NERSC PLAYED KEY ROLE IN NOBEL LAUREATE'S DISCOVERY

NERSC, Berkeley Lab Now Centers for Computational Cosmology Community

OCTOBER 4, 2011

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In the 1990s, Saul Perlmutter discovered that the universe is expanding at an accelerating rate. He confirmed his observational conclusions by running thousands of simulations at the National Energy Research Scientific Computing Center (NERSC) at Lawrence Berkeley National Laboratory (Berkeley Lab). As a result of this groundbreaking work, Perlmutter was awarded the 2011 Nobel Prize in Physics. His research team is believed to have been the first to use supercomputers to analyze and validate observational data in cosmology. This melding of computational science and cosmology sowed the seeds for more projects, establishing Berkeley Lab and NERSC as centers for the emerging field.

The Supernova Cosmology Project

The Supernova Cosmology Project, co-led by Perlmutter, used a robotic telescope equipped with a digital detector instead of photographic plates. Its digital images were compared with earlier images using "subtraction" software. By 1994 the SCP team could discover supernovae "on demand," and Perlmutter realized he would soon need more computing power to analyze the growing flow of data. NERSC's move to Berkeley Lab in 1996 provided the perfect opportunity for his team.

With a Laboratory Directed Research and Development (LDRD) grant, the NERSC and Physics divisions jointly hired a postdoc. Peter Nugent—now leader of the NERSC Analytics Team and co-leader of Berkeley Lab's Computational Cosmology Center (C3)—helped the group develop parallel algorithms that could run on 128 cores at once, taking great advantage of NERSC's "Mcurie" system, a 512-processor Cray T3E-900 supercomputer.

Perlmutter (far left) with members of the Supernova Cosmology Project team. Nugent, now group lead for NERSC Analytics and head of the Computational Cosmology Center at Berkeley Lab, stands center rear. (Roy Kaltschmidt, LBNL)

To analyze the data from 40 supernovae for errors or biases, Nugent simulated 10,000 exploding supernovae at varying distances under varying circumstances. These were then plotted and compared with the observed data to detect any biases affecting observation or interpretation. The Cray T3E supercomputer was also used to check and recheck their work by resampling the data and running calculations that helped determine the reliability of their measurements thousands of times.

These rigorous, supercomputer-powered analyses of potential biases reduced the uncertainties in the data and helped Perlmutter's team win widespread acceptance of their conclusions in the scientific community.

Computational Cosmology Legacy

The story, however, doesn't end there. Perlmutter's work inspired a profusion of computational cosmology research centered at Berkeley and NERSC:

- **BOOMERANG**, a 1999 balloon-based Cosmic Background Radiation survey, made close to one billion measurements of CMB temperature variations. Analysis of the BOOMERANG dataset at NERSC established that the Universe is flat— its geometry is Euclidean, not curved. Nearly all CMB experiments launched since have used NERSC for data analysis in some capacity, and today NERSC supports around 100 researchers from a dozen CMB experiments.
- **Planck**, the European Space Agency's satellite observatory is yielding 300 billion samples per year. The C3 team spent nearly a decade developing the supercomputing infrastructure for the U.S. Planck Team's data and analysis operations at NERSC (and received a **NASA Public Service Group Award** for their efforts).
- **Nearby Supernova Factory** (SNfactory), an international collaboration between several groups in the United States and France, collects detailed observations of low-redshift supernovae. By 2003 the SNfactory was discovering eight supernovae per month, a rate made possible by a high-speed data link, custom data pipeline software and NERSC's ability to store and process 50 GB of data per night. Sunfall, a collaborative visual analytics system developed jointly by the Computational Research and Physics divisions,, has eliminated 90 percent of the human labor once involved in supernova identification and follow-up, while cutting false-positives by a factor of 10.
- **Palomar Transient Factory** (PTF), an innovative sky survey, is the first project dedicated solely to finding "transient" astronomical events, including supernovae. A team at Caltech worked with NERSC to develop an automated system that sifts through terabytes of astronomical data every night to find interesting events. PTF has discovered more than 1,300 supernovae, three of which form new classes of these objects. Last month PTF discovered one of the closest Type Ia supernovae in the last 40 years, **SN 2011fe, in the nearby Pinwheel galaxy**.
- **Deep Sky Project** is a Web-accessible collection of 11 million astronomical images (70 terabytes of data) housed at NERSC. The brainchild of Nugent, who was on Perlmutter's SCP team, the database is made up of images taken over a decade and covering nearly all of the northern sky, about 20,000 square degrees. Astronomers from around the world can download these composite images at the Deep Sky Project web site.

