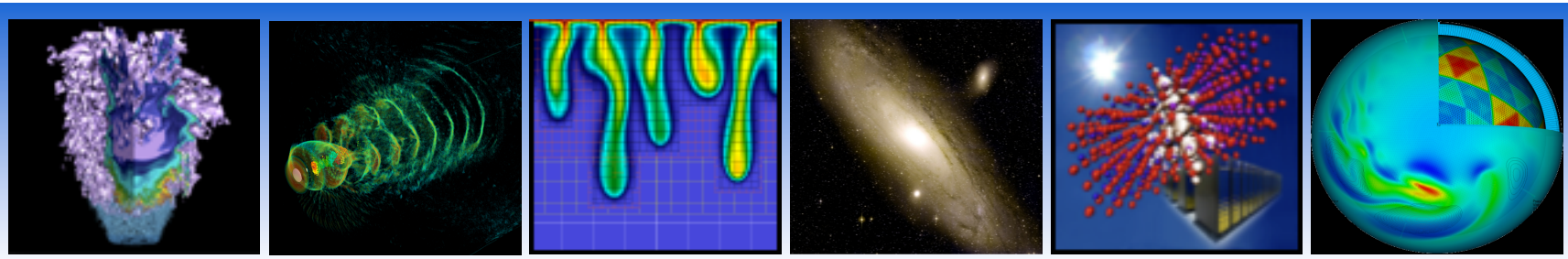

NERSC Science Highlights

A selection of scientific results produced by NERSC users.

June, 2011

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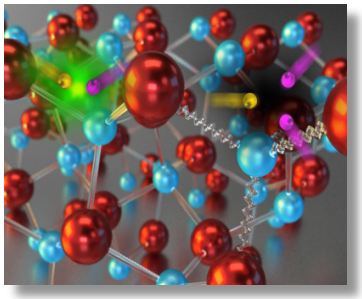
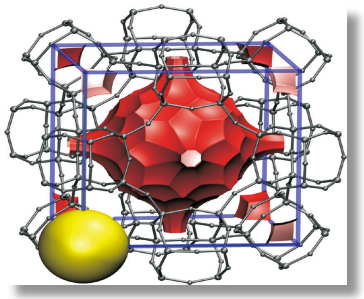
NERSC Scientific Accomplishments, Q2CY2011



Energy Resources

NERSC users have explained the cause of LED droop; this may lead to less-expensive higher efficiency LED lighting.

(Kioupakis / Van de Walle, UC SB)



Carbon Capture

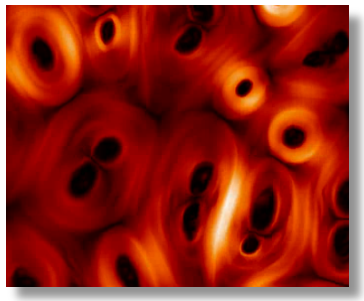
A new automated method developed at NERSC promises to speed the identification of porous materials for carbon dioxide separation.

(M. Haranczyk, LBNL)

Fusion Energy

Magnetic reconnection simulations done at NERSC along with NASA Voyager probe data help shake up prevailing views of the solar system's outer reaches.

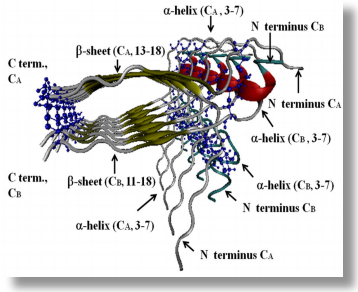
(J. Drake, U. Maryland)

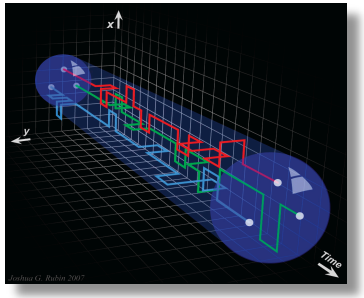


Proteins

Molecular dynamics studies show how the Insulin molecule misfolds and provide the first *in-silico* mutagensis studies of this key protein.

