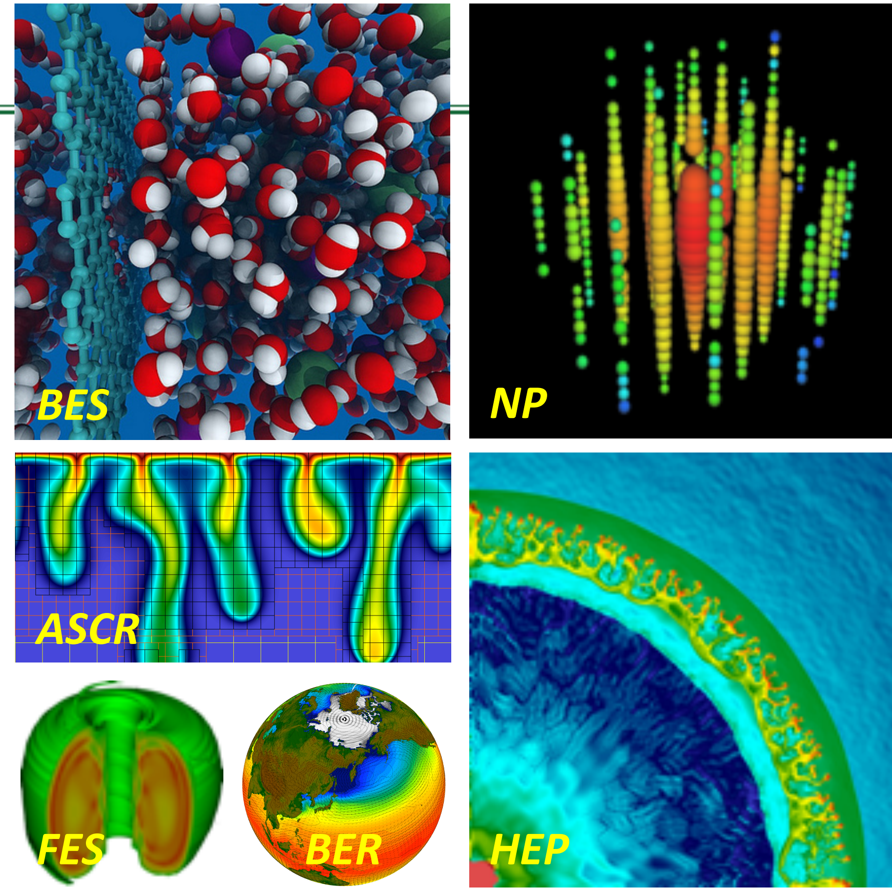
NERSC Science Highlights



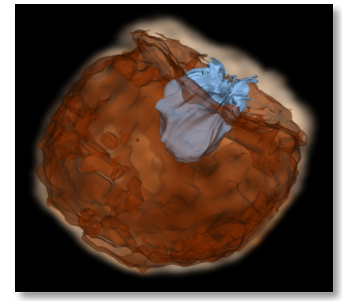
Selected User Accomplishments

June 2015

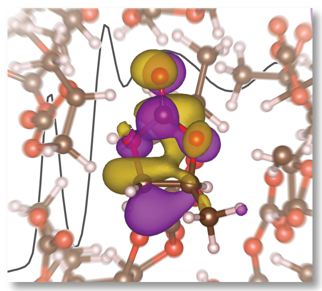
NERSC User Science Highlights

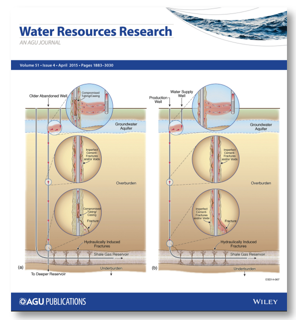
Materials
Simulations reveal structural defects from irradiation that can't be seen in experiments
(R. Devanathan, PNNL)

Astrophysics
Sophisticated data analysis pipeline allows rapid detection of a rare cosmic event
(P. Nugent, LBNL)

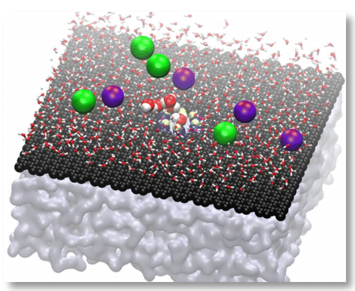


Chemistry
Predictions combine with experiment data to provide new insight into chemistry relevant to batteries and water
(R. Saykally, UCB)



