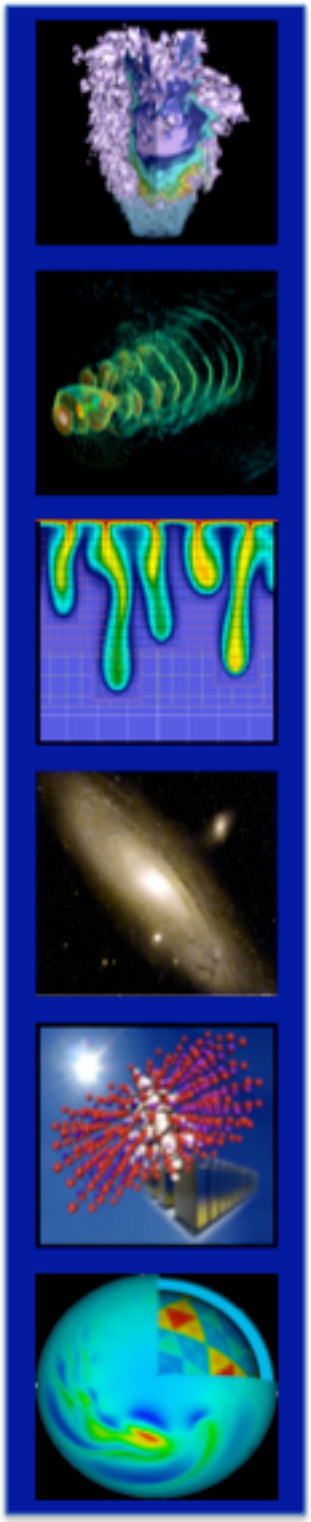


NERSC Science Highlights
March 2010

A selection of scientific results produced by NERSC users.

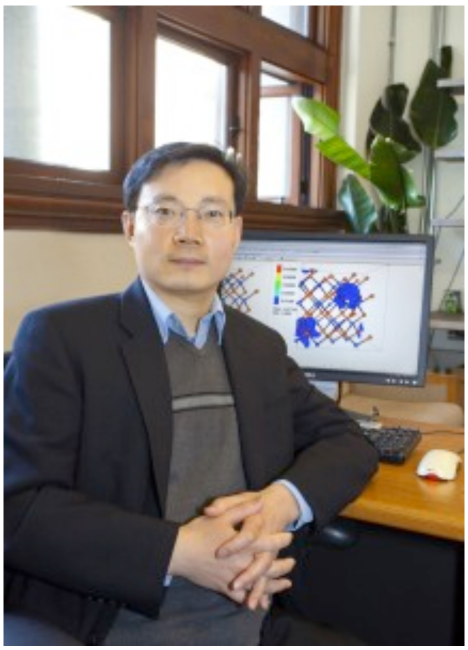
Prepared by the
National Energy Research Scientific Computing Center
Lawrence Berkeley National Laboratory
Berkeley, CA 94720

Mismatched alloys are a good match for thermoelectrics

Posted By lcyarris On January 25, 2010 @ 11:06 am In Feature Stories | Comments Disabled

Employing some of the world's most powerful supercomputers, scientists at Lawrence Berkeley National Laboratory have shown that mismatched alloys are a good match for the future development of high performance thermoelectric devices. Thermoelectrics hold enormous potential for green energy production because of their ability to convert heat into electricity.

Computations performed on "Franklin," a Cray XT4 massively parallel processing system operated by the National Energy Research Scientific Computing Center (NERSC), showed that the introduction of oxygen impurities into a unique class of semiconductors known as highly mismatched alloys (HMAs) can substantially enhance the thermoelectric performance of these materials without the customary degradation in electric conductivity.



[1]

Junqiao Wu, a Berkeley Lab/UC Berkeley physicist, used a NERSC supercomputer to show that the thermoelectric performance of highly mismatched alloys can be substantially enhanced by the introduction of oxygen impurities. (Photo by Roy Kaltschmidt, Berkeley Lab Public Affairs)

"We are predicting a range of inexpensive, abundant, non-toxic materials in which the band structure can be widely tuned for maximal thermoelectric efficiency," says Junqiao Wu, a physicist with Berkeley Lab's Materials Sciences Division and a professor with UC Berkeley's Department of Materials Science and Engineering who led this research.

"Specifically, we've shown that the hybridization of electronic wave functions of alloy constituents in HMAs makes it possible to enhance thermopower without much reduction of electric conductivity, which is not the case for conventional thermoelectric materials," he says.

Collaborating with Wu on this work were Joo-Hyoung Lee and Jeffrey Grossman, both now at the Massachusetts Institute of Technology. The team published a paper on these results in Physical Review Letters titled, "Enhancing the Thermoelectric Power Factor with Highly Mismatched Isoelectronic Doping."