About NERSC and Berkeley Lab
The National Energy Research Scientific Computing Center (NERSC) is the primary high-performance computing facility for scientific research sponsored by the U.S. Department of Energy's Office of Science. Located at Lawrence Berkeley National Laboratory, the NERSC Center serves more than 4,000 scientists at national laboratories and universities researching a wide range of problems in combustion, climate modeling, fusion energy, materials science, physics, chemistry, computational biology, and other disciplines. **Berkeley Lab** is a U.S. Department of Energy national laboratory located in Berkeley, California. It conducts unclassified scientific research and is managed by the University of California for the U.S. DOE Office of Science. For more information about computing sciences at Berkeley Lab, please visit **www.lbl.gov/cs**.

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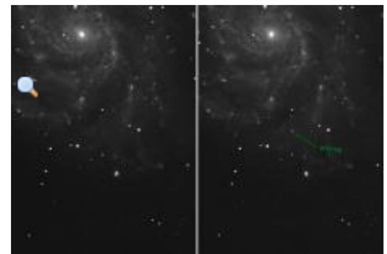
SUPERNOVA CAUGHT IN THE ACT

Earliest-ever Detection Made Possible by Computing, Networks

AUGUST 25, 2011

Contact: Linda Vu, +1 510 495 2402, lvu@lbl.gov

A supernova discovered yesterday is closer to Earth—approximately 21 million light-years away—than any other of its kind in a generation. Astronomers believe they caught the supernova within hours of its explosion, a rare feat made possible by a specialized survey telescope and state-of-the-art computational tools.



Before and after images of supernova PTF 11kly as it appeared in the nearby M101 galaxy. Click to enlarge. (Images: Peter Nugent)

The discovery of such a supernova so early and so close has energized the astronomical community as they are scrambling to observe it with as many telescopes as possible, including the Hubble Space Telescope.

Joshua Bloom, assistant professor of astronomy at the University of California, Berkeley, called it "the supernova of a generation." Astronomers at Lawrence Berkeley National Laboratory (Berkeley Lab) and UC Berkeley, who made the discovery predict that it will be a target for research for the next decade, making it one of the most-studied supernova in history.

The supernova, dubbed PTF 11kly, occurred in the Pinwheel Galaxy, located in the "Big Dipper," otherwise known as the Ursa Major constellation. It was discovered by the Palomar Transient Factory (PTF) survey, which is designed to observe and uncover astronomical events as they happen.

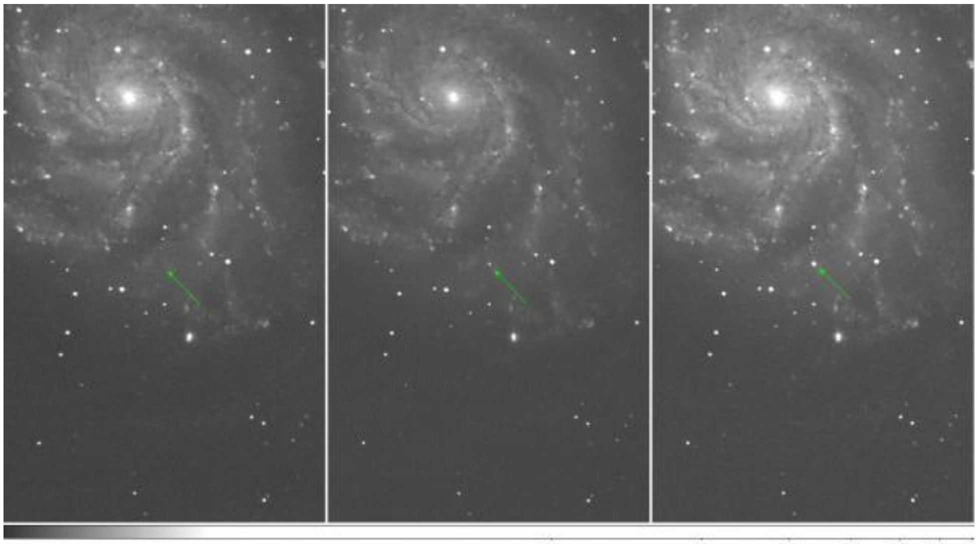
Want to see it for yourself? Berkeley Lab astronomer Peter Nugent explains how

"We caught this supernova very soon after explosion. PTF 11kly is getting brighter by the minute. It's already 20 times brighter than it was yesterday," said Peter Nugent, the senior scientist at Berkeley Lab who first spotted the supernova. Nugent is also an adjunct professor of astronomy at UC Berkeley. "Observing PTF 11kly unfold should be a wild ride. It is an instant cosmic classic."

He credits supercomputers at the National Energy Research Scientific Computing Center (NERSC), a Department of Energy supercomputing center at Berkeley Lab, as well as high-speed networks with uncovering this rare event in the nick of time.

