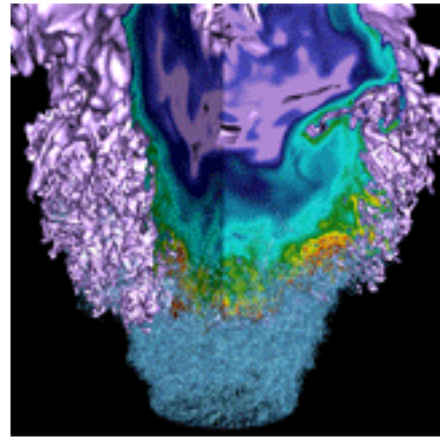
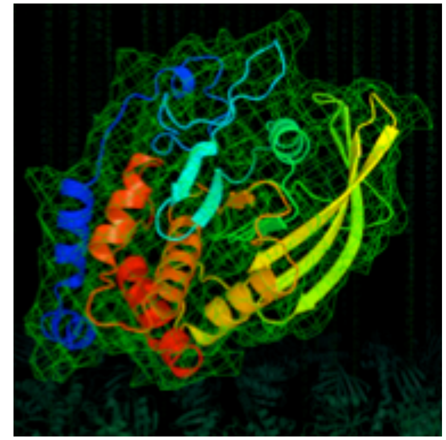
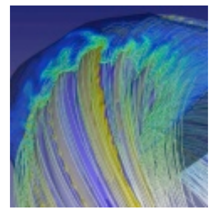
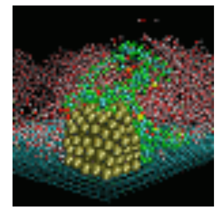
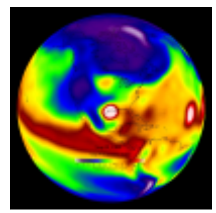
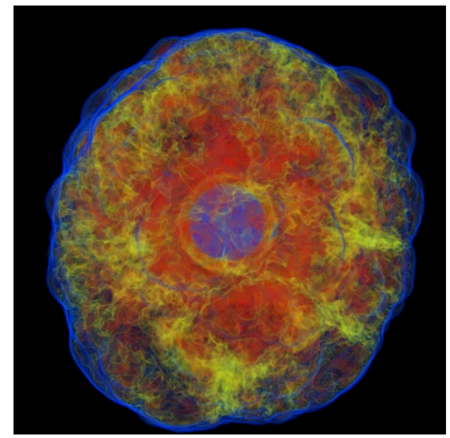
NERSC Science Highlights



NERSC

Selected User Accomplishments

June 2013

U.S. DEPARTMENT OF ENERGY | Office of Science

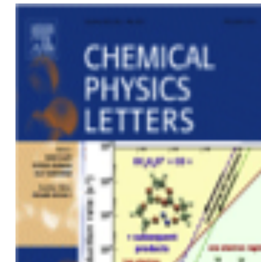
BERKELEY LAB
Lawrence Berkeley National Laboratory

NERSC User Science Highlights

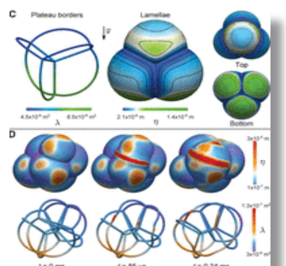
NERSC

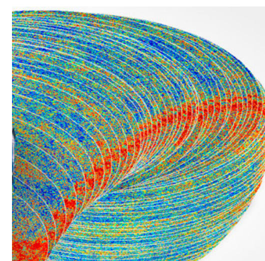
Climate
Spread of taller vegetation could exacerbate warming in northern latitudes
(C. Bonfils, LLNL)

Materials
Using computation to improve lithium batteries
(K. Leung, Sandia Nat'l Labs)



Math and Computing
New method improves simulations of complex, multiphase phenomena.
(J. Sethian, UCB / LBNL)

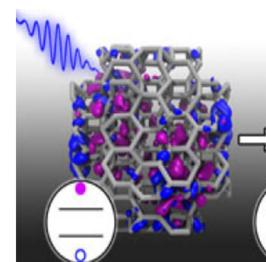




High Energy Physics
PLANCK mission changes fundamental understanding of universe's age and composition
(J. Borrill, LBNL)