Seebeck Effect and Green Energy

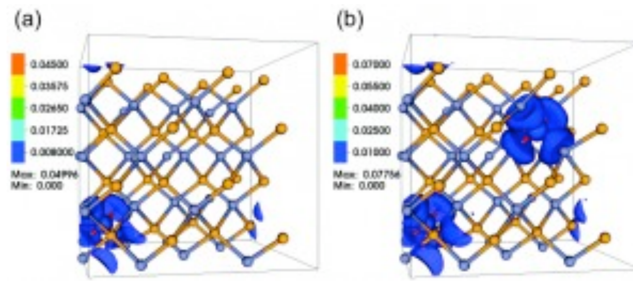
In 1821, the German-Estonian physicist Thomas Johann Seebeck observed that a temperature difference between two ends of a metal bar created an electrical current in between, with the voltage being directly proportional to the temperature difference. This phenomenon became known as the Seebeck thermoelectric effect and it holds great promise for capturing and converting into electricity some of the vast amounts of heat now being lost in the turbine-driven production of electrical power. For this lost heat to be reclaimed, however, thermoelectric efficiency must be significantly improved.

"Good thermoelectric materials should have high thermopower, high electric conductivity, and low thermal conductivity," says Wu. "Enhancement in thermoelectric performance can be achieved by reducing thermal conductivity through nanostructuring. However, increasing performance by increasing thermopower has proven difficult because an increase in thermopower has typically come at the cost of a decrease in electric conductivity."

To get around this conundrum, Wu and his colleagues turned to HMAs, an unusual new class of materials whose development has been led by another physicist with Berkeley Lab's Materials

Sciences Division, Wladyslaw Walukiewicz. HMAs are formed from alloys that are highly mismatched in terms of electronegativity, which is a measurement of their ability to attract electrons. The partial replacement of anions with highly electronegative isoelectronic ions makes it possible to fabricate HMAs whose properties can be dramatically altered with only a small amount of doping. Anions are negatively charged atoms and isoelectronic ions are different elements that have identical electronic configurations.

"In HMAs, the hybridization between extended states of the majority component and localized states of the minority component results in a strong band restructuring, leading to peaks in the electronic density of states and new sub bands in the original band structure," Wu says. "Owing to the extended states hybridized into these sub bands, high electric conductivity is largely maintained in spite of alloy scattering."



[2]

Contour plots showing electronic density of states in HMAs created from zinc selenide by the addition of (a) 3.125-percent oxygen atoms, and (b) 6.25 percent oxygen. The zinc and selenium atoms are shown in light blue and orange. Oxygen atoms (dark blue) are surrounded by high electronic density regions. (Image provided by Junqiao Wu)

In their theoretical work, Wu and his colleagues discovered that this type of electronic structure engineering can be greatly beneficial for thermoelectricity. Working with the semiconductor zinc selenide, they simulated the introduction of two dilute concentrations of oxygen atoms (3.125 and 6.25 percent respectively) to create model HMAs. In both cases, the oxygen impurities were shown to induce peaks in the electronic density of states above the conduction band minimum. It was also shown that charge densities near the density of state peaks were substantially attracted toward the highly electronegative oxygen atoms.

Wu and his colleagues found that for each of the simulation scenarios, the impurity-induced peaks in the electronic density of states resulted in a "sharp increase" of both thermopower and electric conductivity compared to oxygen-free zinc selenide. The increases were by factors of 30 and 180 respectively.

"Furthermore, this effect is found to be absent when the impurity electronegativity matches the host that it substitutes," Wu says. "These results suggest that highly electronegativity-mismatched alloys can be designed for high performance thermoelectric applications."

Wu and his research group are now working to actually synthesize HMAs for physical testing in the laboratory. In addition to capturing energy that is now being wasted, Wu believes that HMA-based thermoelectrics can also be used for solid state cooling, in which a thermoelectric device is used to cool other devices or materials.

"Thermoelectric coolers have advantages over conventional refrigeration technology in that they have no moving parts, need little maintenance, and work at a much smaller spatial scale," Wu says.

This project was supported under Berkeley Lab's Laboratory Directed Research and Development Program.

