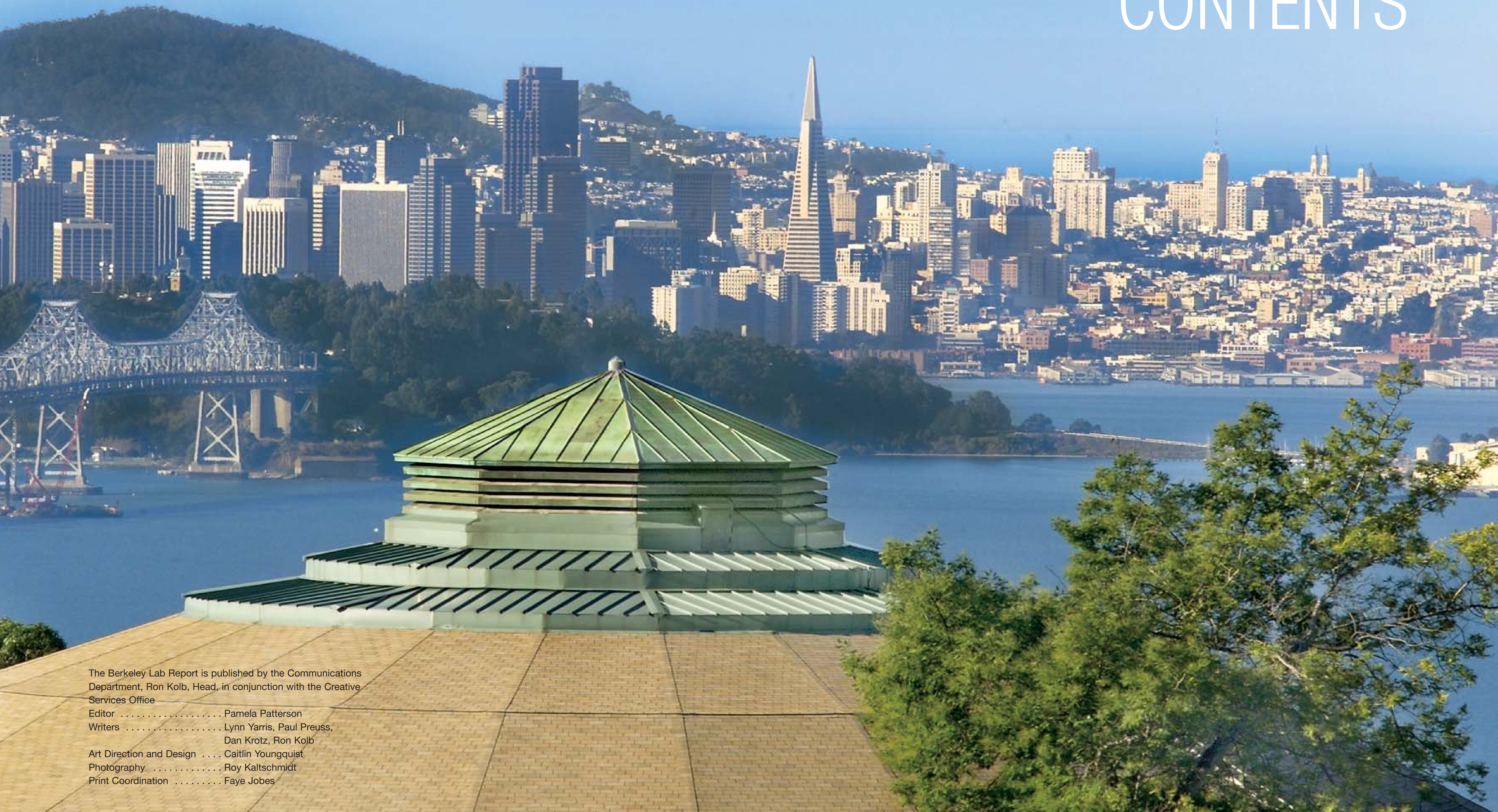
Berkeley Lab

A View to the Future

BERKELEY LAB 2005/2006 REPORT

CONTENTS



The Berkeley Lab Report is published by the Communications Department, Ron Kolb, Head, in conjunction with the Creative Services Office

