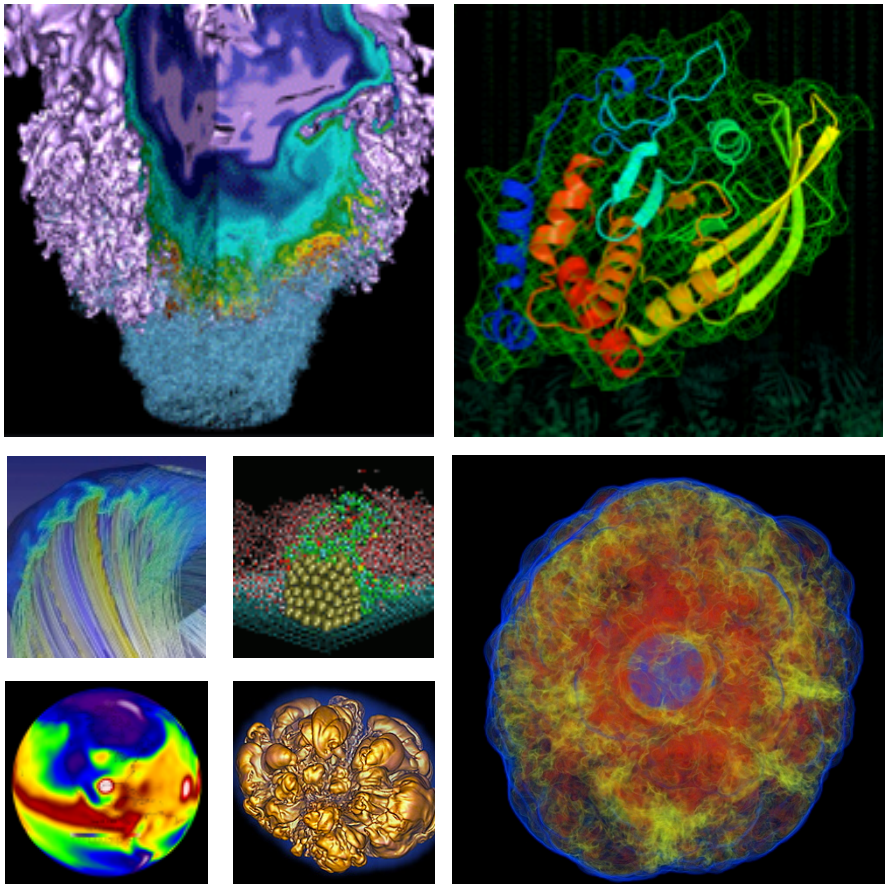
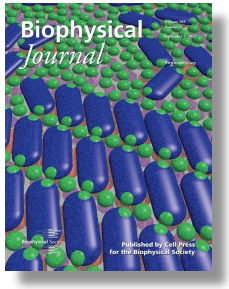
NERSC Science Highlights



Selected User Accomplishments

December 2013

NERSC User Science Highlights

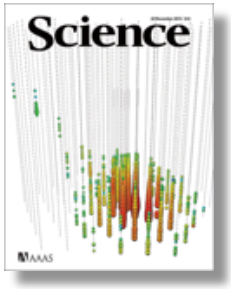


Life Sciences

Model shows arrangement of proteins in photosynthetic membranes
(P. Geissler, UC Berkeley)

Nuclear Physics

Wherein Bert 'n' Ernie are followed by the even more energetic "BigBird"
(L. Gerhardt, NERSC)

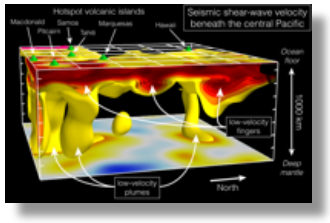


Energy

Simulation couples with experiment to boost bioenergy research
(L. Petridis, ORNL)

Astrophysics

Helping to answer the question, "Are Earths Rare?"
(E. Petigura, UC Berkeley)



Geoscience

Hotspot volcanoes explained
(B. Romanowicz, UC Berkeley)

Materials

NERSC enables simulations that mimic some key features of carbonate crystallization.
L. Hedges (LBNL)