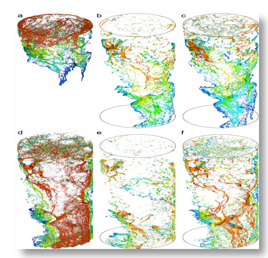


Environment
Numerical simulations are assessing the impact of shale gas reservoir fracture on groundwater quality
(G. Moridis, LBNL)



Chemistry
Multiple computational techniques are used to help explain molecular self assembly and water transport across novel membranes
(A. Striolo, U. Coll. London)

Environment
Simulations of underground flow can accurately capture pore-scale details over large 3-D volumes
(T. Scheibe, PNNL)



Atomistic Models Aid Radiation Damage Studies

Scientific Achievement

Simulations reveal structural defects from irradiation that are barely detectable by electron microscopy

Significance and Impact

Comprehensive understanding of radiation damage in materials is essential for nuclear waste isolation and development and optimization of nuclear fission/fusion reactors.

Research Details

– Classical Molecular Dynamics simulations provide information on density changes, defect evolution, chemical bonding environments, and structural stability in irradiated ceria. This work contributes to our understanding of how energetic particles from radiation slow down via interaction with the material they move through. Insights from this work can inform future studies of irradiated nuclear fuel and aging of spent nuclear fuel during dry cask storage for decades.

On the Cover: Results from a Molecular Dynamics simulation of the effects of irradiation damage in the compound ceria, which serves as a uranium oxide fuel surrogate. Blue spheres represent the process by which highly energetic particles from nuclear fission slow down, creating damage tracks that result in structural defects and dislocations.

R. Devanathan, et al., J. Mater. Res., Vol. 30, No. 9, May 14, 2015

New Insights from Method that Uses Supercomputers to Analyze Synchrotron Experiment Data

Scientific Achievement

Predictions combine with X-ray absorption data to provide key insights in geological, biological, and energy processes

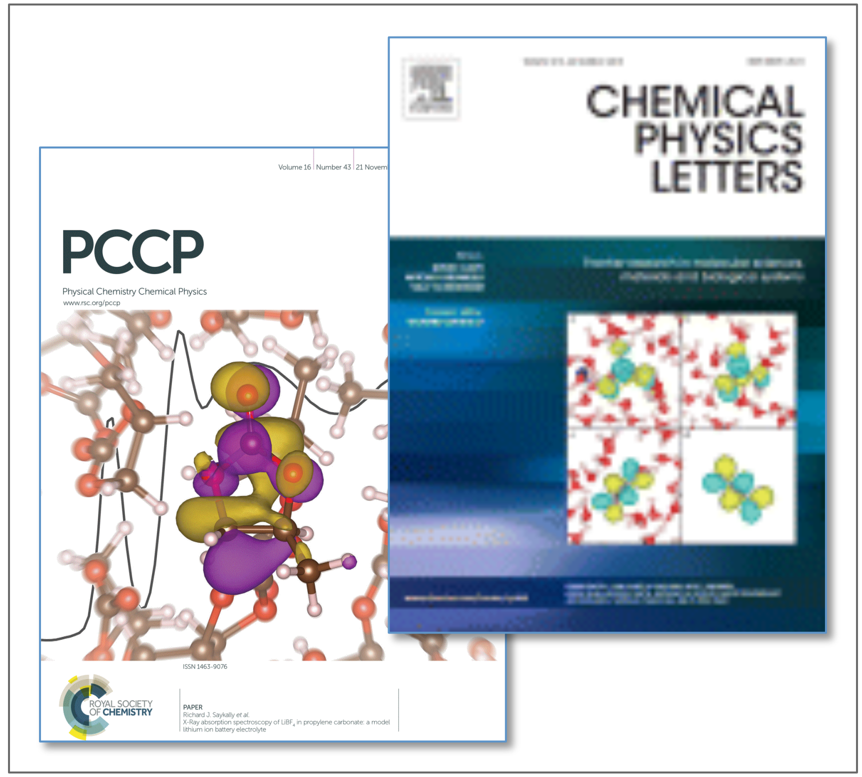
Significance and Impact

Study of hydration properties of carbonic acid will benefit the development of carbon sequestration and mitigation technologies; study of a model lithium electrolyte opens a possible avenue to better lithium ion batteries

Research Details

- Molecular dynamics and density functional theory simulations provided interpretation of $LiBF_4$/propylene carbonate spectroscopy data and revealed the lithium ion solvation structure in this model battery electrolyte
- A similar effort yielded the hydration structure of the extremely short-lived aqueous carbonic acid (H_2CO_3) system that is the centerpiece of the global carbon cycle.