The PTF survey uses a robotic telescope mounted on the 48-inch Samuel Oschin Telescope at Palomar Observatory in Southern California to scan the sky nightly. As soon as the observations are taken, the data travels more than 400 miles to NERSC via the National Science Foundation's High Performance Wireless Research and Education Network and DOE's Energy Sciences Network (ESnet). At NERSC, computers running machine learning algorithms in the Real-time Transient Detection Pipeline scan through the data and identify events to follow up on. Within hours of identifying PTF 11kly, this automated system sent the coordinates to telescopes around the world for follow-up observations.

Three hours after the automated PTF pipeline identified this supernova candidate, telescopes in the Canary Islands (Spain)



These images (click to enlarge) show Type Ia supernova PTF 11kly, the youngest ever detected, over the past three nights. The left image taken on August 22, 2011, shows the star (to the lower right of the glaxay) shortly before it exploded, approximately 1 million times fainter than the human eye can detect. The center image taken on August 23 shows the supernova at about 10,000 times fainter than the human eye can detect. The right image taken on August 24 shows the event six times brighter than the previous day. In two weeks time it should be visible with a good pair of binoculars. (images: Peter Nugent)

had captured unique “light signatures,” or spectra, of the event. Twelve hours later, his team had observed the event with a suite of telescopes including the Lick Observatory (California), and Keck Observatory (Hawaii) had determined the supernova belongs to a special category, called Type Ia. Nugent notes that this is the earliest spectrum ever taken of a Type Ia supernova.

“Type Ia supernova are the kind we use to measure the expansion of the Universe. Seeing one explode so close by allows us to study these events in unprecedented detail,” said Mark Sullivan, the Oxford University team leader who was among the first to follow up on this detection.

“We still do not know for sure what causes such explosions,” said Weidong Li, senior scientist at UC Berkeley and collaborator of Nugent. “We are using images from the Hubble Space Telescope, taken fortuitously years before an explosion to search for clues to the event’s origin.”

The team will be watching carefully over the next few weeks, and an urgent request to NASA yesterday means the Hubble Space Telescope will begin studying the supernova’s chemistry and physics this weekend.

Catching supernovae so early allows a rare glimpse at the outer layers of the explosion, which contain hints about the star it once was. “When you catch them this early, mixed in with the explosion you can actually see unburned bits from the star that exploded! It is remarkable,” said Andrew Howell of UC Santa Barbara/Las Cumbres Global Telescope Network. “We are finding new clues to solving the mystery of the origin of these supernovae that has perplexed us for 70 years. Despite looking at thousands of supernovae, I’ve never seen anything like this before.”

“The ability to process all of this data in near real-time and share our results with collaborators around the globe through the **Deep Sky Science Gateway** at NERSC is an invaluable tool for following up on supernova events,” says Nugent. “We wouldn’t have been able to detect and observe this candidate as soon as we did without the resources at NERSC.”

At a mere 21 million light-years from Earth, a relatively small distance by astronomical standards, the supernova is still getting brighter, and might even be visible with good binoculars in ten days' time, appearing brighter than any other supernova of its type in the last 30 years.

“The best time to see this exploding star will be just after evening twilight in the Northern hemisphere in a week or so,” said Oxford’s Sullivan. “You’ll need dark skies and a good pair of binoculars, although a small telescope would be even better.”

The scientists in the PTF have discovered more than 1,000 supernovae since it started operating in 2008, but they believe this could be their most significant discovery yet. The last time a supernova of this sort occurred so close was in 1986, but Nugent notes that this one was peculiar and heavily obscured by dust.

"Before that, you'd have to go back to 1972, 1937 and 1572 to find more nearby Type Ia supernovae,” says Nugent.

The **Palomar Transient Factory** is a survey operated a Palomar Observatory by the California Institute of Technology on behalf of a worldwide consortium of partner institutions. Collaborators on PTF 11kly with Nugent, Bloom and Li are Brad Cenko, Alex V. Filippenko, Geoffrey Marcy, Adam Miller (UC Berkeley), Rollin C. Thomas (Lawrence Berkeley National Laboratory), Sullivan (Oxford University), and Andrew Howell (UC Santa Barbara/Las Cumbres Global Telescope Network).

Read more about **how NERSC supports the Palomar Transient Factory**.

