



NERSC Science Highlights

A selection of scientific results
produced by NERSC users

September, 2011



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National Energy Research
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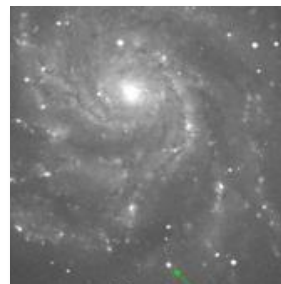


NERSC User Scientific Accomplishments, Q3CY2011



Astrophysics

NERSC played a key role in the discovery that led to the 2011 Nobel Prize in Physics.
(S. Perlmutter, UC Berkeley/LBNL)

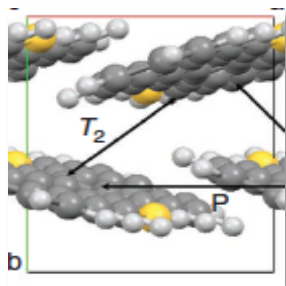


Astrophysics

The earliest-ever detection of a supernova was made possible by NERSC and Esnet.
(P. Nugent, LBNL)

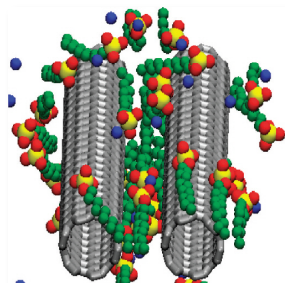
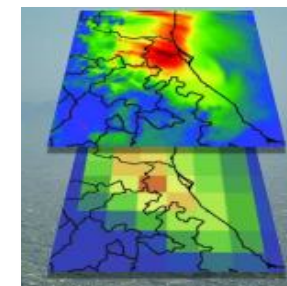
Materials

A vastly improved organic semiconductor discovery is a key proof of principle for rational design of new materials.
(A. Aspuru-Guzik, Harvard)



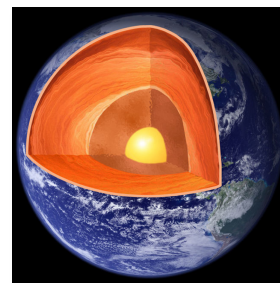
Climate

Atmospheric scientists have shown how small-scale effects of aerosols contribute to errors in climate models.
(W. Gustafson, PNNL)



Chemistry

Molecular dynamics simulations show how certain surfactants can be used to separate out bundles of carbon nanotubes with important properties.
(A. Striolo, U. Oklahoma)



Nuclear Physics

The KamLAND neutrino experiment showed that radioactivity cannot be Earth's only heat source; it accounts for only 1/2 of it.
(S. Freedman, LBNL)



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NERSC Played Key Role in Nobel Prize-Winning Discovery



- Accelerating Expansion of the Universe subject of 2011 Prize
- Type Ia supernovae are used as “standard candles” to measure the distance to remote galaxies.
- Simulations run at NERSC in the late 90s modeled how Type Ia supernovae should appear from Earth.
- This provided the crucial calibration needed to enable the Nobel Prize-winning discovery.

When NERSC moved to Berkeley 1996, this project's work was one of the first funded in a new computational science program created to encourage collaborations between physical and computer scientists.



Berkeley Lab's Saul Perlmutter was awarded the 2011 Nobel Prize in Physics along with two others for their discovery.

It implies the existence of so-called dark energy, a mysterious force that acts to oppose gravity.

The nature of dark energy is unknown and has been termed the most important problem facing 21st century physics.

<http://www.nersc.gov/perlmutter>



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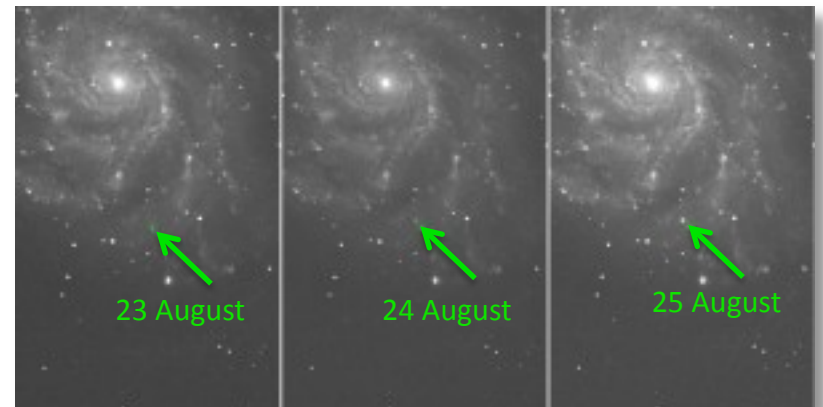


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Earliest-ever Detection of Supernova Made Possible by NERSC and ESnet

- Observed *within hours* of its explosion; will allow a rare glimpse at the supernova's outer layers that contain hints about what kind of star exploded
 - *The last time a supernova of this type occurred so close was 1972. Before that: 1937, 1898 and 1572.*
- NERSC resources used:
 - NERSC data transfer nodes accept telescope data (300GB/night); HPSS archives;
 - Data (~150 TB now) reside on NERSC Global Filesystem;
 - Subtraction pipeline on Carver (iDataPlex) system to process images and detect new transients;
 - Science gateway nodes serve the DeepSky database to astronomers worldwide.



“Before” and “After” images showing the discovery.