Biological Science
Electronic structure computation at NERSC helps explain how our biological clocks work
(V. Batista, Yale)

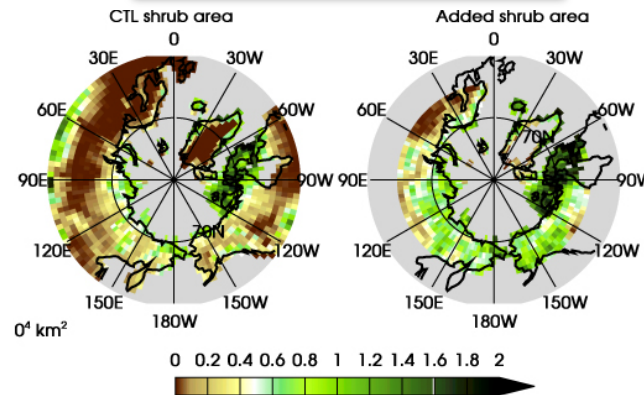
Materials
Studies suggest the possibility of solar cells with efficiencies much higher than that available today
(J. Galli, UC Davis)



Tundra Bushes Add Fuel to Northern Thaw

NERSC

- **Finding: Spread of taller vegetation could exacerbate warming in northern latitudes**
- **Simulations at NERSC are the first to investigate long-term climate effects of shrub expansion into the tundra**
  - Community Climate System Model runs analyzed expansion of existing short shrubs in tundra and invasion of taller shrubs due to warming
  - Two key effects: greater surface sunlight absorption and plant-induced increase in atmospheric moisture content
- **Suggests that tall shrub invasion will systematically increase soil temperature, shorten the freezing season, and trigger permafrost degradation**
- **Article chosen as an Institute of Physics (IOP) Select Paper**

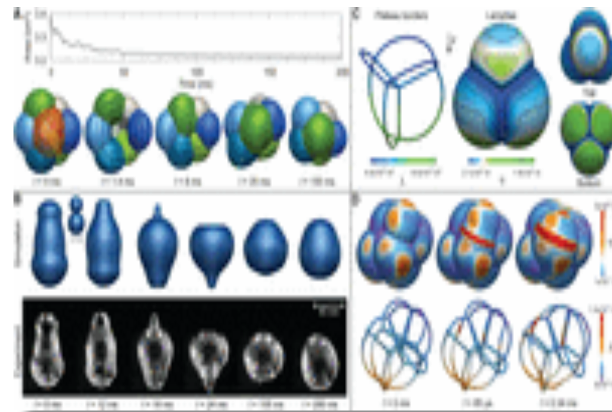


Simulations suggest that an invasion of shrubs can further warm the northern high latitudes

Environmental Research Letters
Vol 7, 011005 (2012)

New Method Improves Simulations of Foams, Membranes, Detergents, and More

- **Allows simulation of many complex phenomena that cover a wide range of time and length scales:**
  - How grains develop in metals and ceramics;
  - Formation bubbles and foams, which have applications in industry and materials design
  - Design of fire retardants
- **Awarded "Cozzarelli Prize" by National Academy of Science for papers that reflect scientific excellence and originality**
- **Could help modeling of industrial processes where liquids mix or in the formation of solid foams such as those used to cushion bicycle helmets.**



Computer simulation of soap bubble formation. Experimental image is in the lower left. The new method, developed in part using NERSC resources, allows computer modeling of processes that take place over six orders of magnitude in space and time.

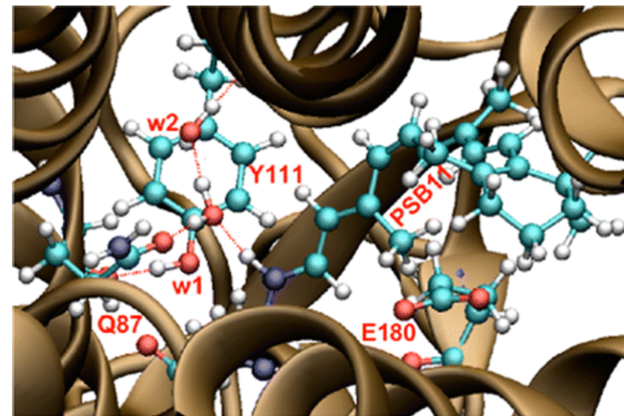
Proc. National Academy of Science December 6, 2011
Journal of Computational Physics 231 (2012) 6051–6085
Science 10 May 2013