Saykally, David Prendergast, et al,
Phys. Chem. Chem. Phys 2014,
Chemical Physics Letters 2014



On the Covers: Results from two studies using supercomputer simulation to interpret data from experiments that probe the local electronic environment of important materials. Both works represent a collaboration between the Molecular Foundry, NERSC and the Advanced Light Source (ALS), all DOE Office of Science national user facilities hosted at Berkeley Lab.

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

PI: R. Saykally (UC Berkeley)
1.9 M Hours

NERSC

Simulation Insights into Water and Soft Matter

Scientific Achievement

An arsenal of computational techniques yields key information on how large molecules self assemble on non-uniform surfaces and how chemically modified graphene can act as a superior water desalination device.

Significance and Impact

Concepts revealed in these studies will help the design and engineering of advanced materials that are central to the increasingly important water-energy nexus.

Research Details

- Equilibrium dissipative particle dynamics simulation of surfactants adsorbed on model heterogeneous surfaces reveal previously-unreported structures
- MD simulations show that hydroxylated graphene pores exclude Cl^{-} ions even at moderate ionic strength.

On the Covers: Left: Molecular Dynamics simulation results that could be useful for the design of water desalination membranes. Right: Simulation results that could be useful for the manufacture of new coatings and other materials

A. Striolo, et al
Langmuir 2013, 29, 11884–11897
J. Phys. Chem. B 2015, 119, 5467–5474

Astronomers Observe a Supernova Colliding with its Companion Star

Scientific Achievement

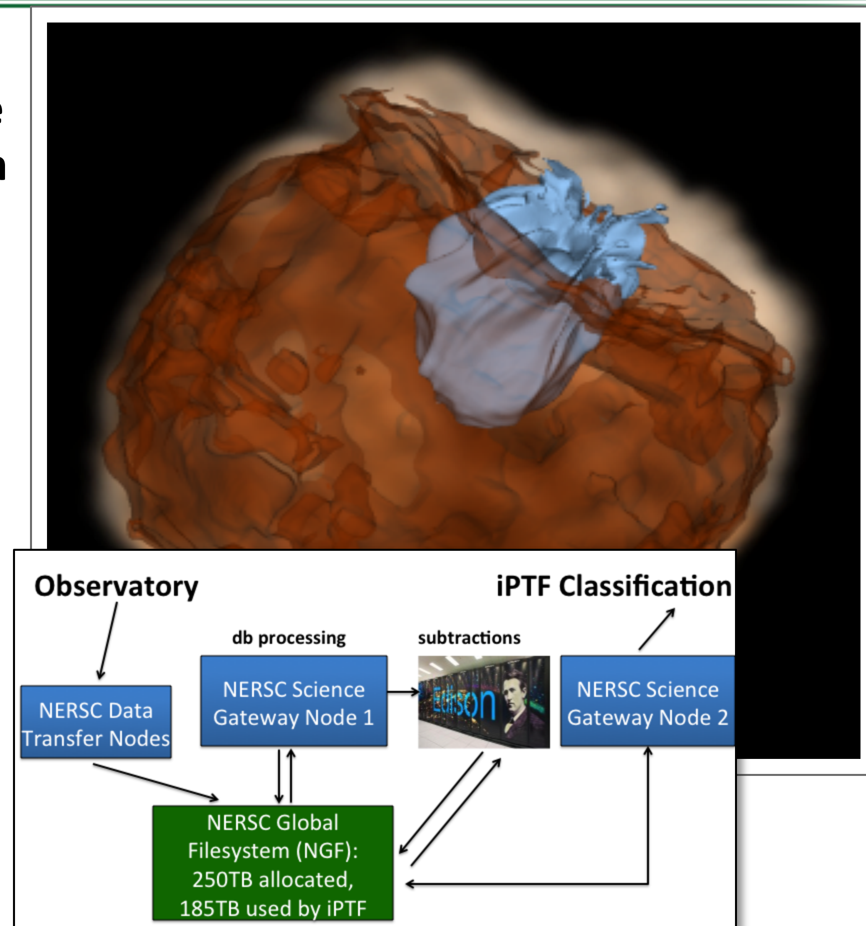
NERSC machine-learning data analysis pipeline allowed the first ever observation of light from a supernova slamming into a neighboring star.

Significance and Impact

Although thousands of Type Ia supernovae have been found, how they form has been unclear. Results from this work lend support to one of two competing formation theories.