(A. Masunov, U. Florida)

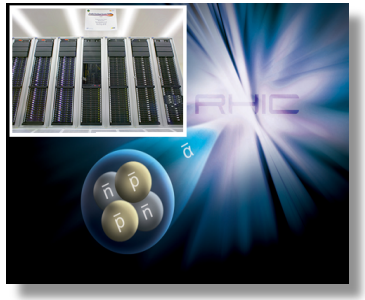




Nuclear Theory

Computations done primarily at NERSC suggest the possible existence of a so-called H-dibaryon bound state, an exotic nucleus first envisaged in 1977.

(M. Savage, U. Washington)



Nuclear Physics

The heaviest antimatter particle has been discovered with NERSC help. Antihelium-4 is likely to hold the title for decades.

(STAR Collaboration, BNL/LBNL)

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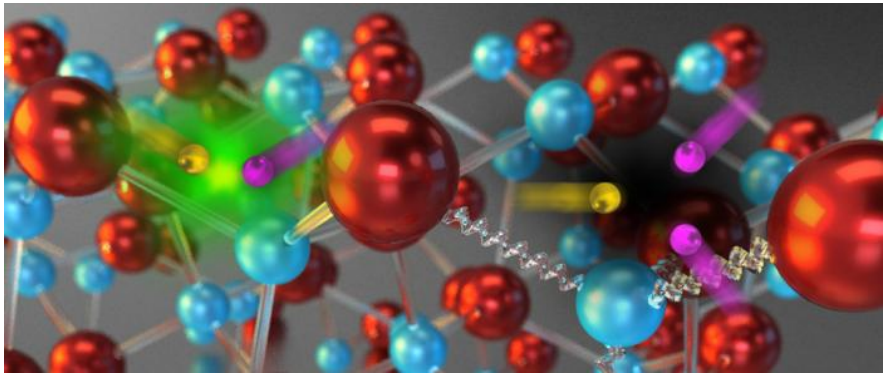
Material Science for Energy Efficient Lighting

- **LEDs are up to 3x more energy efficient than fluorescent lights and last 10x longer**
  - ***"LED droop" makes them unusable for lighting rooms, since efficiency drops when current is scaled.***
  - ***Science discovery: Indirect Auger recombination combined with carrier scattering***
- **Explains cause of droop, allowing university and industry researchers to work on solutions.**



E. Kioupakis,
C. Van de Walle
(UC Santa Barbara)

Schematic of an LED crystal. At left, an electron and electron hole recombine and release light. In Auger recombination (right) the electron and hole combine with a third carrier, releasing no photon. The energy loss is also assisted by indirect processes, vibrations in the crystal lattice shown as squiggles.

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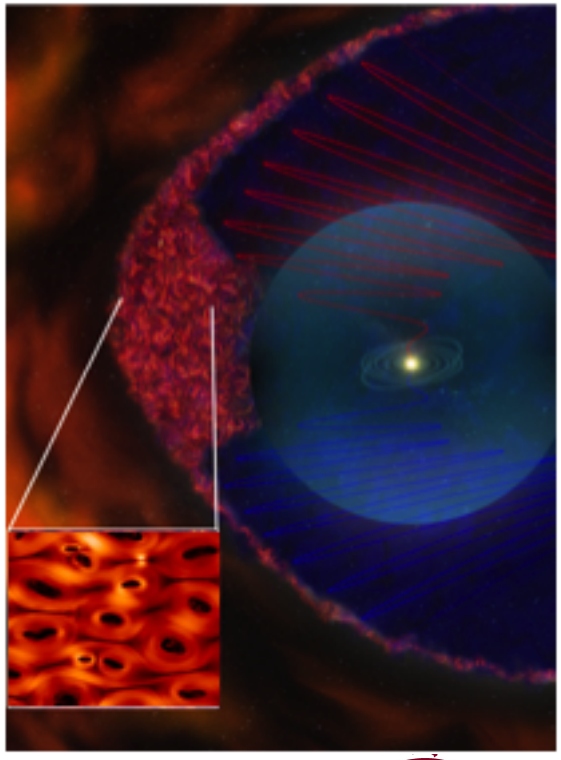
A Revised Picture of the Solar System's Edge