PI: R. Saye, J. Sethian (UC Berkeley/LBNL)

Using Computation to Understand the Basis of Circadian Rhythm

- **A quantum/molecular mechanics study done at NERSC has revealed the structure of the molecule *melanopsin*, a protein believed to be at the heart of regulating the biological clock.**

- **The molecule's structure had not been pinned down by any experimental method.**
  - Melanopsin is present in the eye, but is not involved in vision. Instead, it responds to light and and sends a signal to a region of the brain known to be at the heart of matching hormones to the natural cycle of a 24-hour day.
  - The new study explains how the molecule's structure relates to its photo-activation, which has been a fundamental research challenge.
- **Similar molecules are sometimes used for photosynthesis; this work could help produce "bioinspired" materials for solar energy conversion.**



Structure of the nonvisual ocular photoreceptor melanopsin, which is found in cells of the retina, absorbs blue light, and triggers the "biological clock" of mammals by activating a small region of the brain that regulates neuronal and hormonal rhythms over 24-h cycles.

Journal of the American Chemical Society 2012, 134 (48), pp 19536–19539

U.S. DEPARTMENT OF ENERGY | Office of Science

BES

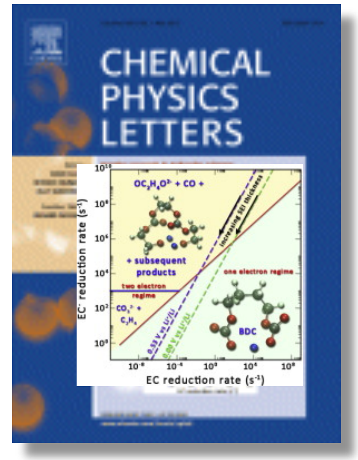
PI: V. Batista (Yale)

BERKELEY LAB

Computation Improves Lithium Batteries

NERSC

- **Accomplishment: Detailed computational study accurately predicts chemical decomposition products during battery charging.**
- **Significance: Most commercial lithium ion batteries use materials that decompose on the electrode surface. One particular material, "Ethylene Carbonate (EC)," is unique in its ability to form a stable layer that prevents further decomposition.**
- **How such layers form has been largely unclear.**
- **Understanding EC and its electrochemical behavior contributes to the selection of additives and/or coatings that inhibit early aging, degradation and failure of lithium-ion batteries.**



On the Cover: A NERSC startup allocation leads to a "Frontiers Article" and journal cover; included are computational results that may lead to extensive revision of existing theories for chemical decomposition in lithium ion batteries.

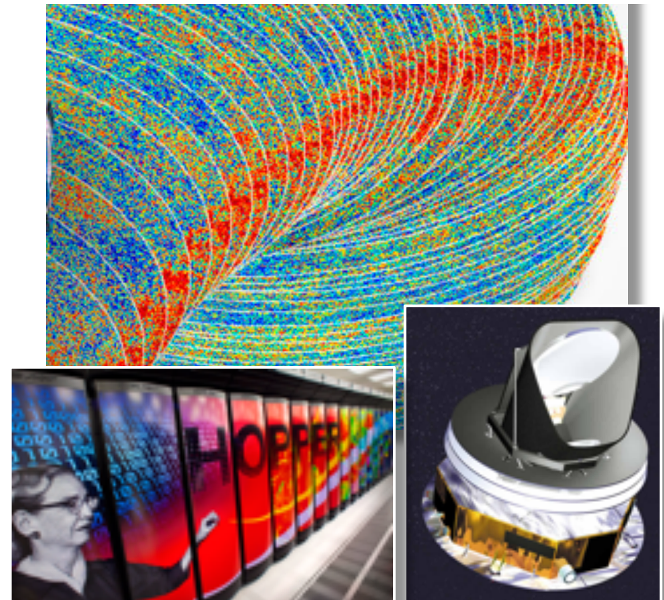
NERSC Helps Planck Mission Expose Ancient Light