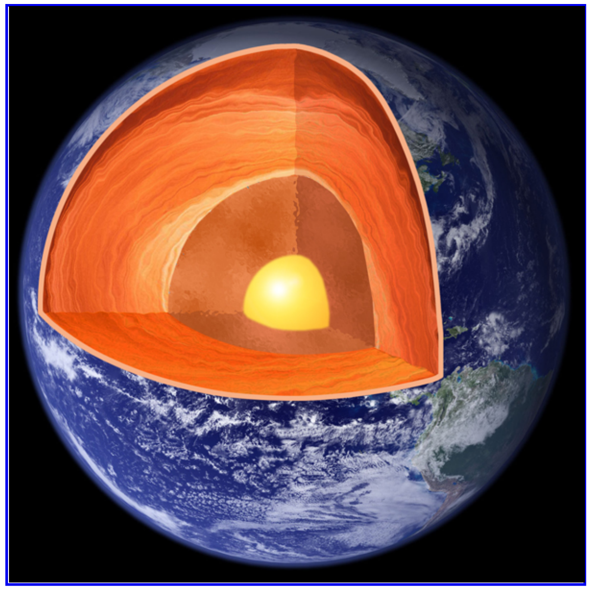
About NERSC and Berkeley Lab

The National Energy Research Scientific Computing Center (NERSC) is the primary high-performance computing facility for scientific research sponsored by the U.S. Department of Energy's Office of Science. Located at Lawrence Berkeley National Laboratory, the NERSC Center serves more than 4,000 scientists at national laboratories and universities researching a wide range of problems in combustion, climate modeling, fusion energy, materials science, physics, chemistry, computational biology, and other disciplines. **Berkeley Lab** is a U.S. Department of Energy national laboratory located in Berkeley, California. It conducts unclassified scientific research and is managed by the University of California for the U.S. DOE Office of Science. For more information about computing sciences at Berkeley Lab, please visit **www.lbl.gov/cs**.

What Keeps the Earth Cooking?

Posted By paulpreuss On July 17, 2011 @ 11:25 am In News Releases | Comments Disabled

What spreads the sea floors and moves the continents? What melts iron in the outer core and enables the Earth's magnetic field? Heat. Geologists have used temperature measurements from more than 20,000 boreholes around the world to estimate that some 44 terawatts (44 trillion watts) of heat continually flow from Earth's interior into space. Where does it come from?



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A main source of the 44 trillion watts of heat that flows from the interior of the Earth is the decay of radioactive isotopes in the mantle and crust. Scientists using the KamLAND neutrino detector in Japan have measured how much heat is generated this way by capturing geoneutrinos released during radioactive decay.

Radioactive decay of uranium, thorium, and potassium in Earth's crust and mantle is a principal source, and in 2005 scientists in the KamLAND collaboration, based in Japan, first showed that there was a way to measure the contribution directly. The trick was to catch what KamLAND dubbed geoneutrinos – more precisely, geo-*anti*neutrinos – emitted when radioactive isotopes decay. (KamLAND stands for Kamioka Liquid-scintillator Antineutrino Detector.)

"As a detector of geoneutrinos, KamLAND has distinct advantages," says Stuart Freedman of the U.S. Department of Energy's Lawrence Berkeley National Laboratory (Berkeley Lab), which is a major contributor to KamLAND. Freedman, a member of Berkeley Lab's Nuclear Science Division and a professor in the Department of Physics at the University of California at Berkeley, leads U.S. participation. "KamLAND was specifically designed to study antineutrinos. We are able to discriminate them from background noise and detect them with very high sensitivity."

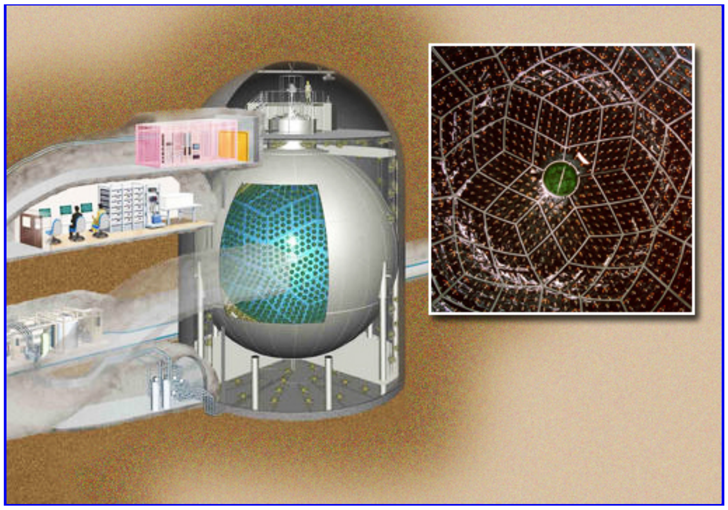
KamLAND scientists have now published new figures for heat energy from radioactive decay in the journal *Nature Geoscience*. Based on the improved sensitivity of the KamLAND detector, plus several years' worth of additional data, the new estimate is not merely "consistent" with the predictions of accepted geophysical models but is precise enough to aid in refining those models.

One thing that's at least 97-percent certain is that radioactive decay supplies only about half the Earth's heat. Other sources – primordial heat left over from the planet's formation, and possibly others as well – must account for the rest.

