



News from the National Energy Research Scientific Computing Center

November 2006

Depositing a Slice of Universe

NERSC will keep terabytes of data from outer space

Data from the world's largest radio telescope, which scans the sky for signs of pulsars, black holes and extraterrestrial civilizations, have found a new home in NERSC's vast storage system.

Led by Dan Werthimer, a scientist at UC Berkeley's Space Sciences Laboratory, the "Berkeley High Resolution Neutral Hydrogen Sky Survey" recently began feeding hundreds of gigabytes of data daily to the High Performance Storage System (HPSS).

Collected by the Arecibo telescope in Puerto Rico, the radio signal data will provide valuable information to astrophysicists, cosmologists and other researchers who aim to solve some of the most intriguing mysteries about the universe. Arecibo, a 305-meter dish, is operated by Cornell University under an agreement with the National Science Foundation.

"Before we received assistance from NERSC, our sky survey data was stored on over 1,000 tapes. So it was very difficult to access," Werthimer said. "NERSC will allow us to



Serving up the cosmos: The Arecibo dish in Puerto Rico detects radio signals emitted from space and helps researchers understand stars, dark energy and everything in between.

make our data accessible to the scientific community for a variety of research projects."

For Werthimer and his research team, the

data will help advance three projects: SETI@home, AstroPulse and hydrogen mapping. SETI@home, launched in 1995, seeks (continued on page 2)

Fast and Furious

Particle accelerator research yields impressive images

A project to create 3D simulations of laser-driven wakefield particle accelerators has produced new images clarifying the three-dimensional evolution of the laser driver and accelerated electron beam. The project won an allocation of 2.5 million hours on NERCS' Seaborg supercomputer this year as part of DOE's Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program.



Cameron Geddes

Led by Cameron Geddes, a scientist at the Accelerator and Fusion Research Division at Berkeley Lab, the research aims to improve (continued on page 3)

Mining for Calculations

Model for impurities analysis will advance material sciences

Researchers at the Colorado School of Mines and Northwestern University have developed a novel way to quantify the kinetics of interfaces—or defects—in materials, a feat that was recently chronicled in the journal Science.

Moneesh Upmanyu and his research team used NERSC and other resources to create the mathematical model that can determine the impact of interfaces on the mechanical, chemical, and other properties of otherwise pristine materials, whether they occur naturally or are man-made.

The research, described in a paper titled, "Interface Mobility from (continued on page 2)



Universe (continued from page 1)

evidence of extraterrestrial civilizations by searching for certain types of radio signals that, because of their narrow bandwidths, don't occur naturally.

The SETI (Search for Extraterrestrial Intelligence) project has created a global distributed computing network spanning 226 countries that invites anyone with an Internet-connected computer to join. So far, it has attracted more than 5.2 million participants, whose personal computers help to crunch the data from Arecibo.

AstroPulse, on the other hand, will look for a type of dispersed radio pulses that are shorter than the ones sought by SETI@home. The microsecond pulses could come from rapidly spinning pulsars, black holes or extraterrestrial intelligence.

Both SETI@home and AstroPulse run on BOINC, an open-source software. BOINC, developed by David Anderson and his team at the Space Sciences Lab, makes it easy to develop and manage distributed computing projects. Projects that take advantage of BOINC include Einstein@home at the University of Wisconsin and LHC@home at CERN.

The third project maps the galactic distribution of hydrogen. The high-resolution map will provide a wealth of three-dimensional information such as the density and temperature of interstellar objects, enabling researchers to better understand the structure and dynamics of our galaxy.

"We recognize the importance of Dan's projects to advance a wide-range of space research," said Francesca Verdier, Associate General Manager for Science Driven Services at NERSC. "The data from Arecibo will be put to good use by the scientific community worldwide."

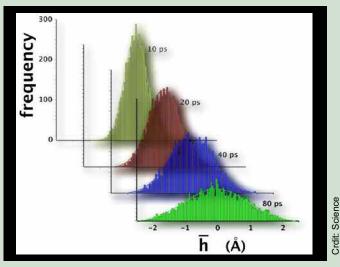
Werthimer plans to store 200 terabytes of data over two years at HPSS. HPSS, which was put in place in 1998, currently has a theoretical capacity of 30 petabytes. It's capable of swallowing up data at 450 megabytes per second.

Find out more about Werthimer's projects and BOINC at http://www.ssl.berkeley.edu/research/index.php.