- **Our sun's magnetic field helps protect us from galactic cosmic rays. But is this field smooth and continuous or is it permeable?**
  - ***Science discovery: the edge of the solar system is a turbulent place, filled with a roiling sea of huge magnetic bubbles that act as particle traps.***
- **Shakes up prevailing views of the solar system's outer reaches; shows that magnetic reconnection is ubiquitous in space.**



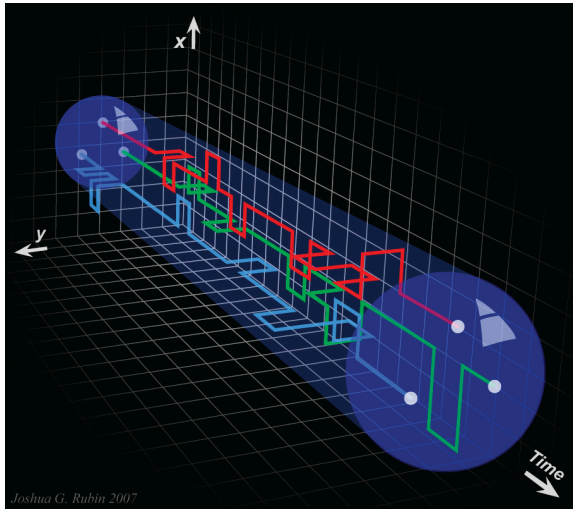
Artist's impression of the heliosphere, showing its outer region filled with magnetic bubble "foam" in red (credit: NASA). The inset shows the results of a visualization of the bubbles, 100 million miles across, created on NERSC's Franklin system.

J. Drake
(Univ. Maryland)

Evidence for Bound Dibaryon from LQCD

- **Quantum chromodynamics (QCD) is the fundamental quantum field theory describing interactions of quarks and gluons.**
  - ***Computations have provided the first reliable prediction of a two-baryon bound state starting from first principles (albeit at unphysical quark masses).***
  - ***Suggests the possible existence of the so-called H-dibaryon bound state, an exotic nucleus first envisaged in 1977.***

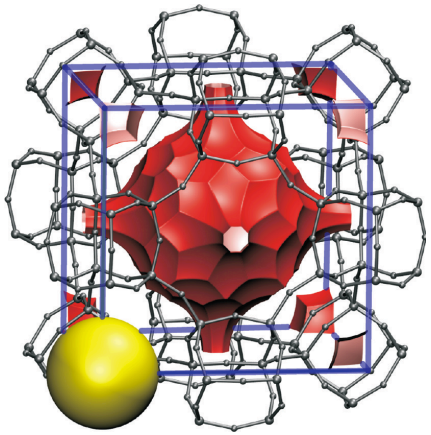
M. Savage
(Univ. Washington);
W. Detmold
(College of William & Mary)



The QCD theory is addressed numerically using Lattice QCD, which is illustrated schematically on the left, showing Monte Carlo tracks in three of the four dimensions of the space-time lattice.

Speeding Up Materials Evaluation for Carbon Capture

- **Objective: High-throughput screening of databases of porous materials to determine suitability for carbon capture**
- **Developed an automated method to bypass a manual, time-consuming, visual analysis of void spaces in porous materials, enabling high-throughput, unsupervised molecular simulations.**
  - ***NERSC resources can now be used at a larger scale to characterize many more materials***
  - ***BES/ASCR SciDAC SAP project "Knowledge Guided Screening Tools for Identification of Porous Materials for CO_2 Separations"***



Schematic of a candidate porous material showing a suitable gas capture area (center) and unsuitable areas (corners). A new method developed at NERSC can differentiate between suitable and unsuitable areas, thereby speeding up discovery of new materials.