Hunting for neutrinos from deep in the Earth

Antineutrinos are produced not only in the decay of uranium, thorium, and potassium isotopes but in a variety of others, including fission products in nuclear power reactors. In fact, reactor-produced antineutrinos were the first neutrinos to be directly detected (neutrinos and antineutrinos are distinguished from each other by the interactions in which they appear).

Because neutrinos interact only by way of the weak force – and gravity, insignificant except on the scale of the cosmos – they stream through the Earth as if it were transparent. This makes them hard to spot, but on the very rare occasions when an antineutrino collides with a proton inside the KamLAND detector – a sphere filled with a thousand metric tons of scintillating mineral oil – it produces an unmistakable double signal.



[2]

The KamLAND antineutrino detector is a vessel filled with scintillating mineral oil and lined with photomultiplier tubes (inset), the largest scintillation detector ever constructed, buried deep underground near Toyama, Japan.

The first signal comes when the antineutrino converts the proton to a neutron plus a positron (an anti-electron), which quickly annihilates when it hits an ordinary electron – a process called inverse beta decay. The faint flash of light from the ionizing positron and the annihilation process is picked up by the more than 1,800 photomultiplier tubes within the KamLAND vessel. A couple of hundred millionths of a second later the neutron from the decay is captured by a proton in the hydrogen-rich fluid and emits a gamma ray, the second signal. This "delayed coincidence" allows antineutrino interactions to be distinguished from background events such as hits from cosmic rays penetrating the kilometer of rock that overlies the detector.

Says Freedman, "It's like looking for a spy in a crowd of people on the street. You can't pick out one spy, but if there's a second spy following the first one around, the signal is still small but it's easy to spot."

KamLAND was originally designed to detect antineutrinos from more than 50 reactors in Japan, some close and some far away, in order to study the phenomenon of neutrino oscillation. Reactors produce electron neutrinos, but as they travel they oscillate into muon neutrinos and tau neutrinos; the three "flavors" are associated with the electron and its heavier cousins.

Being surrounded by nuclear reactors means KamLAND's background events from reactor antineutrinos must also be accounted for in identifying geoneutrino events. This is done by identifying the nuclear-plant antineutrinos by their characteristic energies and other factors, such as their varying rates of production versus the steady arrival of geoneutrinos. Reactor antineutrinos are calculated and subtracted from the total. What's left are the geoneutrinos.

Tracking the heat

All models of the inner Earth depend on indirect evidence. Leading models of the kind known as bulk silicate Earth (BSE) assume that the mantle and crust contain only lithophiles ("rock-loving" elements) and the core contains only siderophiles (elements that "like to be with iron"). Thus all the heat from radioactive decay comes from the crust and mantle – about eight terawatts from uranium 238 (^{238}U), another eight terawatts from thorium 232 (^{232}Th), and four terawatts from potassium 40 (^{40}K).

KamLAND's double-coincidence detection method is insensitive to the low-energy part of the geoneutrino signal from ^{238}U and ^{232}Th and completely insensitive to ^{40}K antineutrinos. Other kinds of radioactive decay are also missed by the detector, but compared to uranium, thorium, and potassium are negligible contributors to Earth's heat.

Additional factors that have to be taken into account include how the radioactive elements are distributed (whether uniformly or concentrated in a "sunken layer" at the core-mantle boundary), variations due to radioactive elements in the local geology (in KamLAND's case, less than 10 percent of the expected flux), antineutrinos from fission products, and how neutrinos oscillate as they travel through the crust and mantle. Alternate theories were also considered, including the speculative idea that there may be a natural nuclear reactor somewhere deep inside the Earth, where fissile elements have accumulated and initiated a sustained fission reaction.

KamLAND detected 841 candidate antineutrino events between March of 2002 and November of 2009, of which about 730 were reactor events or other background. The rest, about 111, were from radioactive decays of uranium and thorium in the Earth. These results were combined with data from the Borexino experiment at Gran Sasso in Italy to calculate the contribution of uranium and thorium to Earth's heat production. The answer was about 20 terawatts; based on models, another three terawatts were estimated to come from other isotope decays.

This is more heat energy than the most popular BSE model suggests, but still far less than Earth's total. Says Freedman, "One thing we can say with near certainty is that radioactive decay alone is not enough to account for Earth's heat energy. Whether the rest is primordial heat or comes from some other source is an unanswered question."

Better models are likely to result when many more geoneutrino detectors are located in different places around the globe, including midocean islands where the crust is thin and local concentrations of radioactivity (not to mention nuclear reactors) are at a minimum.

Says Freedman, "This is what's called an inverse problem, where you have a lot of information but also a lot of complicated inputs and variables. Sorting those out to arrive at the best explanation among many requires multiple sources of data."