Editor . . . . Pamela Patterson
Writers . . . . Lynn Yarris, Paul Preuss, Dan Krotz, Ron Kolb
Art Direction and Design . . . . Caitlin Youngquist
Photography . . . . Roy Kaltschmidt
Print Coordination . . . . Faye Jobes

About "A View to the Future"

When I first arrived at Berkeley Lab as its Director in August of 2004, I knew of this Laboratory's distinguished history — its nine Nobel Prizes, the pioneering "team science" created by founder Ernest Lawrence. We have a legacy of seminal contributions in the fields of high energy and nuclear physics, chemistry, accelerator science and, in more recent times, energy efficiency, advanced computing, materials, and the biosciences. I inherited an outstanding lab from my predecessor, Chuck Shank.

I knew that LBNL was a special place, but I did not know how special until I began to attend division reviews, Laboratory Directed Research and Development meetings, and began to work closely with the talented staff on the science and operations sides of the house. It became apparent to me why Berkeley Lab is regarded by the DOE as a national treasure.

Soon after I arrived, I became embroiled in the contract competition for continued management of Berkeley Lab by the University of California. Working with UC in its bid to retain the contract with the Department of Energy, our senior management team began to realize the exciting opportunities available because of the extraordinary resources of our Lab: the scientists and supporting staff, the national facilities, and the close proximity of UC Berkeley and UCSF.

In order to capture the full potential of these opportunities, we have formed alliances among the Lab's centers of excellence to attack various scientific and technological challenges. There are many outstanding examples of interdisciplinary work being done at the Lab that bring together areas in the biological sciences, the physical sciences, and the computational sciences. Many of these areas are outlined in the body of this report.

When I worked at Bell Laboratories, we were immersed in a culture of interdisciplinary problem-solving where research partnerships formed spontaneously over lunch in the cafeteria, after seminars, and in social events. While at Stanford, I wanted to duplicate this atmosphere and helped start Bio-X, the largest interdisciplinary initiative on campus, with several hundreds of millions of dollars of University support. Following Dr. Lawrence's collaborative approach to science, I see that a major part of my job is to make our collaborative environment even better.

A new Lab-wide initiative is starting to develop sustainable, CO_2– neutral sources of energy that will draw upon many of the core strengths of the Berkeley Lab. While energy efficiency will play a huge role in defining how much energy we will need, we must also have a diversified portfolio of investments in energy sources. Among America's most serious concerns are national security (intimately tied to energy security), long-term economic competitiveness, and the dangers of global warming. The need for CO_2– neutral energy is central to all of these concerns, and thus is the single most important societal problem that science and technology must solve.

There appear to be no magic bullets to solve this problem. Already, we are contributing to fusion research, the waste storage problems associated with fusion energy, and carbon sequestration of the combustion products of fossil fuel. Answers may also lie in greatly improved photovoltaic generation, efficient methods to convert electricity into chemical energy, and synthetic mimics of photosynthesis. Another promising avenue is to apply advances in molecular biology to develop faster-growing, self-fertilizing plants and more efficient methods to convert biomass (including biowaste) into more useful forms of energy.

Berkeley Lab is uniquely positioned to tackle this challenge, with its strengths in the biological, chemical and computational sciences; world-class facilities like the Advanced Light Source, the National Center for Electron Microscopy, NERSC, the Molecular Foundry; its distinguished corps of engineers; and its leadership in material science and nanotechnology. This is collectively a prodigious scientific resource, and we are capable of attacking this problem in a way reminiscent of Bell Laboratory's development of a solid state electronic switch (the transistor) to replace the vacuum tube.

There are more examples of interdisciplinary work that can be done at our Lab. In this Berkeley Lab Report, our scientific directions are summarized and our core competencies are described. Including goals for the next five years in six different areas, the Report is designed to help those who may not fully understand our work to appreciate the value that LBNL can continue to bring to our world. It is also my hope that those responsible for investing in scientific research in this country can learn about what we do and how we are impacting science, society and our future generations.