Mining (continued from page 1)

Interface Random Walk," is critical for engineering high-performing materials, such as thin films, composites, and polycrystals. Those materials are building blocks for the next-generation solar energy generators and batteries, for example.

To create a more accurate comparison, scientists need to factor in more realistic driving forces and include the effect of impurities. The formalism developed by Upmanyu and his team has done just that. They based their find on theoretical work by Einstein,



The time evolution in picoseconds (ps) of the distribution of the average grain boundary position. The distributions are normal, as predicted by the theory.

The microstructure of the interfaces, in turn, is affected by several forces. These driving forces can cause the microstructure to move and evolve. A quantitative measure of interface kinetics is the interface mobility, the ratio of the interface velocity to the driving force.

Past studies on individual homophase crystalline interfaces (or grain boundaries) in several highly pure metals show an interesting trend: the experimental mobilities are orders of magnitude smaller than those extracted via computations. The discrepancy is often attributed to the presence of impurities, fueling speculation that even minute quantities of impurities significantly slow down the interface motion.

"An often overlooked fact is that computations are limited to tens of nanoseconds," said Upmanyu, the lead researcher and an assistant professor in the engineering division and material sciences program at the Colorado School of Mines. "As a result, they are performed at driving forces orders of magnitude greater than those commonly observed in experiments."

Smulochowski and Langevin on Brownian motion in the early 1900s.

Previous experiments and calculations also show that the retarding effect of impurities is much more severe than previously thought. Upmanyu and his team plan to use their findings to directly quantify the impurity drag effect. The team, which has been using NERSC resources for over two years and running its data mainly on the Seaborg supercomputer, also includes Zachary Trautt, a graduate student in engineering at the Colorado School of Mines and Alain Karma, a physics professor at Northwestern University.

"We also utilized the NERSC on-line help to extend our in-house molecular dynamics code to a multi-threaded version (using Open MP), which enabled us to run large-scale parallel jobs." Upmanyu said.

You can learn more about the calculations and simulations done by the researchers here: http://www.sciencemag.org/cgi/content/abstract/314/5799/632.



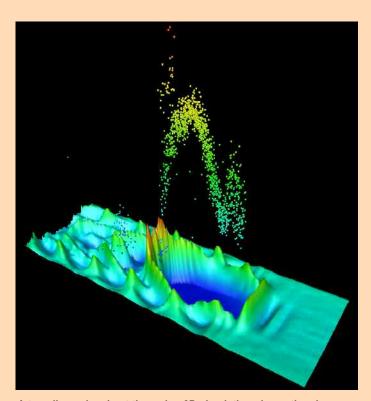
Fast (continued from page 1)

designs for next-generation accelerators that use laser-driven plasma waves to accelerate particles.

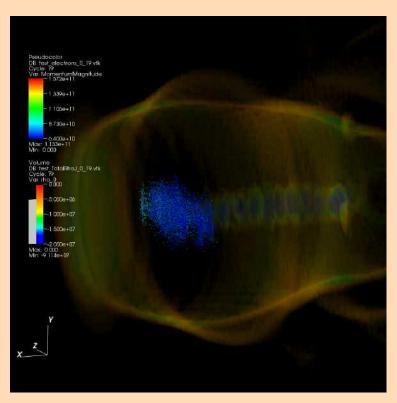
The high accelerating fields of these machines may lead to more compact accelerators for high-energy physics, which answers the questions about the origin of the universe and how it works.

The machines' compactness, and the ultra-short electron bunches produced, may revolutionize the use of accelerators in chemistry and biology by providing laboratory scale ultrafast radiation sources. Applications of these radiation sources include new medical diagnostic tools, materials and drugs.

Recent experiments have demonstrated high-quality beams from such accelerators, with accelerating fields thousands of times greater than those produced by conventional machines. Large-scale, 3D particle simulations done under INCITE clarify mechanisms of beam formation and evolution, and they have begun to identify potential optimizations in this emerging field.



A two-dimensional cut through a 3D simulation shows the plasma wave density (surface height) and reveals the particle momentum distribution versus position (spheres, height and color = momentum). Simulation by Cameron Geddes. Visualization by Cameron Geddes and Peter Messmer.



A 3D visualization showing the density of the plasma wave driven by the laser (volume shading), and positions of particles accelerated by that wave (blue spheres). Simulation by John Cary and Cameron Geddes. Visualization by Cristina Siegerist.

NERSC News

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