Research Details

- Original theoretical computation predicting that this kind of observation might be possible was also done at NERSC back in 2010 by UC Berkeley Prof. Daniel Kasen.
- The intermediate Palomar Transient Factory (iPTF) analysis pipeline found the light signal from the supernova just hours after it ignited in a galaxy about 300M light years away from Earth. iPTF depends on NERSC computation and global storage resources.



Simulation of the expanding debris from a supernova explosion (shown in red) running over and shredding a nearby star (shown in blue). Image credit: Daniel Kasen, Berkeley Lab/ UC Berkeley. Inset shows NERSC contribution to iPTF processing pipeline

Nature | Vol521 | May 21, 2015
The Atrophysical Journal 708:1025–1031, 2010 January 10

PI: P. Nugent (LBNL)
250k Hours

Assessing Potential Impact of Fracking on Drinking Water

Scientific Achievement

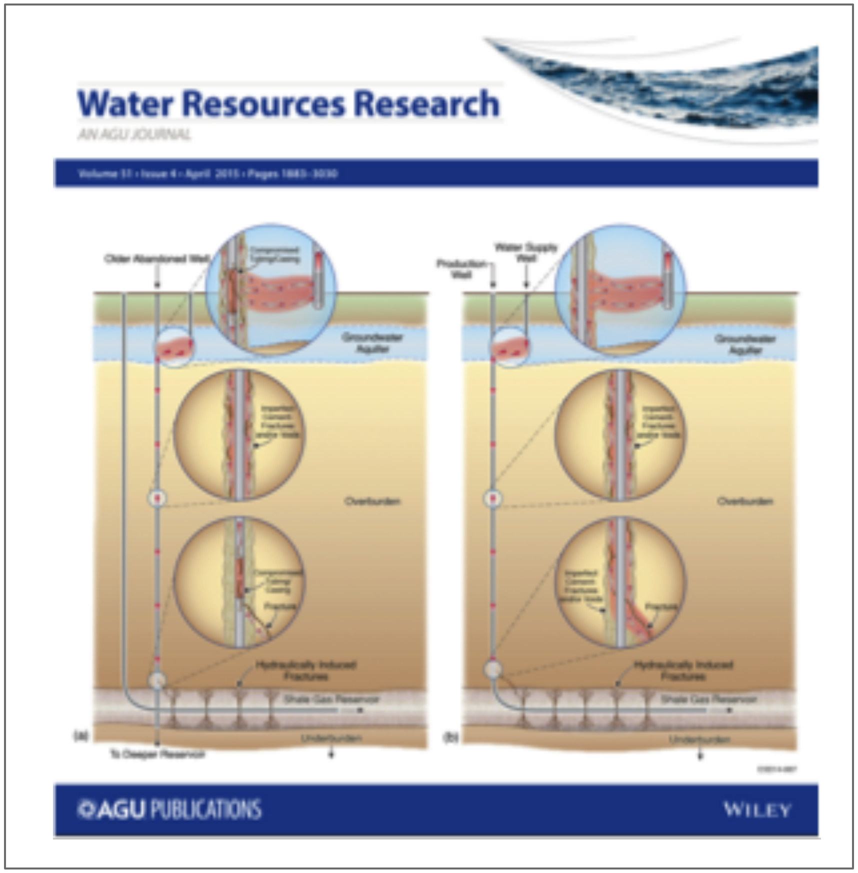
EPA-funded study used numerical simulation to investigate geomechanical failure scenarios that might allow potential gas and water transport between a tight-gas reservoir and an overlying fresh-water aquifer

Significance and Impact

Hydraulic fracturing of oil/gas reservoirs may create permeable pathways between the reservoir and shallower fresh-water aquifers, resulting in groundwater contamination

Research Details

- Used the TOUGH code that describes two-phase nonisothermal flow of a water and real gas mixture
- Key factors driving short-term transport of gas include high permeability for the connecting pathway, reservoir pressure, and the overall volume of the connecting feature



On the Cover: schematic showing two possible failure scenarios whereby reservoir stimulation could create environmental threats through creation of a pathway connecting the stimulated reservoir with shallower fresh-water aquifers, thus resulting in the contamination of potable groundwater by escaping hydrocarbons or other reservoir fluid.