Model Shows Arrangement of Proteins in Photosynthetic Membranes

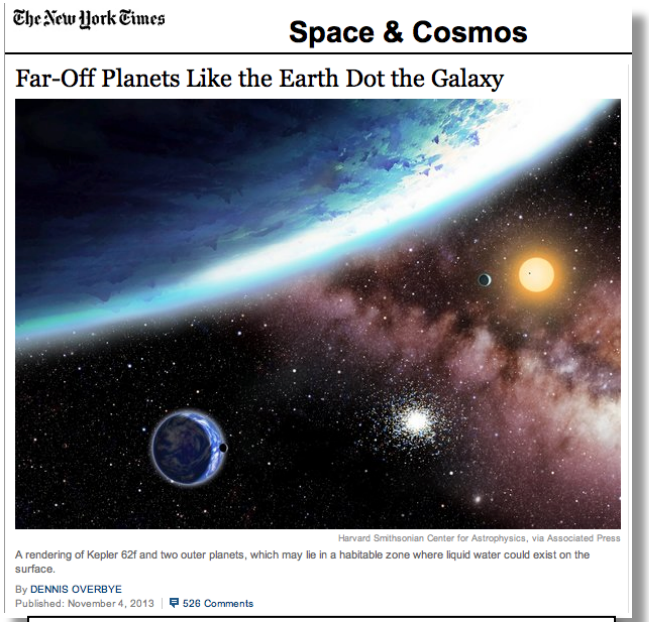
- Simulations show coexistence of crystalline and fluid phases in photosynthetic membranes.
- Significance: Photosynthetic efficiency relies on precise spatial organization of certain pigment-proteins but how the proteins know to arrange themselves is unclear. This work provides chemical understanding of the rearrangement pathways.
- General goal is to understand how photosynthesis works in plants to help improve man-made systems that could absorb light and generate chemical fuels.
- The computing challenge involves being simple enough to capture huge length scales, yet rich enough to provide detailed thermodynamic predictions that could affect photosynthetic function.

On the Cover: The image shows the structural arrangement of proteins in a statistical-mechanical model of a grana stack, which is part of the photosynthetic light-harvesting system

Biophysical Journal 105 (5), 2013

How Many Earths Are There?

- **Accomplishment: Three-year analysis of space observatory data suggests that one out of every five sunlike stars in the galaxy has a planet the size of Earth circling it with conditions that might permit surface liquid water.**
- **Significance: Provides important evidence regarding a fundamental scientific question - whether planets suitable for biochemistry are common or rare in the universe.**
- **Software developed for this study has the potential to perform very high quality analysis of future DOE wide-field digital data from DES and LSST surveys, enhancing Cosmic Frontier science.**
- **Finding that Earth- and Neptune-size planets are ten times more common than Jupiter-size planets, challenges existing theories of planet formation and migration**



The New York Times

Space & Cosmos

Far-Off Planets Like the Earth Dot the Galaxy

Harvard Smithsonian Center for Astrophysics, via Associated Press

A rendering of Kepler 62f and two outer planets, which may lie in a habitable zone where liquid water could exist on the surface.

By DENNIS OVERBYE

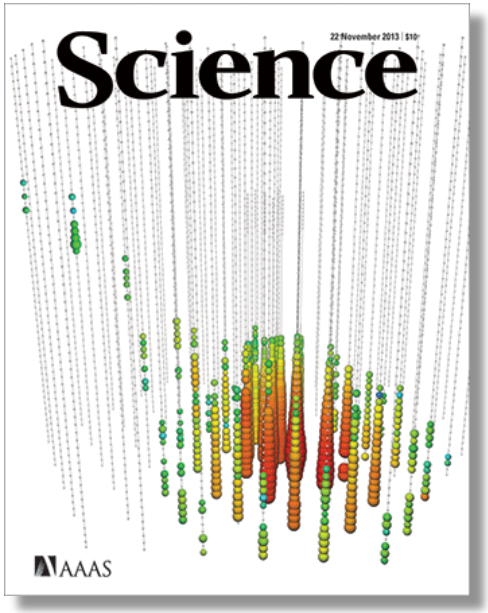
Published: November 4, 2013 | 526 Comments

News of The Times: entry describing graduate student Erik Petigura's NERSC results appeared in the New York Times on November 4, 2013. Image shows a rendering of 3 outer planets that may lie in a habitable zone where liquid water could exist on the surface

Proceedings of the National Academy of Sciences November 4, 2013

NERSC Supports Physics World Breakthrough of the Year 2013

- Analysis of more recent data from the IceCube detector has revealed a new neutrino event with almost double the energy of the PeV events reported in November.
- NERSC Carver, PDSF, and HPSS resources were used for Monte Carlo simulation and data analysis to sift out neutrino signals from cosmic “noise” in the IceCube observations.
- Significance: NERSC resources are helping to usher in an era of "neutrino astronomy" where particles are used instead of radiation to study the most energetic engines in the cosmos.
- The energies of the neutrinos detected are almost 100 times the energy of the most energetic collision achievable in the Large Hadron Collider.



On the Cover: IceCube detector (pictured) found the first solid evidence for cosmic neutrinos, subatomic particles created in violent events at the far reaches of the universe

Science Nov. 22, 2013

Simulation Couples with Experiment to Boost Energy Research

- **Accomplishment: Supercomputing and neutron scattering combined to reveal two fundamental processes in steam pretreatment of biomass.**
- **Motivation: Although woody biomass is abundant, current processes for using it are expensive due to recalcitrance of the plant cell walls.**
- **Challenge: Molecular-level understanding of bioprocesses that span huge time and spatial scales, from atomistic levels to larger cellulose and lignin polymer structures, is required.**
- **Significance: The physical details revealed in this work could enable scientists to engineer improved pretreatment processes and ultimately bring down the costs of biofuel production; also: important synergy between theory and experiment and collaboration between users of two key DOE facilities (SPNS and NERSC)**

On the Cover: graphical representation of lignocellulosic biomass based on supercomputer models