Berkeley Lab is a U.S. Department of Energy national laboratory located in Berkeley, California. It conducts unclassified scientific research for DOE's Office of Science and is managed by the University of California. Visit our Website at www.lbl.gov/

Additional Information

For more information on the research of Junqiao Wu, visit his Website at www.mse.berkeley.edu/~jwu/ [3]

The paper "Enhancing the Thermoelectric Power Factor with Highly Mismatched Isoelectronic Doping" can be viewed on the Website of Physical Review Letters at http://www2.me.berkeley.edu/~jwu/publications/Lee-PRL-10.pdf [4]

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[1] Image: **http://newscenter.lbl.gov/wp-content/uploads/Junqiao-Wu.jpg**
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[3] www.mse.berkeley.edu/~jwu/: **http://www.mse.berkeley.edu/%7Ejwu/**
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NERSC Helps Researchers Discover a Potential On-Off Switch for Nanoelectronics

December 22, 2009

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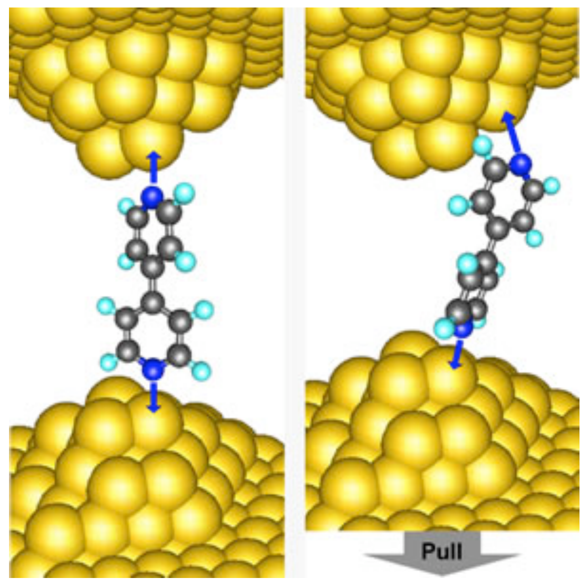
Computing Sciences Contact: Linda Vu, lvu@lbl.gov, 510-495-2402
Molecular Foundry Contact: Aditi Risbud, ASRisbud@lbl.gov, 510-486-4861

Researchers at the Lawrence Berkeley National Laboratory's (Berkeley Lab) Molecular Foundry and Columbia University found that electrical resistance through a molecular junction—a nanometer scale circuit element consisting of a single molecule contacted with gold wires—can be turned on and off by simply pushing and pulling the junction. Experts believe that this newly demonstrated molecular-scale control could be leveraged for future nanoscale electronic devices.



These schematics illustrate the vertical and angled molecular junction configurations for mechanically induced switching. A study has revealed that electrical resistance through such a junction can be turned on and off simply by pushing (left) so that the configuration is vertical or by pulling the junction (right) so that the configuation is angled.

The switching phenomenon was initially discovered in experiments conducted by a team of researchers led by Latha Venkataraman of Columbia University. But the underlying physics would only later be understood when a group of theorists led by Jeff Neaton at Berkeley Lab's Molecular Foundry teamed up with the Columbia researchers to develop a theory to describe the conductance of individual molecules trapped between gold electrodes. This work was done with the help of the National Energy Research Scientific Computing Center's (NERSC) Cray XT4 system, named Franklin.

"If we wish to ultimately design circuit elements at the molecular scale, we need to understand how the intrinsic properties of a molecule or junction are actually connected to its measured resistance," said Neaton. "Knowing where each and every atom is in a single-molecule junction is simply beyond what's possible with experiments at this stage. For these sub-nanometer scale junctions—just a handful of atoms—theory can be valuable in helping interpret and understand resistance measurements."

Experiments Meet Theory

In traditional electronic devices, charge-carrying electrons diffuse through circuits in a well understood fashion, gaining or losing energy through transactions with impurities or other particles they encounter. Electrons at the nanoscale, however, can travel by a mechanism called quantum tunneling in which, due to the small length scales involved, it becomes possible for a particle to disappear through an energy barrier and suddenly appear on the other side, without expending energy. Tracking such tunneling of electrons through individual molecules in nanoscale devices has proven difficult.

"The high throughput and magnitude of the NERSC resources facilitated a highly interactive back-and-forth with experimentalists, allowing us to rapidly modify our calculations and compare with experimental results as they became available."

—Jeff Neaton, Facility Director of the Theory of Nanostructured Materials Facility at The Molecular Foundry

"You can't use a microscope to see that a molecule is trapped, you can only sense it indirectly through electrical conductivity data, for example. For more than a decade, researchers have been 'wiring up' individual molecules and measuring their electrical conductance," said Neaton.

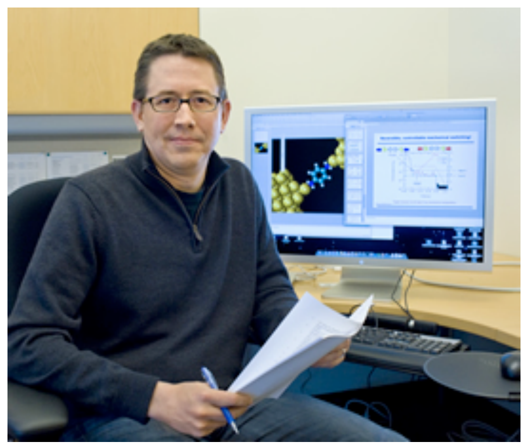
He notes that routine formation of high quality electrical contacts, or "alligator clips," between nanostructures and electrical leads is extremely challenging. This makes experiments difficult to interpret; as a result, the reported conductance values-in experiment and theory often varied by an order of magnitude or more. The time was ripe for a quantitative comparison between theory and an experiment with well defined contacts, a collaboration made possible by the Molecular Foundry User Program.