AGU Water Resources Research 51, 2543–2573, 2015
doi:10.1002/2014WR016086

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

PI: G. Moridis (LBNL)
1.5M Hours

NERSC

Expanding the Impact of Pore-scale Simulations

Scientific Achievement

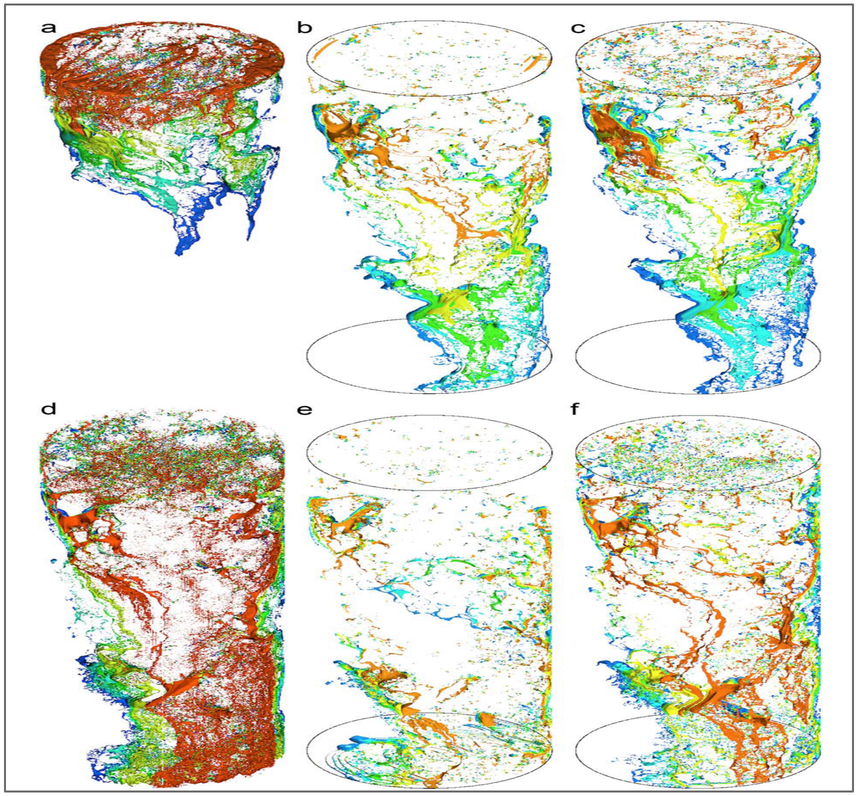
Numerical simulations of underground flow are now able to accurately capture pore-scale details over large 3-D volumes

Significance and Impact

By bridging the gap between pore scale (10s of microns—the size of solid soil grains and pore spaces) and true field scales, simulations will be able to provide accurate assessments of groundwater contamination risk and effective remediation strategies.

Research Details

– Performed multiscale simulations over a decimeter-scale volume of natural porous media with a wide range of grain sizes using a combination of Stokes flow in large open pores and Darcy-like flow in porous solid regions and compared computed hydraulic conductivity, tracers, and breakthrough curves with column experiments containing the same sample, imaged with computed tomography.



Visualizations of tracer concentration at two simulation times (top images: 55 min, bottom images 515 min) for three alternative simulation cases with accuracy improving going left to right. Colored surfaces are isosurfaces of concentration. Images c and f (on the right) utilize a method that resolved porous solids with pores smaller than the experiment imaged resolution and are the most accurate representations.

Scheibe, et al., AGU Water Resources Research February 2015

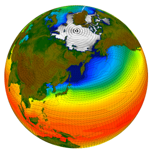
U.S. DEPARTMENT OF ENERGY | Office of Science BER

PI: T. Scheibe (PNNL)
500k Hours

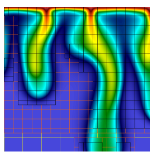
NERSC

About the Title Slide Images

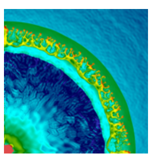
Evolution of electrical current density, parallel to magnetic field, in the Pegasus Toroidal Experiment; provided by John O'Bryan and Carl Sovinec, University of Wisconsin-Madison;
Sponsored by Office of Fusion Energy Sciences



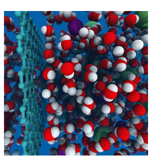
A single month from a simulation of the 20th century by the CCSM capturing wind directions, ocean surface temperatures, and sea ice concentrations. Image courtesy Gary Strand (NCAR) and copyright University Corporation for Atmospheric Research. ***Sponsored by Office of Biological and Environmental Research***



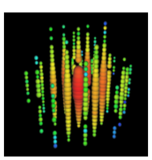
Simulation of density-driven flow for CO_2 storage in saline aquifers. Shown is a snapshot of the CO_2 concentration after onset of convection overlayed on the AMR grid. Image courtesy of George Pau and John Bell (LBNL). ***Sponsored by Office of Advanced Scientific Computing Research.***



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