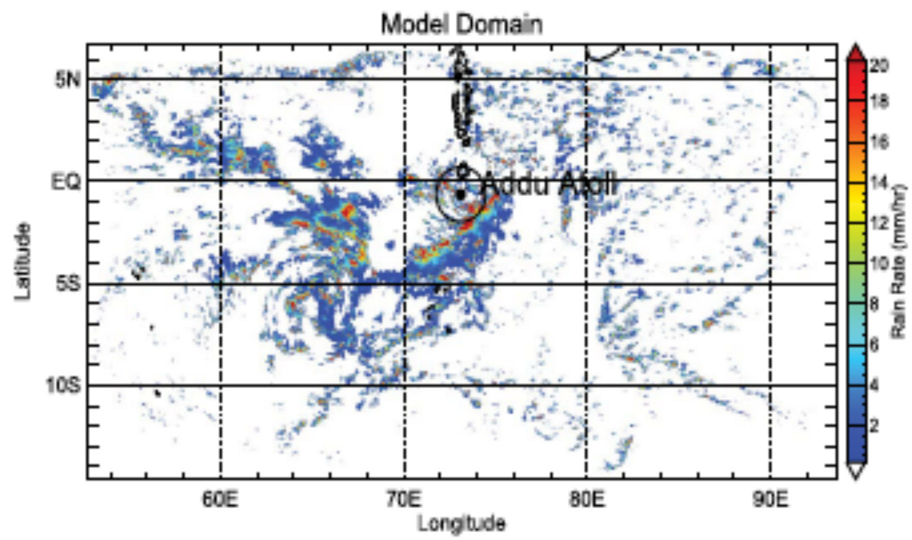
Phys. Status Solidi B 251, No. 8, 1480–1497 (2014) / DOI 10.1002/pssb.201451226

BES

(Y-M. Ching/U. Missouri)

Tracking Tropical Clouds to Polish Climate and Weather Prediction

- High-resolution cloud modeling at NERSC and the OLCF has revealed the cause of a moisture buildup that initiates and propels an important tropical disturbance called the Madden-Julian Oscillation (MJO).
- The MJO is a regular, intra-seasonal (30–90 day) variation in tropical atmosphere but it has a big effect on U.S. weather.
- Understanding initiation and propagation of the MJO will mean better prediction of severe U.S. West Coast winter storms, summer monsoons in the U.S. Southwest, Pacific hurricanes, and perhaps even the El Niño weather event.



The figure shows the both the domain of the simulations in this work (range in latitude/ longitude) and a snapshot of predicted precipitation at an arbitrary time. The results have led to better understanding of the Madden-Julian Oscillation, something that has been referred to as the "holy grail" of tropical meteorology.

J. Adv. Modeling Earth Sys. 06(3):938-949. DOI:10.1002/2014MS000335

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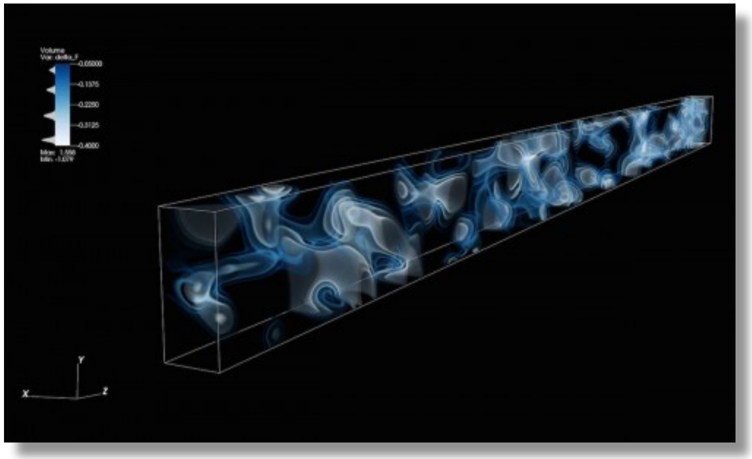
(S. Hagos/PNNL)

'CT Scan' of Distant Universe Reveals Cosmic Web in 3D

- Astronomers have created the first 3-D map of the 'adolescent' Universe, just 3 billion years after the Big Bang.
- Used a new technique similar to medical x-ray computer-tomographic (CT) imaging
- This is the first time the cosmic web has been mapped at such a large distance – 11 billion light years away.
- The map provides a tantalizing glimpse of giant structures extending across millions of light years, and paves the way for more extensive studies that should reveal not only the structure of the cosmic web, but also details of its function – the ways that gas is funneled along the web into galaxies, providing the raw material for the growth of galaxies through the formation of stars and planets.



3D map of the cosmic web at a distance of 10.8 billion years from Earth, generated from imprints of hydrogen gas observed in the spectrum of 24 background galaxies behind the volume. This is the first time large-scale structures in such a distant part of the Universe have been directly mapped. Credit: Casey Stark (UC Berkeley), Khee-Gan Lee (MPIA).

Astrophysical J. Lett., October 16, 2014

(K.-G. Lee/Max Planck)

New Inexpensive Silicon-based Semiconductor for Solar Energy Conversion

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- Detailed first-principles modeling resulted in the prediction of a new, silicon-based molecule that could be used for commercial solar energy conversion.
- The substance was then synthesized and shown to have exceptional light-absorbing properties and thermal stability
- The new material is much better than amorphous silicon; compares well with crystalline silicon; can be synthesized in a straightforward manner; and is composed entirely of elements abundant in nature.
- NERSC resources were used to model the defects in the crystal structure and the spatial distribution of charge carriers – two key characteristics for solar energy conversion.

On the Cover: Computation has helped engineer an inexpensive new silicon-based semiconductor for solar Energy conversion. The material has a promising "band gap" for visible light absorption and electron/hole mobilities much superior to those of amorphous silicon, a system already in use in solar cell devices.

Energy & Environmental Science, August 2014

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(G. Galli, U.Chicago)

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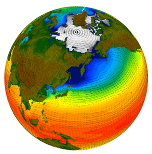
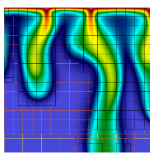
About the Title Slide Images

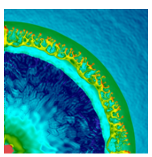
Evolution of electrical current density, parallel to magnetic field, in the Pegasus Toroidal Experiment; provided by John O'Bryan and Carl Sovinec, University of Wisconsin-Madison; Sponsored by Office of Fusion Energy Sciences



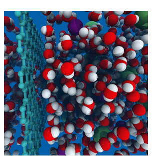
A single month from a simulation of the 20th century by the CCSM capturing wind directions, ocean surface temperatures, and sea ice concentrations. Image courtesy Gary Strand (NCAR) and copyright University Corporation for Atmospheric Research. Sponsored by Office of Biological and Environmental Research



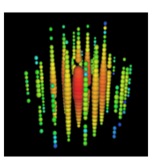
Simulation of density-driven flow for CO_2 storage in saline aquifers. Shown is a snapshot of the CO_2 concentration after onset of convection overlayed on the AMR grid. Image courtesy of George Pau and John Bell (LBNL). Sponsored by Office of Advanced Scientific Computing Research.



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

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