NERSC

- **Using a sensitive space telescope and NERSC supercomputing, scientists from the international Planck collaboration have have created the most detailed maps ever of relic radiation that still exists from the Big Bang.**
- **Preliminary results suggest that the universe is 80 million years older than we thought, with more matter and less dark energy.**
- **NERSC played a crucial role in the findings allowing *hundreds* of users to analyze the data.**
  - Simulations running on more than 10,000 processors using over 10 million compute hours.
- **Said to be "a goldmine containing stunning confirmations and new puzzles," with "data that will form the cornerstone of our cosmological model for decades to come."**

The New York Times

Universe as an Infant: Fatter Than Expected and Kind of Lumpy

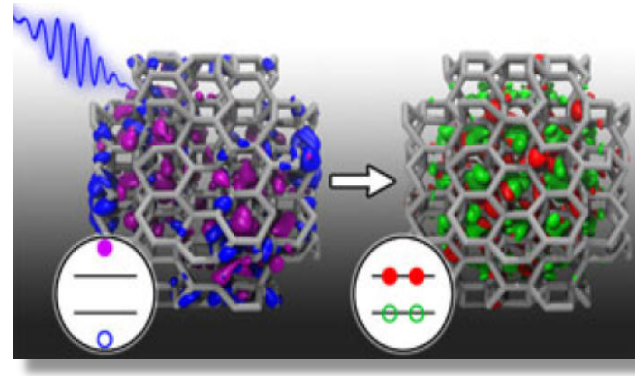


Some of the many thousands of simulations that have been run using a NERSC supercomputer (left) to analyze data from the Planck satellite (right)

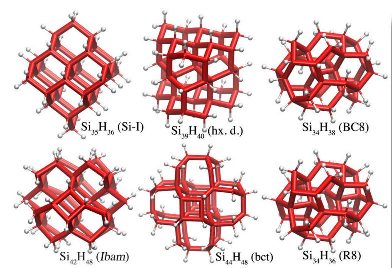
Studies Suggest Super-Efficient Solar Cells

- **Simulations done at NERSC suggest that using an exotic form of silicon could substantially improve the efficiency of solar cells.**

- **The NERSC-allocated (NISE) project examined electronic and optical properties of silicon nanoparticles generated using high-pressure methods.**
- **Solar cells currently in use generate one "electron-hole" pair per incident photon of light, making them capable of a theoretical maximum efficiency of only 33%.**
- **The NERSC-facilitated discovery of processes leading to generation of <u>multiple</u> electron-hole pairs per photon could extend efficiency to 42%, possibly even 70%.**



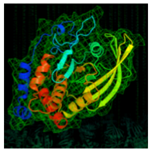
Simulations done at NERSC show that when light (blue wave on left) hits a crystal of a high-pressure form of silicon, it releases two electron-hole pairs (red circles/ green rings). Below are the nanoparticle structures studied.



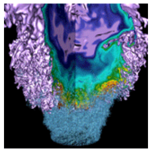
Phys. Rev. Lett. 110, 046804 (2013)

S. Wippermann, J. Galli (UC Davis)

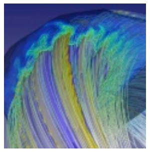
About the Title Slide Images



Snapshot from a simulation of a protein folding to its preferred shape, one of many such simulations done at NERSC as part of the Dynameomics Project (Valerie Daggett, U. Washington)

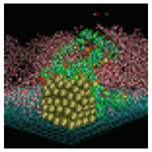


Detailed structure of a flame from a Low swirl burner combustion simulation. Image courtesy of John Bell, LBNL.

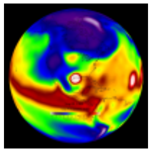


Representation of a plasma from a magnetic fusion energy simulation. Magnetic fields within the plasma are represented as white lines and the temperature is shown as blue/yellow surface (Linda Sugiyama, MIT)

Simulation of the blast resulting from a core collapse supernova. This image, generated by NERSC's Hank Childs, was carried on the TIME Magazine web site following the publication of these simulations.



Various components of a fuel cell from a simulation to help improve the fuel cell membrane (PNNL)



Plot of precipitation on Sept. 9, 1900 from the 20th Century Reanalysis Project, Gilbert Compo (U. Colorado)

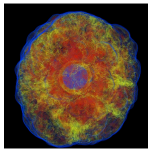


Image depicting a central engine model used in simulation of core-collapse supernovae and long gamma-ray bursts, from Christian Ott (Caltech)

National Energy Research Scientific Computing Center