One tool experimental researchers use to probe changes in nanostructure currents is called a scanning tunneling microscope (STM), which has a conductive gold tip. Previous work had shown a gold STM tip could repeatedly be plunged into a gold surface containing a solution of molecules and retracted, until the contact area between the tip and gold surface reduces to a single strand, like a necklace. When this strand finally breaks, nearby molecules can hop into the gap between strands and contact the gold electrodes, resulting in a sudden change in conductance. Using this technique, Venkataraman and her colleagues discovered that the conductance of molecules terminated by amines (related to ammonia) in contact with gold electrodes could be reliably measured.

Using a new theoretical approach, Neaton and his collaborators also began to study the conductance of a junction between gold electrodes and bipyridine—an aromatic molecule with two benzene-like rings, each containing one nitrogen atom. They hypothesized about the conductance of junctions arranged vertically between gold molecules and sandwiched at angles, working closely with the laboratory researchers to compare their computer-generated predictions with experiments.

According to Neaton, the team used computational methods based on parameter-free first-principles calculations and NERSC's Franklin system to test these hypotheses. First-principles methods are atomic-scale computational approaches with the ability to predict measurable properties of materials with good accuracy from scratch, i.e., through solution of the quantum mechanics of a system of interacting electrons in a field of nuclei. Using a new approach based on these methods, the electrical resistance of bipyridine-gold molecular junctions was evaluated in different conformations.

"Computing properties of bipyridine-gold molecular junctions related to its electrical conductance for different conformations using first-principles approaches is computationally demanding," said Neaton. "The high throughput and magnitude of the NERSC resources facilitated a highly interactive back-and-forth with experimentalists, allowing us to rapidly modify our calculations and compare with experimental results as they became available."



Jeffrey Neaton is Facility Director of the Theory of Nanostructured Materials Facility at the Molecular Foundry.

After the researchers had plugged away for more than a year, the story that emerged was surprisingly detailed: if bipyridine bonded at an angle, more current could flow through the junction compared with the bipyridine bonded in a vertical configuration. This suggests the conductance of bipyridine was linked to the molecule's orientation in the junction. In experiments, these scientists noticed when the final strand of gold atoms breaks and snaps back, the vertical gap is not big enough for bipyridine to insert itself in line, so instead it bonds at an angle. As the gap increases, the molecule jumps to a vertical configuration, causing the conductance to plummet abruptly. Eventually, the molecule straightens even more, and the contact breaks.

"Once we determined this, we wondered,'Could you reverse this behavior?'" said Su Ying Quek, a postdoctoral researcher at the Molecular Foundry who was involved in the theory development.

In experiments, Quek and Neaton were able to demonstrate why pushing the junction to an angle and pulling it straight could repeatedly alter the conductance, creating a mechanical switch with well defined on and off states.

"One of the fascinating things about this experiment is the degree to which it is possible to control the 'alligator clips,'" said Neaton. "For this particular molecule, bipyridine, experiments can reproducibly alter the atomic-scale interface between the molecule and its gold contacts back and forth to switch the conductance of the junction."

Quek and Neaton hope to refine and apply their theoretical framework to promising systems for solar energy conversion and multi-electron heterogeneous catalysis, where controlling charge dynamics at nanoscale interfaces is central.

"Understanding how electrons move through single-molecule junctions is the first step," said Neaton. "Organic-inorganic interfaces are everywhere in nanoscience, and developing a better picture of charge transport in hybrid materials systems will certainly lead to the discovery of new and improved electronic devices."

"Mechanically controlled binary conductance switching of a single-molecule junction," by Su Ying Quek, Maria Kamenetska, Michael L. Steigerwald, Hyoung Joon Choi, Steven G. Louie, Mark S. Hybertsen, J.B. Neaton and L. Venkataraman, appears in Nature Nanotechnology and is available online. **Click here** for the paper.

For more information about this research, please visit:
http://newscenter.lbl.gov/press-releases/2009/03/02/researchers-discover-a-potential-on-off-switch-for-nanoelectronics/

Work at the Molecular Foundry was supported by the Director, Office of Science, Office of Basic Energy Sciences, Division of Materials Science and Engineering, of the DOE under Contract No. DE-AC02-05CH11231, and by the National Science Foundation through its Nanoscale Science and Engineering Initiative.