The knowledge we acquire in science is additive, and at its core is our ability to be stimulated by others. Through our collective efforts, we will do far more than we can separately. By creating a fertile, supporting environment of creativity and innovation, we will accomplish great things as we prepare to celebrate Lawrence Berkeley National Laboratory's 75th year of service.

Steve Chu
Director

Securing a Cleaner Tomorrow

The world is at a crossroads. Each year, energy consumption increases and more greenhouse gases are emitted into the atmosphere. By 2020, one-third of the world's population may lack access to clean water, air, and affordable energy. That same year, it's estimated that U.S. energy demands will have risen 40 percent from today's levels, an increase that far outpaces the nation's energy production capabilities.

If steps aren't soon taken, tomorrow's generation will inherit a world that looks vastly different than today's. That's why Berkeley Lab scientists are spearheading several initiatives designed to mitigate the environmental impacts of the nation's fossil-fuel-dependent economy and more efficiently utilize today's energy sources.

Working in conjunction with partners in industry and academia, they are tackling some of the most pressing problems of the 21st century. They're learning how to trap carbon dioxide, a greenhouse gas, deep underground and possibly in the oceans. They're using state-of-the-art imaging technologies to learn how airborne pollutants influence the planet's climate, and they're using one of the world's most powerful supercomputers to predict climate change.

They're determining how to best extract the vast quantities of natural gas hidden under the world's oceans and permafrost, which could yield far more energy than the earth's remaining reserves of fossil fuel. They're learning how to clean up contaminated sites and facilitate the safe disposal of nuclear waste. And they're developing new ways to more efficiently utilize today's energy sources through the development of energy-saving windows, advanced lighting technology, and software that streamlines a building's energy use.

Their work will help buy the world precious time until carbon-neutral sources of energy become a reality — a goal that Berkeley Lab scientists will pursue in the coming years.

Energy Technologies and Environmental Solutions

A NASA image of Earth as seen by satellite.

Berkeley Lab is leading a multi-institutional initiative, called SECUREarth, which will accelerate the study of subsurface processes that impact water resources, environmental remediation, agriculture, energy production, and climate change. The program's mission is to ensure energy security and environmental protection.

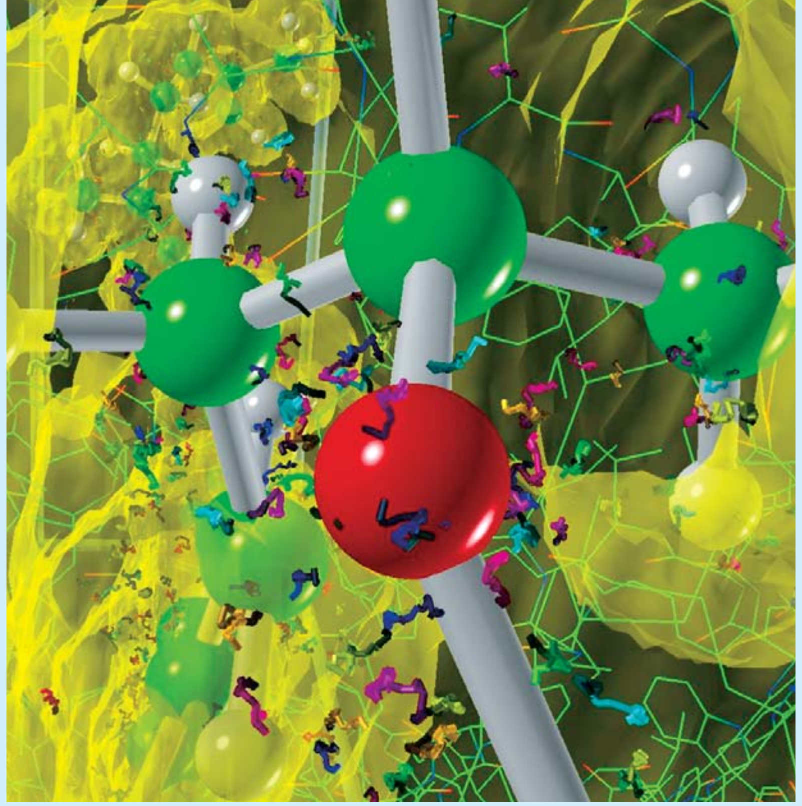
"To meet tomorrow's demands, we need a quantum leap in our understanding of subsurface processes — and SECUREarth can help us do that," says Gudmundur "Bo" Bodvarsson, director of Berkeley Lab's Earth Sciences Division and one of the architects of the program.