Peter Nugent (NERSC) is project PI and Realtime Transient Detection Lead



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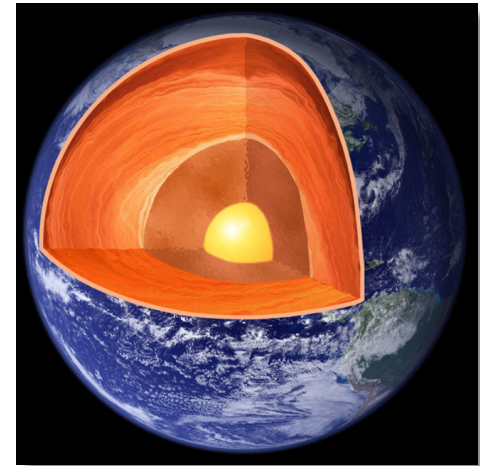


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Understanding Earth's Main Heat Source

- Heat from within Earth is responsible for volcanoes, continental shift, destroying tectonic plates, and more.
Where does this heat come from?
 - Two possible sources: residual primordial heat and radioactive decay
- **Science discovery:** radioactive decay accounts for about $\frac{1}{2}$ Earth's heat energy – about 29 Terawatts.
 - KamLAND measurement of geo-neutrino flux provided this result
- NERSC is the main computing center for U.S. KamLAND research.
- KamLAND has stored about 700TB of data in NERSC HPSS.



KamLAND measured the flux from fission of naturally occurring uranium and thorium.

**Stuart Freedman
(LBNL)**



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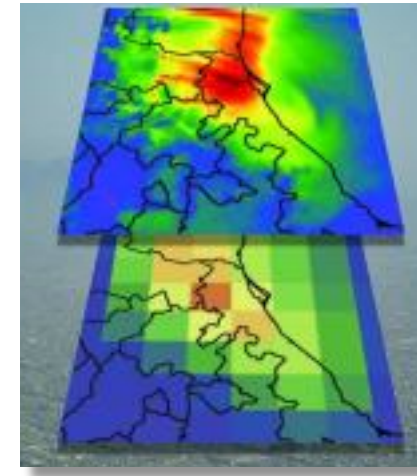
NP

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- Global climate models do not have sufficient resolution to represent aerosols (dust, smoke, pollution) directly.
 - Instead, they must rely on parameterizations, which are statistical representations. What is the effect of this?
- **Science discovery:** Detailed error quantification shows that parameterization error can be large – up to 30%.
 - Error is largest in areas where local processes add aerosols and in regions of complex topography



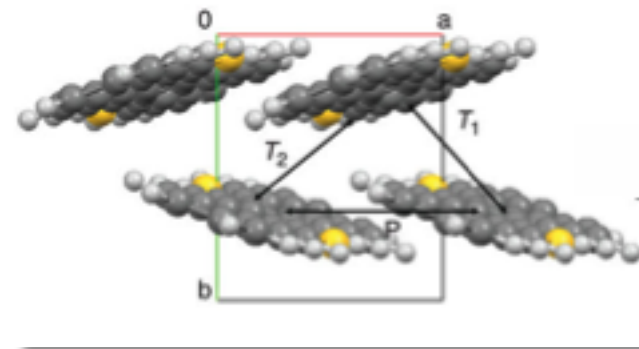
Weather Research and Forecasting (WRF) model simulation for Mexico City. The higher-resolution aerosol model (top) shows the importance of aerosols in climate studies. Colors indicate concentrations of aerosol pollution with red being highest, light green lowest.

**William Gustafson
(PNNL)**



True Rational Materials Design

- Organic semiconductors hold immense promise for use in flexible displays (picture an iPad you could roll up) but they aren't yet fast enough for high-def LCD screens.
- **Science discovery:** a new organic semiconductor that conducts charge more than 30 times faster than the material currently used in liquid crystal displays
 - Can also be used to manufacture less expensive printed solar cells
- Would have taken several years to synthesize and characterize all the candidate compounds studied.



Predicted crystal structure of the semiconductor material

***A key proof of principle:
using HPC to change the
paradigm of materials
discovery from serendipity
to
rational design.***

**Alan Aspuru-Guzik
(Harvard)**



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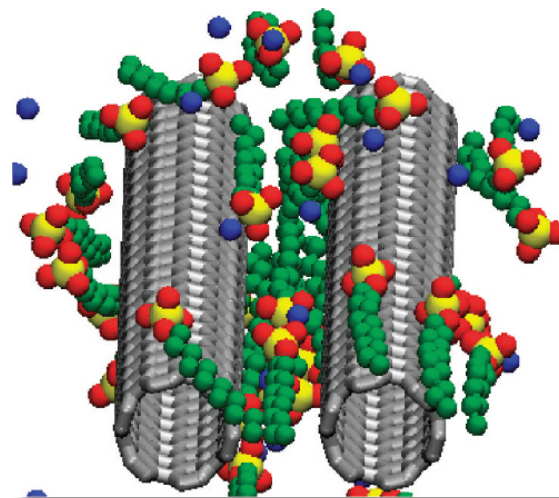
BES

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- When carbon nanotubes (CNTs) are produced, they come as a mixture of “chiralities” (or handedness) with varying electronic properties.
 - Nanotubes need to be rich in one chirality to be useful.
- **Science Discovery:** Molecular dynamics simulations show how certain surfactants can separate out bundles of nanotubes so that the carbon atoms are all arranged in the same way.
- Single-chiral tubes might be used in applications as diverse as high-performance electronics, nanosensors, catalyst supports, hydrogen storage, and gas separation.



Snapshot from a simulation showing how carbon nanotubes can be stabilized in water using a common surfactant (an emulsifier or dispersing agent)

Alberto Striolo
(U. Oklahoma)