"Partial radiogenic heat model for Earth revealed by geoneutrino measurements," by the KamLAND Collaboration, Itaru Shimizu of Tohoku University, Sendai, Japan, corresponding author, is published in *Nature Geoscience* and is available in advanced online publication at http://www.nature.com/ngeo/journal/vaop/ncurrents/abs/ngeo1205.html [3].

Berkeley Lab and UC Berkeley members of the KamLAND Collaboration include Thomas Banks, Thomas Bloxham, Jason Detwiler, Stuart Freedman, Brian Fujikawa, Ke Han, Richard Kadel, Hitoshi Murayama, Thomas O'Donnell, and Herbert Steiner. Besides Tohoku University, Lawrence Berkeley National Laboratory, and the University of California at Berkeley, member institutions of the KamLAND Collaboration are the Institute for the Physics and Mathematics of the Universe, Tokyo University, Kashiwa (of which Hitoshi Murayama is also the director); the University of Alabama, Tuscaloosa; the California Institute of Technology, Pasadena; Colorado State University, Fort Collins; Drexel University, Philadelphia; the University of

Hawaii at Manoa; Kansas State University, Manhattan; Stanford University, Palo Alto, California; the University of Tennessee, Knoxville; Triangle Universities Nuclear Laboratory, Durham, and Duke University, North Carolina Central University, and the University of North Carolina at Chapel Hill; the University of Wisconsin at Madison, and NIKHEF (National Institute for Subatomic Physics), Amsterdam.

KamLAND is supported by the Japanese Ministry of Education, Culture, Sports, Science and Technology and the U.S. Department of Energy's Office of Science.

Lawrence Berkeley National Laboratory addresses the world's most urgent scientific challenges by advancing sustainable energy, protecting human health, creating new materials, and revealing the origin and fate of the universe. Founded in 1931, Berkeley Lab's scientific expertise has been recognized with 12 Nobel prizes. The University of California manages Berkeley Lab for the U.S. Department of Energy's Office of Science. For more, visit www.lbl.gov [4].

URLs in this post:

[1] Image: **http://newscenter.lbl.gov/wp-content/uploads/cutaway-Earth.jpg**
[2] Image: **http://newscenter.lbl.gov/wp-content/uploads/KamLAND-detector.jpg**
[3] http://www.nature.com/ngeo/journal/vaop/ncurrents/abs/ngeo1205.html: **http://www.nature.com/ngeo/journal/vaop/ncurrent/abs/ngeo1205.html**
[4] www.lbl.gov: **http://www.lbl.gov/**

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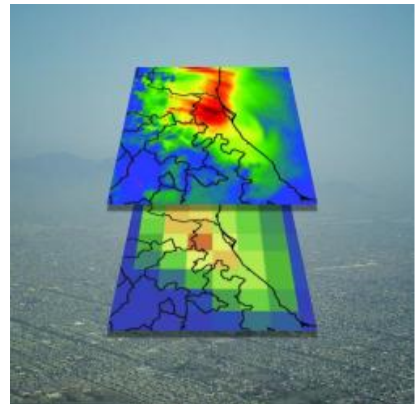
SMALL PARTICLES, BIG IMPACT

Small-scale effects of Aerosols Add up Over Time

AUGUST 24, 2011 | Tags: Climate, Earth Sciences, Environmental Science, Franklin, NERSC
Linda Vu, lvu@lbl.gov, +1 510 495 2402



High-resolution simulation for Mexico City (top), shows a more detailed and accurate picture of aerosol pollution compared to representations of a global climate model (bottom). The deep red to light green colors represent concentrations of aerosol pollution with red being highest, light green lowest.

Using systems at the National Energy Research Scientific Computing Center (NERSC), atmospheric scientists at the Pacific Northwest National Laboratory (PNNL) have found that small scale effects of aerosols—tiny particles of dust or pollution in the atmosphere—can add up and over time and lead to large, accumulated errors in climate prediction models.

"Aerosols like ozone, dust and sea salt in our atmosphere scatter and absorb sunlight. Depending on the type of particle and its elevation above Earth's surface, these particles can tip the energy balance toward heating or cooling," says Dr. William Gustafson, an atmospheric scientist at PNNL and principal investigator of the study, published in the July 2011 ***Journal of Geophysical Research Atmospheres***.

Because global climate models typically calculate atmospheric processes at scales close to 100 by 100 kilometers (62 miles across), the characteristics of aerosols are averaged over a large area. This practice distorts the effects of aerosols in climate predictions because, in reality, these particles act on a much smaller scale and can vary according to local atmospheric or geographic features.

To quantify this error, Gustafson led a collaboration that looked at changes in the net flux of sunlight—the amount of sunlight that is reflected back into space, absorbed or allowed to hit the ground by aerosols—using a regional atmospheric model to emulate grids typical of coarse global climate models, as well as detailed grids at scales of 3 by 3 kilometers (1.6 miles across). The 30-day–long simulations were based on observations collected by the Department of Energy during March 2006.