SECUREarth scientists will harness powerful scientific tools such as deep earth imaging and supercomputers to focus on two broad problems. The first is how best to clean up and isolate subsurface waste, whether it's existing waste such as at the Hanford Site in Washington state, or potential waste, such as at the proposed Yucca Mountain nuclear waste repository. The second problem concerns how to most efficiently locate and extract the subsurface resources that drive the nation's economy. These include methane hydrates, oil and gas, geothermal energy such as hot water and steam, and water for agriculture, power plants, and drinking needs.

Berkeley Lab scientists are also seeking ways to make fuel and electricity directly from sunlight in an effort to create energy without emitting carbon into the atmosphere.

One option is to mimic nature. Through photosynthesis, green plants are able to harvest energy from sunlight and convert it to chemical energy. If scientists can create artificial versions of photosynthesis, the dream of solar power as a clean, efficient and sustainable source of energy for humanity could be realized.

But photosynthesis is a complex process. Fortunately, an important piece of the photosynthesis puzzle is now in place. Researchers with Berkeley Lab and UC Berkeley have identified one of the key molecules that help protect plants from oxidation damage as the result of absorbing too much light. The researchers determined that when chlorophyll molecules in green plants take in more solar energy than they are able to immediately use, molecules of zeaxanthin carry away the excess energy. This study was led by Lab Deputy Director Graham Fleming and Kris Niyogi, who holds a joint appointment with Berkeley Lab and UC Berkeley.



Scientists are using supercomputers at the National Energy Research Scientific Computing Center (NERSC) to calculate and visualize the electronic structures of key molecules involved in the complex reactions of photosynthesis.

If scientists can learn to emulate nature's technique and create artificial versions of photosynthesis, then people could effectively tap into the sun as a clean, efficient, sustainable and carbon-neutral source of energy.

Another promising clean energy idea is a new generation of solar cells that combine nanotechnology with plastic electronics. Such hybrid solar cells will be cheaper and easier to make than their semiconductor counterparts.

"We have demonstrated that semiconductor nanorods can be used to fabricate readily processed and energy-efficient hybrid solar cells together with polymers," says Paul Alivisatos, a chemist who holds a joint appointment with Berkeley Lab's Materials Science Division and UC Berkeley.

Berkeley Lab scientists are also world leaders in learning how to sequester carbon dioxide deep underground and in the ocean, where it can't wreak havoc on the Earth's climate. It's estimated that each year seven billion tons of carbon dioxide enter the atmosphere through the burning of fossil fuels.

Starting in the spring of 2004, approximately 3,000 tons of carbon dioxide, compressed to a liquid, were injected nearly a mile deep into a brine-saturated aquifer that sits above an abandoned oil field near Houston. This test is the first scientific evaluation in the U.S of brine formations as underground carbon sequestration storage sites. Berkeley Lab scientists will spend about a year monitoring what happens to the carbon dioxide plume as it moves throughout the formation, displacing the brine from porous rock.

And other Berkeley Lab scientists look to the oceans, which currently capture a third of the carbon put into the atmosphere — most of it from fossil fuels. Two robotic Carbon Explorer floats tracked patches of iron-fertilized plankton for weeks through the storm-tossed Southern Ocean to test the "iron hypothesis," which proposes that adding iron to some ocean waters will make more aquatic plants bloom — thus trapping enough atmospheric carbon dioxide to offset the greenhouse effect. Around the globe, Carbon Explorers continue to gather evidence about the ultimate fate of carbon absorbed and released by the oceans.