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. 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 DOE Office of Science.

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A Computational Science Approach for Analyzing Culture

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

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February 18, 2010

Just as photography revolutionized the study of art by allowing millions of people all over the world to scrutinize sculptures and paintings outside of museums, researchers from the Software Studies Initiative at the University of California at San Diego (UCSD) believe that a new paradigm called *cultural analytics* will drastically change the study of culture by allowing people to quantify evolving trends across time and countries.

Click here to watch Jeremy Douglass talk about Cultural Analytics.

Inspired by scientists who have long used computers to transform simulations and experimental data into multi-dimensional models that can then be dissected and analyzed, cultural analytics applies similar techniques to cultural data. With an allocation on the Department of Energy's National Energy Research Scientific Computing Center's (NERSC) supercomputers and help from the facility's analytics team, UCSD researchers recently illustrated changing trends in media and design across the 20th and 21st centuries via Time magazine covers and Google logos.

"The explosive growth of cultural content on the web, including social media together with digitization efforts by museums, libraries and companies, make possible a fundamentally new paradigm for the study of both contemporary and historical cultures," says Lev Manovich, Director of the Software Studies Initiative at the University of California, San Diego.

"The cultural analytics paradigm provides powerful tools for researchers to map subjective impressions of art into numerical descriptors like intensities of color, texture and shapes, as well as the organization of images using classification techniques," says Daniela Ushizima of the NERSC Analytics team, who contributed pattern recognition codes to the cultural analytics image-processing pipeline.

Manovich's research, called "Visualizing Patterns in Databases of Cultural Images and Video," is one of three projects currently participating in the Humanities High Performance Computing Program, an initiative that gives humanities researchers access to some of the world’s most powerful supercomputers, typically reserved for cutting-edge scientific research. The program was established in 2008 as a unique collaboration between DOE and the National Endowment for the Humanities.

"For decades NERSC has provided high-end computing resources and expertise to thousands science users annually. These resources have contributed to a number of science breakthroughs that have improved our understanding of nature. By opening up these computing resources to humanities, we will also gain a better understanding of human culture and history," says NERSC Division Director Kathy Yelick.

Visualizing Cultural Changes in Time Covers and Google logos

As relatively inexpensive hardware and software empowers libraries, museums and universities to digitize historical collections of art, music and literature, and as masses of people continue to create and publish their own movies, music and artwork on the Internet, Manovich predicts that the biggest challenge facing cultural analytics will be securing enough computing resources to process, manage and visualize this data at a high-enough resolution for analysis.

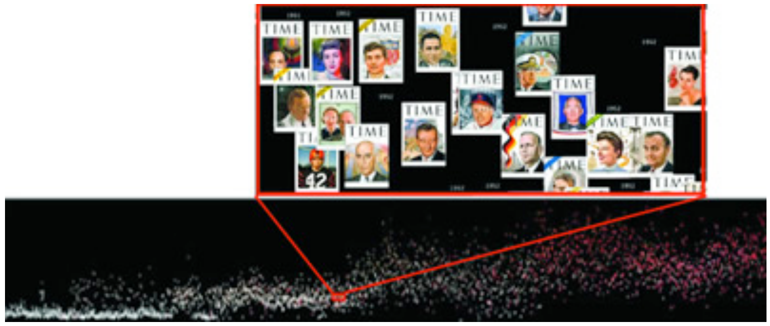

Figure 1. TIME OVER TIME: (Bottom Image) This is a graph of all the Time magazine covers of the 20th century. (Top Image) This is a high resolution cutout from the image below. Click on the image to download a high-resolution version of the graph.

Over the past few months, Manovich and his collaborators leveraged the expertise of NERSC's analytics team to help them to develop a pipeline for processing cultural images and to scale up their existing codes to run on NERSC's high-end computing systems. To test their pipeline, the team mapped out all 4,553 covers of Time magazine from 1923 to 2008 and all the Google logos that have been published on the search engine's homepage around the world from 1998 to 2009.

In the Time magazine visualization (Fig. 1), the X-axis represents time in years, from the beginning of the 20th century shown on the left to the early 21st century on the right. The Y-axis measures the brightness and saturation hue of each cover, with the most colorful covers appearing toward the top.

"Visualizing the Time covers in this format reveals gradual historical changes in the design and content of the magazine," says Manovich. "For example, we see how color comes in over time, with black and white and color covers co-existing for a long period. Saturation and contrast of covers gradually increases throughout the 20th century—but surprisingly, this trend appears to stop toward the very end of the century, with designers using less color in the last decade."