M. Haranczyk, J. Sethian (LBNL)

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EFRC Energy Frontier Research Center for gas separations relevant to clean air technologies
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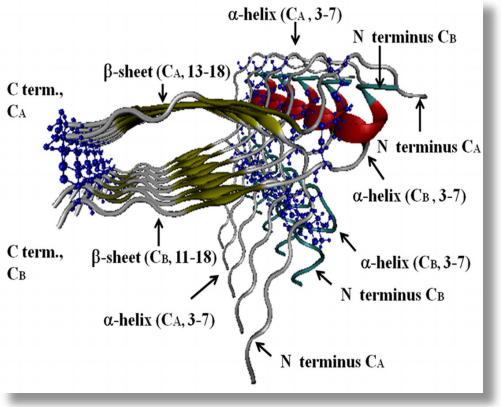
Improving Insulin via Molecular Dynamics

- **During production, transportation, and delivery the insulin protein can misfold, causing it to form fibers that are biologically inactive. How does it happen? What can be done about it?**
  - ***High-resolution molecular dynamics provides detailed atomic-level insight into structural stability and aggregation behavior***
  - ***Shows which parts of the insulin molecule cause fiber formation.***
  - ***First systematic study of mutation effects on insulin stability: in silico mutagenesis.***
- ***Could help in the design of new insulin analogs; may prove useful in the rational design of insulin aggregation inhibitors.***



Initial structure used for the insulin model showing key structural elements with helices shown as magenta ribbons, β-strands as yellow arrows, disulfide bonds indicated by blue lines, and the rest shown as loops.

Workalemahu Mikre, Artëm E. Masunov

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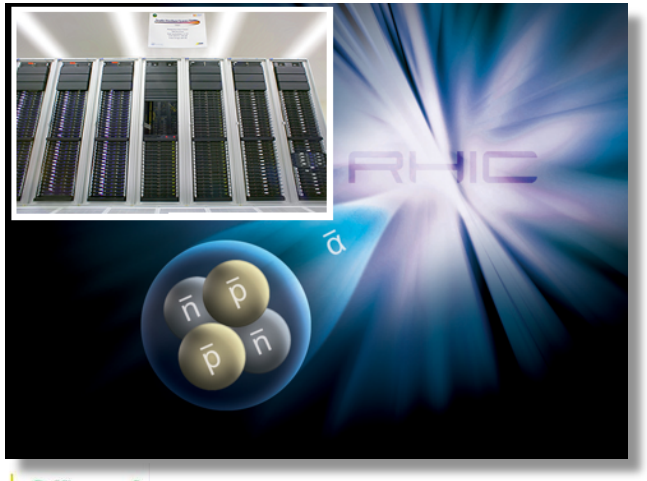
Heaviest Antimatter Nucleus Detected

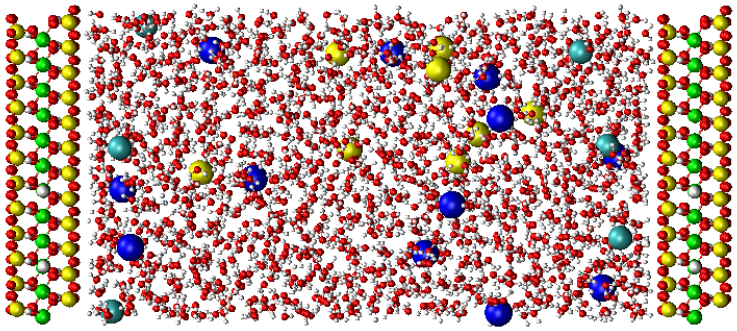
- **The STAR experiment creates high-energy nuclear collisions with energies similar to those microseconds after the Big Bang.**
  - ***Science Discovery: Detected the antimatter partner of the helium nucleus, antihelium-4.***
  - ***It's the heaviest antinucleus ever detected; likely to be heaviest stable antinucleus observed for* decades *to come.***
- **NERSC's PDSF cluster provides about 1/2 of the STAR simulation and analysis capability; NERSC-HPSS and Globus Grid facilities also vital.**



A rendering of an antihelium-4 nucleus emerging from a Relativistic Heavy Ion Collider collision with NERSC's PDSF cluster shown in the inset.