Carbon Explorer floats, called SOLOs, are launched into the sea by Lab researchers to record temperature, salinity, circulation, and carbon biomass concentrations. Such evidence may reveal valuable information about the fate of carbon absorbed and released by the oceans.

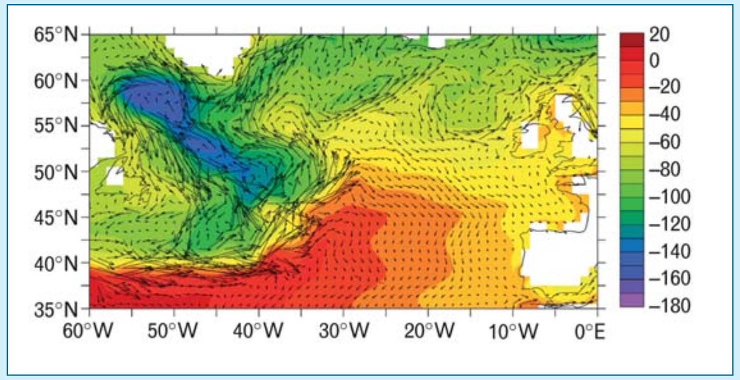
2010

GOAL FOR ENERGY TECHNOLOGIES

Demonstrate Safe and Effective Carbon Sequestration Systems.

To better understand the impacts of climate change, scientists from the National Center for Atmospheric Research recently completed a 1,000-year run of a powerful new climate-system model at Berkeley Lab's National Energy Research Scientific Computing Center (NERSC). The scientists ran the simulation for more than 200 uninterrupted days on NERSC's Seaborg supercomputer. Accurately predicting global climate change demands complex and comprehensive computer simulation codes, the fastest supercomputers available, and the ability to run those simulations long enough to model century after century of the global climate.

Efficient energy use is another Berkeley Lab research cornerstone. Scientists here developed the next generation of energy-efficient windows called transition-metal switchable mirrors, which are glass panels with a coating capable of switching back and forth between transparent and reflective states. Controlling the flow of solar radiation through windows has already saved billions of dollars in energy costs — an estimated $8 billion through the year 2000. Berkeley Lab's new window technology could increase savings even more. Other scientists are developing building energy simulation software, creating efficient lighting technologies, and fine-tuning ventilation systems.



Scientists at the National Center for Atmospheric Research used the computing power of NERSC to extend the Parallel Climate Model (PCM) run to nearly 1,500 years, part of a set of experiments that represents the most extensive 20th century climate simulations ever attempted. In this image, the PCM simulates the sea surface height (in centimeters) and ocean currents in the North Atlantic Ocean.

On the Path to a Healthier World

At the start of the 21st century, scientists now have the tools needed to study living cells at the molecular and atomic levels. The information gained from this ever-expanding array of tools is opening entire new avenues for the prevention and control of some of our deadliest and most pernicious diseases, including major forms of cancer, HIV-AIDS, and malaria. It is also paving the way for learning to repair or replace damaged cells and tissue. The same tools that promise so much for the life sciences offer new possibilities in other arenas as well, most notably carbon-neutral energy production, environmental remediation, and homeland security.

Among the tools now available are spectroscopy techniques for “stopping the action” on biological processes that can take place within a few millionths of a billionth of a second; imaging techniques for capturing the intricate architecture of the proteins that set the composition and chemistry of living cells; genetic sequencing and engineering techniques that can be used to identify and manipulate genes; and new algorithms for faster, more powerful computational resources that enable increasingly sophisticated simulations of the machinery of life.

Berkeley Lab researchers have been at the forefront in the development and use of these tools. Scientists here were major participants in the Human Genome Project, and, through participation in the Joint Genome Institute, are continuing the task of sequencing the DNA of scientifically important organisms and applying this data to the ongoing search for new genes and their associated proteins. Our scientists — often in close collaboration with researchers on the University of California campuses of Berkeley and San Francisco, the California Institute for Quantitative Biomedical Research (QB3), and elsewhere — are unraveling such mysteries as how individual cells interact with each other and their environment to maintain the physical well-being of their host organism.