RSC Green Chemistry, 2014, 16, 63-68

Simulation Captures the Essence of Carbonate Crystallization

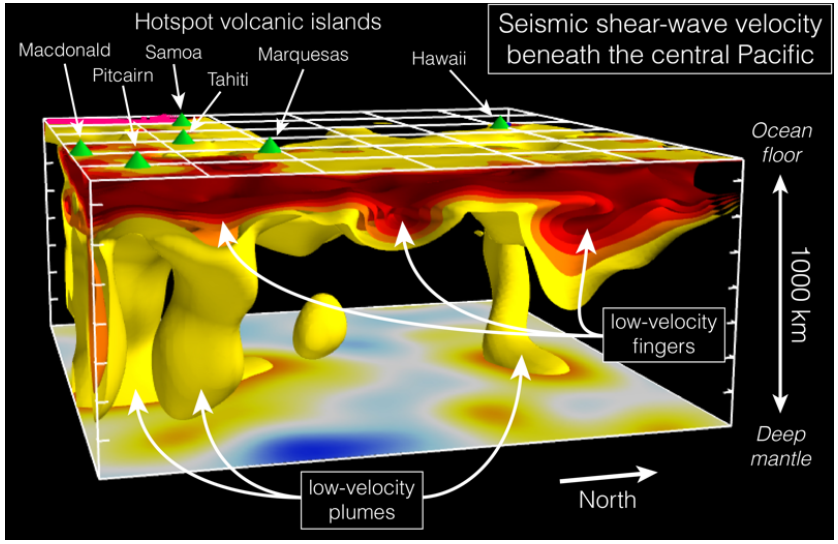
- This study concerns nucleation (the initial part of crystal formation) in porous media, which becomes important when CO_2 is sequestered underground forming limestone crystals.
- Result: pore-mediated nucleation generally happens in two-steps: nucleation within the pore and then nucleation from the filled pore into solution. Nucleation is fastest from pores of a specific size and is markedly slower for sizes much larger or smaller than this sweet spot.
- Important because it suggests how to speed nucleation, to better ensure that carbon capture underground is rapid and permanent.
- NERSC resources enabled simulations in a large phase space (of pore size and shape, and thermodynamic conditions), allowing statistically significant predictions under conditions relevant to experiment.

On the Cover: illustration of nucleation from an ensemble of pores of different size etched into a substrate.

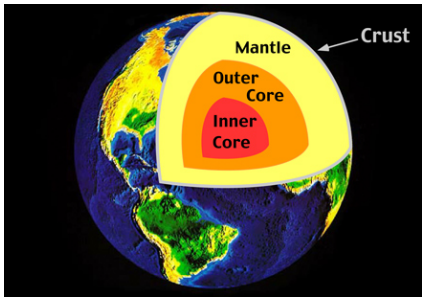
RSC Soft Matter, 2013, 9, 9763-9766

NERSC Project Discovers 'Fingers' of Heat that Help Explain the 'Plumbing' of Earth's Mantle

- Computed images of seismic activity reveal previously-unknown fingerlike structures carrying heat from deep beneath Earth's oceanic plates.
- Helps explain "hotspot volcanoes" that give birth to island chains such as Hawai'i and Tahiti.
- NERSC Director's Reserve (NISE) allocation, 2012-2013
- NERSC resources used to compare seismic waves from a new model of movement within earth's mantle with those from hundreds of earthquakes recorded at locations around the world



3-D rendering of the top 1,000 km below the Pacific Ocean. Slow-moving seismic waves, hotter than surrounding material, interact with plumes rising from the mantle to affect the formation of hotspot volcanic islands.



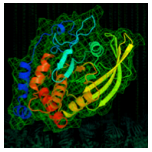
Science 2013 11 October

Science AAAS

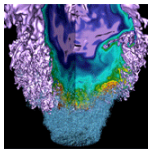
U.S. DEPARTMENT OF ENERGY | Office of Science | BES

B. Romanowicz, S. French (UC Berkeley)

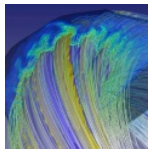
About the Title Slide Images



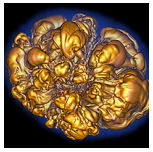
Snapshot from a simulation of a protein folding to its preferred shape, one of many such simulations done at NERSC as part of the Dynameomics Project (Valerie Daggett, U. Washington)



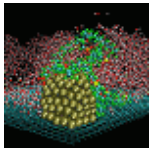
Detailed structure of a flame from a Low swirl burner combustion simulation. Image courtesy of John Bell, LBNL.



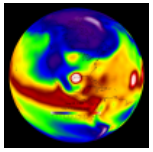
Representation of a plasma from a magnetic fusion energy simulation. Magnetic fields within the plasma are represented as white lines and the temperature is shown as blue/yellow surface (Linda Sugiyama, MIT)



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)

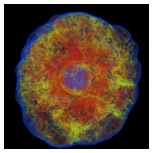


Image depicting a central engine model used in simulation of core-collapse supernovae and long gamma-ray bursts, from Christian Ott (Caltech)

National Energy Research Scientific Computing Center