Nano-scale Modeling for Geologic Carbon Sequestration

- **Clay-rich rock formations play a key role in geologic carbon sequestration by initially preventing CO_2 escape.**
  - ***The sealing capacity of clay-rich materials depends on molecular-scale properties of clay-water interfaces that are not yet fully understood.***
  - ***Molecular dynamics simulations at NERSC yielded an unprecedentedly detailed view of water and ion distribution & dynamics near clay surfaces*.**
- **Provided key insight into mineral surface chemistry at brine concentrations relevant to saline aquifer CO_2 sequestration.**



Ian Bourg and Garrison Sposito (LBNL)

Snapshot of NERSC molecular dynamics simulation showing brine confined in a nanopore between two clay surfaces.

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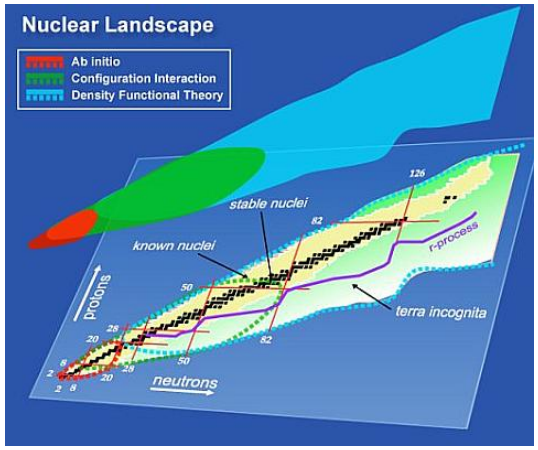
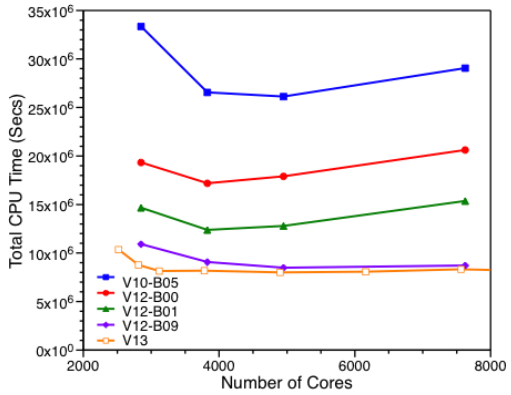
The Speculative ^{14}F Nucleus: Simulation Precedes Experiment

- **Many fundamental properties of nuclei are poorly understood today. Examining proton-rich light nuclei that are far from the "valley of stability" is a most demanding test of existing theory**
  - ***Prediction of the unstable ^{14}F nucleus was supported by ^{6}Li nucleus calculations done at NERSC.***
  - ***Served as motivation for experiments that ultimately observed fluorine-14***
  - **The Many Fermion Dynamics–nuclear (MFDn) code developed, optimized at NERSC; uses ≤ 23,980 cores (Franklin), ≤ 129,168 cores (Hopper)**





Scalability of various versions of the code on Franklin; v13 is hybrid MPI/OpenMP