Living Systems and Quantitative Biology

Mamala trees like this, found in Samoa, produce a promising anti-AIDS drug, originally discovered by Samoan healers, called prostratin. Chemical Engineer Jay Keasling, pictured, is synthesizing genes from the mamala to produce a cheaper and more plentiful synthetic version of prostratin. Keasling is the director of Berkeley Lab's Physical Biosciences Division, and also heads the Lab's new Synthetic Biology Department, the first of its kind in the world.

"Synthetic biology" aims to design and construct novel organisms and biologically inspired systems that can solve problems natural biological systems cannot. Synthetic biological systems can also provide important new insights into how natural systems work. Berkeley Lab established the world's first Synthetic Biology Department, and the research is already paying big dividends, with far greater rewards on the horizon.

According to the World Health Organization, each year nearly 500 million people become infected with malaria, and nearly three million — mostly children — die from it. Jay Keasling, director of Berkeley Lab's Physical Biosciences Division and a professor of chemical engineering at UC Berkeley, has led the development of a simple and much less expensive means of making one of the most promising and potent of all the new antimalarial drugs. By adding new genes and engineering a new metabolic pathway in *E. coli* bacteria, he and his colleagues can quickly and cheaply synthesize a precursor to the chemical compound artemisinin. This next-generation antimalarial drug has proven to be effective even against strains of the malaria parasite resistant to the current front-line drugs, but it is far too expensive right now for the countries in Africa and South America where it is needed most.

The Bill and Melinda Gates Foundation recently awarded a $42.6 million grant to further the development of microbial artemisinin production. Meanwhile, Keasling and his colleagues have obtained similar results with prostratin, a rare chemical compound that holds enormous therapeutic potential as an anti-AIDS drug.

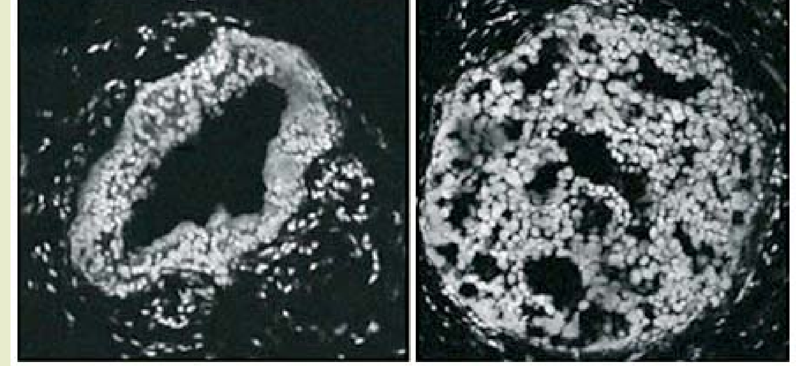
Despite continuing advances in diagnostics and treatment, cancer in all its many forms remains one of the leading causes of premature death. For women in this country, breast cancer is especially threatening, as it strikes one out of every seven. Berkeley Lab has a long history in breast cancer research. Scientists here discovered the critical link between tumor development and extracellular communications, uncovered vital new information on the damaging effects of ionizing radiation, identified new oncogenes and tumor-suppressing proteins, and developed new imaging techniques for tracking the spread of cancer. Most recently, a collaboration led by Joe Gray, director of Berkeley Lab's Life Sciences Division, and including researchers with UC San Francisco and the National Cancer Institute, found a way to precisely identify the onset of the "telomere crisis," an important early event in the development of breast cancer. Telomeres are the structures that protect the ends of chromosomes and prevent inappropriate cell growth that can lead to cancer. The work of Gray and his colleagues suggests that women at higher risk of developing breast cancer can be identified in advance by measuring telomerase activity. Early detection is the key to surviving any form of cancer.