"This net flux quantity is important because it directly relates to changes in the atmosphere's energy balance, and thus the potential impact of the aerosol on atmospheric temperatures and climate," says Gustafson. "In the short term, the impact of aerosol is less dramatic than clouds, but their effects add up in the long term and are important when considering mitigation and adaptation strategies for climate change due to the longer-lived greenhouse gasses, such as carbon dioxide."

The team's results revealed a 30 percent discrepancy between the coarse and detailed models for aerosol direct radiative forcing—rate of energy change at the top layer of the atmosphere due to the aerosols—over portions of Mexico.

"Until recently, computers weren't fast enough to incorporate detailed effects of aerosols in climate models. These calculations are very computationally expensive," says Gustafson. "On average, if you are trying to predict climate without these particles, there may be 15 variables to consider. With aerosols, there are anywhere between 50 and 500 variables."

He notes that the detailed Mexico City models used about 250 computer cores, and were done over a several month period on NERSC's Cray XT4 Franklin system. Ultimately, with more funding and compute power Gustafson says he would like to measure these effects on a global level, as well as be able to include the impact on clouds, which was excluded in the present study. In addition to Gustafson, other authors of this paper include Drs. Yun Qian and Jerome Fast, also of PNNL.

This article was adapted from a story written by Jennifer Ovink, a communications specialist at PNNL's Atmospheric Sciences & Global Change Division. ***Read more***.

HarvardScience
SCIENCE AND ENGINEERING AT HARVARD UNIVERSITY

Electrical conductor sparks interest

Researchers say flexible compound has broad potential in electronics

By Alvin Powell
Harvard Staff Writer
Tuesday, August 16, 2011

Chemists at Harvard and three other institutions have created a purified version of an organic semiconductor with electrical properties that put it among a small handful of organic compounds and that provides an important proof of concept for a screening process to find new compounds for solar panels.

Alán Aspuru-Guzik, associate professor of chemistry and chemical biology, worked with colleagues at Stanford University, Haverford College, and Clark University to identify, synthesize, and characterize the compound. It was based on a compound created several years ago by a team from Japan. The compound, with the tongue-twisting name of dinapthothienothiophene, intrigued Aspuru-Guzik and Haverford colleague Joshua Schrier, who decided to use computers to model several variations and screen them for improved electrical properties.

That process resulted in seven candidate compounds, from which they selected one, whose synthesis was originally devised by Sergio Granados-Focil, an assistant professor of chemistry at Clark, and was synthesized in the lab of Zhenan Bao, an associate professor in Stanford's Chemical Engineering Department. Initial measurements by Bao's group of the compound's "hole mobility" — a measure of how quickly electrons move analogous to current in a metallic material — showed it was among a small handful of top-performing organic molecules.

"It would have taken several years to both synthesize and characterize all the seven candidate compounds. With this approach, we were able to focus on the most promising candidate … as predicted by theory," Bao said. "This is a rare example of 'truly rational' design of new high performance materials."

The Japanese team that created the original compound, led by Kazuo Takimiya, also recently reported that it had created the same compound, though its measurements showed that the compound had lower electrical properties.

Though the discovery, reported today in the journal Nature Communications, may have creative applications in electronics, where organic semiconductors are used in thin film transistors and to create extremely thin television screens, Aspuru-Guzik was just as enthusiastic that it provided confirmation of the screening process, based on computer modeling, that he is using to find new materials for solar panels. Sule Atahan, a postdoctoral fellow working with Aspuru-Guzik, said that the close match between the predicted and measured crystal structures of the compound is key, and that theoretical screening is crucial to identify new materials for clean-energy applications.

From a cost standpoint, organic semiconductors still cannot compete with the silicon typically used in photovoltaic panels. But organics — a family of typically large, complex molecules built around a backbone of carbon atoms — have many advantages over rigid, heavy silicon. Organic semiconductors can be used to make flexible display screens and can be sprayed like paint or ink, opening a broad range of applications.

If a compound can be identified for use in photovoltaics, Aspuru-Guzik said, it may find applications where the rigid structure and equipment needed for traditional solar panels preclude their use, such as in the developing world, where more than 2 billion people still don't have access to reliable electricity.

To identify such a compound, Aspuru-Guzik several years ago began the Clean Energy Project, a distributed computing effort, conducted in collaboration with the IBM World Community Grid, that uses the surplus computing power of idle desktop machines to screen 2.7 million possible candidates. So far, Aspuru-Guzik said, they've identified about 5,000 compounds predicted more than 10 percent efficient at converting sunlight to electricity. Additionally, Aspuru-Guzik and Bao have a joint research project, sponsored by the Stanford Global Climate and Energy Program, to use this approach for accelerating the discovery of high performance organic solar cell materials.