He notes that there are also various changes in magazine content revealed by the visualization. "We see when women and people of color start to be featured, how the subjects diversify to include sports, culture, and topics besides politics, and so on. Since our high-resolution visualizations show the actual covers rather than using points or other graphical primitives typical of standard quantitative graphics, a single visualization reveals many trends at once; it is also accessible to a wider audience than statistical graphs," adds Manovich.

Using NERSC computers, Jeremy Douglass, a post-doctoral researcher with Software Studies, also applied cultural analytics techniques to hundreds of Google logos that have appeared on the search engine's homepage all over the world from 1998 to the present (fig. 2). Artists periodically reinterpret logos on the Google homepage to mark a cultural milestone, a holiday or a special occasion. In the visualization, the X-axis measures how much the various logos deviate from the original design. Images toward the left show very little modification and those toward the right have been significantly modified. Meanwhile, the images toward the bottom of the Y-axis illustrate artistic changes that affect the bottom of the word "Google," and those toward the top show changes toward the upper portion of the word.

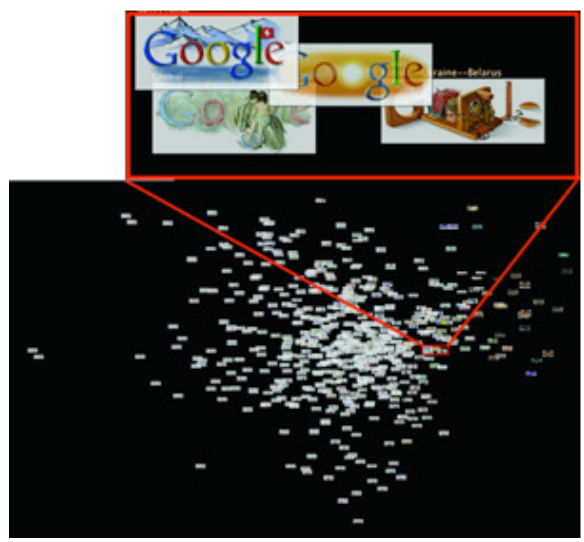

Figure 2. ANALYZING GOOGLE: (Bottom) This graphic shows hundreds of Google logos that have appeared on the search engine's homepage all over the world from 1998 to the present. (Top) This is a high-resolution cutout from the image below. Click on the image to download a high-resolution version of the graph.

"Google logos are relatively small, and there have so far only been less than 600 of them, so the act of rendering full-resolution maps is quite doable with a desktop workstation. However, we were interested in using data exploration to tackle ideas about visual composition and statistical concepts like centroid, skewness, kurtosis, and so forth," says Douglass.

To explore how these and other concepts might contribute to mapping the "space of aesthetic variation," Douglass notes that the team needed to experiment. "That's where the ability to iterate with NERSC's analytics team becomes so important. When you want to repeatedly re-render 4553 high-resolution images and be able to see how they evolve over time according to various features, 'How long will this take?' become a very big deal, and there's no such thing as too much power," he adds.

The cultural analytics team ultimately hopes to create tools that will allow digital media schools and universities to compare hundreds of thousands of videos and images in real time to facilitate live discussions with students. They also hope to create visualizations that will measure in many millions of pixels and show patterns across tens of millions of images. Although they are currently only beginning to develop software for cultural analytics, Manovich says the NERSC runs showed him that supercomputers are a "game changer" and will be vital to achieving this goal.

"Datasets that would take us months to process on our local desktop machines can be completed in only a few hours on the NERSC systems, and this significantly speeds up our workflow," says Manovich. "The NERSC analytics team has been incredibly helpful to our work. In addition to helping us develop the technical tools to process our data, they also share in our excitement, often sending us information that might be useful to the project."

Currently Manovich and his collaborators are using NERSC computers to analyze and visualize patterns across 10 million comic book images from around the globe.

"Contemporary culture is constantly evolving with the advancement of technology. Billions of pictures, video and audio files are uploaded to the Internet every day by ordinary people all over the world. Cultural analytics is an emerging paradigm to make visible patterns contained in this ocean of media," says Manovich.

"Working with Lev Manovich gave me a lot to think about in terms of how high performance computing is underutilized in the humanities and how it could potentially accelerate knowledge discovery," says Janet Jacobsen of the NERSC analytics group. "All in all, this has been a really fun project to be involved with. These researchers are doing something that no one else in their field is doing."

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Hopper (Phase 1) Prepares NERSC for Petascale Computing

February 26, 2010

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Contact: Linda Vu, lvu@lbl.gov, (510)495-2402

After several months of rigorous scientific testing, the Department of Energy's (DOE) National Energy Research Scientific Computing Center (NERSC) has accepted a 5,312-core Cray XT5 machine, called Hopper (Phase 1).