P. Maris, A. M. Shirokov and J. Vary (Iowa State)

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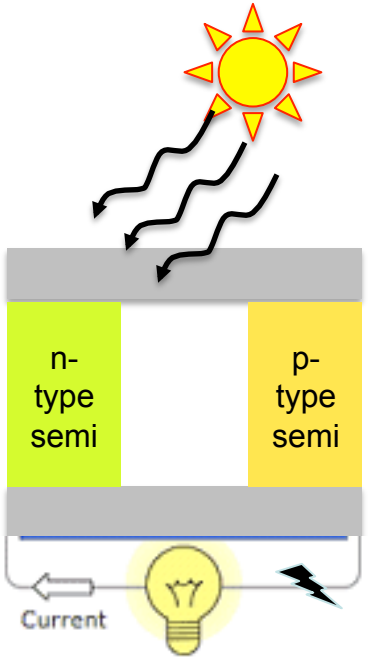
Thermoelectric Materials to Recycle Energy

- **Thermoelectric materials can convert heat directly to electricity.**
  - ***Already used in space but efficiencies are too low for commercial waste energy conversion on Earth. Why are efficiencies so low?***
  - ***NERSC science discovery: Calculations show that there can be a surprisingly strong coupling between lattice vibrations and electronic structure in some candidate thermoelectrics.***

- **Combination of simulation and scattering measurements provides insight that helps us better understand how heat is transported in thermoelectric materials.**



Thermoelectric device schematic. A heat source creates a temperature differential across two semiconductors which then drives a flow of current, thereby converting heat to electrical power.

P. Kent (ORNL)

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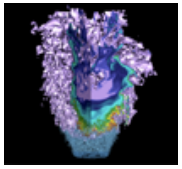
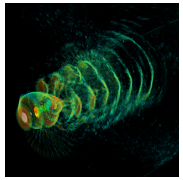
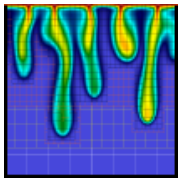
About the Cover



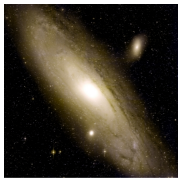
Low swirl burner combustion simulation. Image shows flame radical, OH (purple surface and cutaway) and volume rendering (gray) of vortical structures. Red indicates vigorous burning of lean hydrogen fuel; shows cellular burning characteristic of thermodiffusively unstable fuel. Simulated using an adaptive projection code. Image courtesy of John Bell, LBNL.



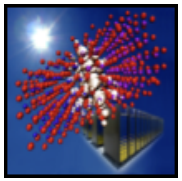
Hydrogen plasma density wake produced by an intense, right-to-left laser pulse. Volume rendering of current density and particles (colored by momentum orange - high, cyan - low) trapped in the plasma wake driven by laser pulse (marked by the white disk) radiation pressure. 3-D, 3,500 Franklin-core, 36-hour LOASIS experiment simulation using VORPAL by Cameron Geddes, LBNL. Image courtesy of Cameron Geddes..



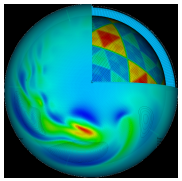
Numerical study of density driven flow for CO_2 storage in saline aquifers. Snapshot of CO_2 concentration after convection starts. Density-driven velocity field dynamics induces convective fingers that enhance the rate by which CO_2 is converted into negatively buoyant aqueous phase, thereby improving the security of CO_2 storage. Image courtesy of George Pau, LBNL



False-color image of the Andromeda Galaxy created by layering 400 individual images captured by the Palomar Transient Factory (PFT) camera in February 2009. NERSC systems analyzing the PTF data are capable of discovering cosmic transients in real time. Image courtesy of Peter Nugent, LBNL.



The exciton wave function (the white isosurface) at the interface of a ZnS/ZnO nanorod. Simulations performed on a Cray XT4 at NERSC, also shown. Image courtesy of Lin-Wang Wang, LBNL.



Simulation of a global cloud resolving model (GCRM). This image is a composite plot showing several variables: wind velocity (surface pseudocolor plot), pressure (b/w contour lines), and a cut-away view of the geodesic grid. Image courtesy of Professor David Randall, Colorado State University.