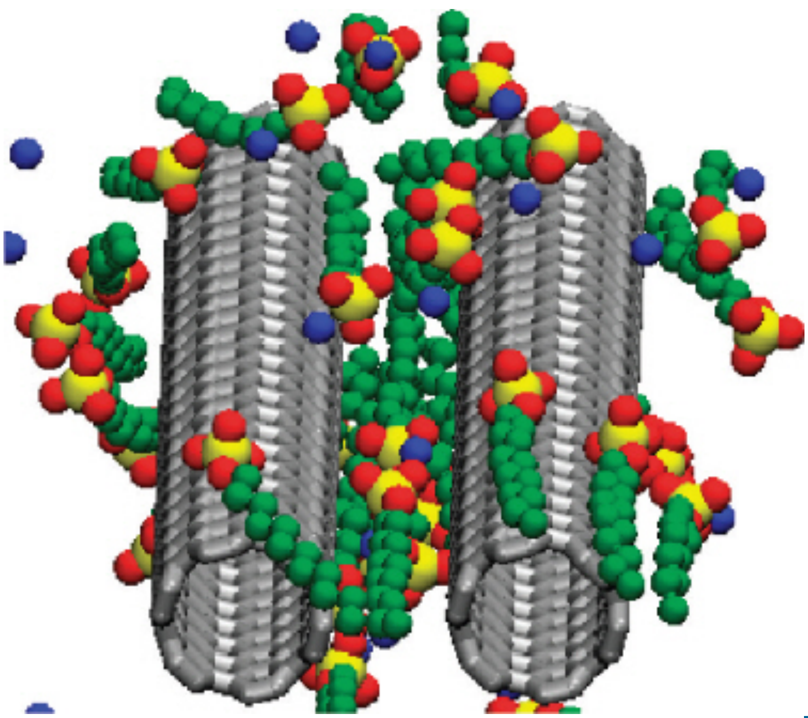
When the screening is complete, Aspuru-Guzik said, researchers plan to publish a list of the 1,000 most promising compounds. After that will come the labor-intensive process of making them and checking for properties that improve on materials used in solar panels today.

“We need only one for the world to be happy,” Aspuru-Guzik said.

Dec 17, 2010

Surfactants separate CNTs

When carbon nanotubes are produced, they come in a mix of "chiralities" (or handedness) with varying electronic properties. However, the nanotubes need to be rich in one chirality if they are to be used to make devices. Using computer simulations, researchers at the University of Oklahoma in the US now suggest that certain surfactants could effectively separate out bundles of nanotubes in which the carbon atoms are then all arranged in the same way. Single-chiral tubes might be used in applications as diverse as drug delivery, biosensors and in high-performance electronics.



(http://images.iop.org/objects/ntw/news/9/12/13/AStriolo.jpg)

The simulations (http://images.iop.org/objects/ntw/news/9/12/13/AStriolo.jpg)

A single-walled carbon nanotube (SWCNT) is a sheet of carbon just one atom thick rolled up into a tube that has a diameter of about 1 nm. The atoms in the sheet are arranged in a hexagonal lattice. The relative orientation of the lattice to the axis of the tube, or its chirality, determines whether the tube is a metal or a semiconductor and so what type of electronic properties it has.

SWCNTs are ideal for use in a variety of applications, such as sensors and transistors, thanks to their extremely high surface area and excellent charge transport properties. However, to make such devices, the tubes need to be rich in one chirality. This is difficult to achieve.

Increasing nanotube repulsion

Now, Alberto Striolo and colleagues say that surfactants, such as sodium cholate and flavin mononucleotide (FMN) could efficiently separate out SWCNTs based on diameter and chirality. Using molecular dynamics simulations, the researchers related the structure of the surfactant adsorbed on aqueous nanotubes to the effective repulsion/attraction between the tubes. They suggest that increasing the repulsion between individual nanotubes yields more stable dispersions of single-chiral tubes. Based on these theoretical simulations, Striolo says he and his team can now start designing molecules to make dispersions containing only the nanotubes they are interested in.

“Although the technique is not yet ready, our strategy is clear – we will design small molecules of surfactants that form aggregates with well-defined morphologies on nanotubes as a function of tube diameter and chirality,” he explained.

The researchers say that the aqueous surfactant aggregates should be rigid and that the hydrophilic parts of the surfactants (the parts that like to remain in contact with water) should be as far away as possible from the nanotubes. Such a recipe should produce nanotubes of the desired diameter and chirality.

The team is now busy designing such optimal surfactants. “We are building a library to describe the behaviour of several known surfactants,” Striolo told *nanotechweb.org*. “Some of these surfactants are known to be effective in stabilising nanotube dispersions – for example, FMN, sodium dodecyl benzene sulphonate and bile salts – while others are not (sodium dodecyl sulphate).”

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