Credit: Photo by Roy Kaltschmidt

(Left) Hopper (Phase 1) is a Cray XT5 with 664 compute nodes each containing two 2.4 GHz AMD Opteron quad-core processors. (Left) The Hopper external Lustre File System contains 2 PB of disk space.

Innovatively built with external login nodes and an external filesystem, Hopper Phase 1 will help NERSC staff optimize the external node architecture before the second phase of the Hopper system arrives. Phase 2 will be a petascale system comprised of 150,000 processor cores and built on next generation Cray technology.

"Working out the kinks in Phase 1 will ensure a more risk-free deployment when Phase 2 arrives," says Jonathan Carter, who heads NERSC's User Services Group and led the Hopper system procurement. "Before accepting the Phase 1 Hopper system, we encouraged all 300 science projects computing at NERSC to use the system during the pre-production period to see whether it could withstand the gamut of scientific demands that we typically see."

According to Katie Antypas, a consultant in the NERSC User Services Group, the new external login nodes on Hopper offer users a more responsive environment. Compared to the Cray XT4 platform, called Franklin, the external login nodes have more memory, and in aggregate, have more computing power. This allows users to compile applications faster and run small post-processing or visualization jobs directly on the login nodes without interference from other users.

Because Hopper has 2 PB of disk space and 25 GB/sec of bandwidth on the external filesystem, users with extreme data demands will see few bottlenecks when they move their data in and out of the machine. Additionally, the availability of dynamically loaded libraries enables even more applications to run on the system and adds support for popular frameworks like Python. This feature helps ensure that the system is optimized for scientific productivity.

"Hopper turned out to be a lot faster than we anticipated, which allowed us to run more simulations at higher resolutions," says Yi-Min Huang, a research scientist in the Space Plasma Theory Group at the University of New Hampshire.

With pre-production computing time on Hopper, Huang and his colleague Amitava Bhattacharjee, professor of physics at the University of New Hampshire, ran extremely detailed simulations of magnetic reconnection, a process by which magnetic field lines break and rejoin, releasing tremendous amounts of energy along the way. This research is vital for understanding solar flares that can disrupt long-range radio communications on Earth, and will help researchers refine the design of magnetic confinement devices for creating zero-emission fusion energy.

"The computing time on Hopper encouraged us to explore magnetic reconnection in the high-Lundquist-number regime in greater detail that we wouldn't have done otherwise. In fact, our high-resolution runs on Hopper showed us that some of our previous simulations were not fully resolved, and thus not as reliable as we believed," says Huang. "The experience we gained from these simulations is invaluable for our future pursuit in this area with our NERSC allocations."

Meanwhile professor Artem Masunov, of the University of Central Florida's NanoScience Technology Center, and his graduate student Workalemahu Mikre, used the free pre-production time on Hopper to better understand the force that drives peptide aggregation into amyloid fibrils, a process which causes neurodegenerative diseases like Alzheimer's, Parkinson's and Type II diabetes. In addition to understanding peptide aggregation, Mikre is also designing small molecules to prevent it.

"With the free pre-production time on Hopper, I could run my simulation on 300 to 400 processor cores for about 12 to 24 hours. As a result, my adviser and I identified which small molecules and mutations led to the fastest disaggregation of decamer assemblies composed of several hexapeptides, including insulin, tau, and Aβ fragments," says Mikre. "This knowledge could contribute to the rational design of drugs for Alzheimer's treatment and amyloid-specific biomarkers for diagnostic purposes."

"The primary reason for architecting Phase-1 of Hopper differently was to make it more productive and user-friendly for our diverse set of science users," says Carter. "Although the technology that makes up the compute portion of Phase 1 of Hopper is newer, it does not differ significantly from the hardware on Franklin. The increase in usability is largely due to the external node architecture."

The hardware for Phase-2 will be delivered later this year.

For more information about Hopper, please visit:
http://www.lbl.gov/cs/CSnews/CSnews103009a.html
http://www.lbl.gov/cs/Archive/news080509.html
http://www.nersc.gov/nusers/systems/hopper/

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Historic Sudbury Neutrino Observatory Data, Carried by ESnet, Lives on at NERSC

February 26, 2010

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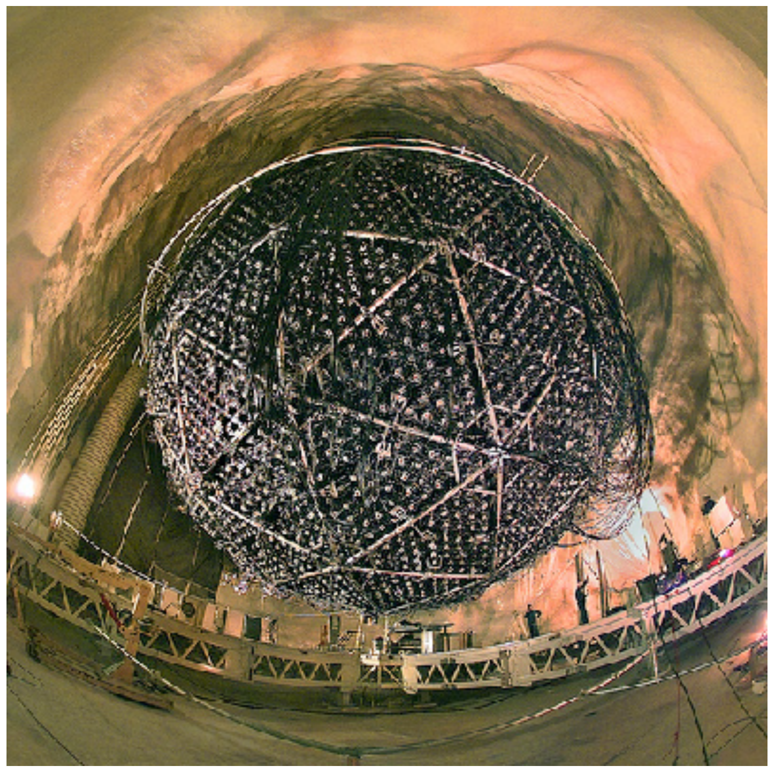
Contact: Linda Vu, lvu@lbl.gov, (510)495-2402

Tunneled 6,800 feet underground in Canada's Vale Inco Creighton mine, the Sudbury Neutrino Observatory (SNO) was designed to detect neutrinos produced by fusion reactions in the Sun. Although the observatory officially "switched off" in August 2006, a copy of all the data generated for and by the experiment will live on at the National Energy Research Scientific Computing Center (NERSC).



Credit: Photo by Roy Kaltschmidt

SNO onsists of an 18-meters-in-diameter stainless steel geodesic sphere inside of which is an acrylic vessel filled with 1000 tons of heavy water (deuterium oxide or D2O). Attached to the sphere are 9,522 ultra-sensitive light-sensors called photomultiplier tubes. When neutrinos passing through the heavy water interact with deuterium nuclei, flashes of light are emitted. The photomultiplier tubes detect these light flashes and convert them into electronic signals that scientists can analyze for the presence of all three types of neutrinos.

"NERSC has been providing great support to SNO for over a decade. We used the PDSF cluster do some of the early analyses and were really appreciative of the support that we received from NERSC staff. When we looked around at different facilities and talked to colleagues that have used the center's High Performance Storage System [HPSS] extensively, we immediately concluded that one copy of our data should be stored at NERSC," says Alan Poon, a member of the SNO collaboration at the Lawrence Berkeley National Laboratory (Berkeley Lab).

"The Department of Energy invested a lot of resources into SNO, and we believe that preserving these datasets at NERSC will afford the best protection of the agency's investment," he adds.

According to Poon, the SNO experiment has made tremendous contributions to humanity's understanding of neutrinos, invisible elementary particles that permeate the cosmos. Before the observatory started searching for solar neutrinos on Earth, all experiments up to that point detected only a fraction of the particles predicted to exist by detailed theories of energy production in the Sun. Results from the SNO experiment eventually revealed that the total number of neutrinos produced in the Sun is just as predicted by solar models, but the neutrinos are oscillating in transit, changing in type or "flavor" from electron neutrinos (the flavor produced in the Sun) to muon or tau neutrinos. In 2001, Science Magazine identified SNO's solution to the solar neutrino mystery as one of their 10 science breakthroughs of the year.

"SNO data will be unique for decades to come. There will not be another experiment in the foreseeable future that would provide the same measurement with better precision and accuracy," says Ryan Martin, a postdoctoral researcher at the Berkeley Lab who helped migrate data from disks at the SNO facility in Sudbury, Canada, to the NERSC facility in Oakland, Calif. "It is important to preserve this data for the scientific community, in case a new theory would require further studies of the data."

Martin worked closely with Damian Hazen of NERSC's Storage Systems Group to transfer 26 terabytes of data across the DOE's Energy Sciences Network (ESnet) to NERSC's HPSS. This set includes everything from the raw data generated by the experiment and processed data used during analysis to the computer codes and simulations used for detector design and scientific computation.

"From testing the transfer speed, tuning the network and identifying packet losses, to the final archiving at HPSS, the center's expertise saved us a lot of headache," says Martin. "These are technical issues that laymen like us would take a long time to solve, if at all. We have been really pleased with the help that NERSC staff have provided."

For more information about SNO, please visit:
http://newscenter.lbl.gov/feature-stories/2003/09/23/a-dash-of-salt-enhances-sno-results/

For more information about Computing Sciences at Berkeley Lab, please visit:
http://www.lbl.gov/cs