(Left) Jay Keasling's research on the rare Artemisia annua tree, pictured, led to the development of a less expensive, synthetic anti-malarial drug, to be produced and distributed thanks to a $42.6 million grant from the Bill and Melinda Gates Foundation. (Right) Members of a Samoan village council listen to a presentation given in their language describing how genetic material from their mamala tree coupled with synthetic biology techniques could produce an anti-AIDS drug and bring them revenue without endangering their rain forest.

2010

GOAL FOR QUANTITATIVE BIOLOGY

Engineer Biological Systems to Advance Health Care, Carbon-Neutral Fuel Supplies, and Environmental Remediation.



Using 3-D confocal microscopy and working with breast-cancer tissue samples, researchers assessed the genomic instability known to play a role in breast cancer. These images highlight regions of chromosomes in cells of a breast duct exhibiting hyperplasia (left) and one exhibiting carcinoma *in situ* (right).

It is estimated that close to 100 trillion cells make up a typical adult human body, and the collective properties of these cells that keep each of us alive emerge as a result of multiple interactions and linked variables. Computational models and simulations are ideal for studying the complex phenomena of life, and Berkeley Lab has been at the forefront of these so-called experiments *in silico*. The Laboratory has established a Scientific Cluster Support Program, in which individual microcomputers are connected through software to perform as a single high-performance processor. This program provides researchers with a cost-effective midrange computing alternative to expensive supercomputers and has already been used to obtain valuable new information about the human immune system. Berkeley Lab-UC Berkeley researcher Arup Chakraborty led a study that showed in detail how the body's immune system is triggered into action. It was found that an intercellular junction, called the "immunological synapse," controls the strength and duration of the signals that activate T-cells, one of the body's principal lines of defense against infections. If problems arise at the immunological synapse, T-cell activation will be misregulated. This information could help in the treatment of autoimmunity, when T-cells mistake the body's own cells for invaders and attack them.

In a separate *in silico* experiment, another group of Berkeley Lab-UC Berkeley researchers, led by bioengineer Adam Arkin, used computers to design a genetically modified form of the HIV virus that could prevent HIV infections from developing into AIDS. While not yet ready for synthesis into an AIDS therapy, their model, called crHIV-1 for conditionally replicating HIV-1, has performed well in computer simulations. It is yet another demonstration of why synthetic biology and *in silico* experiments are generating so much excitement.

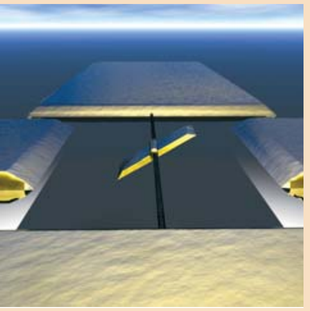
To clean up toxic waste sites and study the creatures that thrive there, researchers from Berkeley Lab, the Department of Energy's Joint Genome Institute (JGI) and UC Berkeley recently reported the first genomic characterization of a microbial community. They revealed the genetic identities of microorganisms that live in toxic conditions recovered from a natural biofilm growing in runoff from an abandoned mine. Until this work, four out of the five microbes characterized had defied laboratory culture and had only been studied in their natural habitat.

Jillian Banfield, an Earth Sciences Division scientist and a professor in UC Berkeley's Department of Earth and Planetary Science, retrieved the sample from the depths of one of the nation's worst Superfund sites in Iron Mountain, California. Banfield's team then applied the screening technique known as FISH (fluorescence *in situ* hybridization), a microscopic technique for a gross assessment of the microbial composition, before sequencing at the JGI.

The genomes of several microbial species were sequenced from this pink biofilm community, collected from acid mine drainage. Such information will help researchers in their efforts to clean up toxic waste sites.

"We extensively sampled the genomes of the dominant members of one of the microbial communities we were studying. Our analyses of the assembled data have revealed a great deal about the population structure, as well as the nature of pathways central to survival of the microbial community," says Banfield.

Eddy Rubin, Director of the Joint Genome Institute and Berkeley Lab's Genomics Division, says , "For the first time we have managed to tease out genetic information directly from an environmental sample."



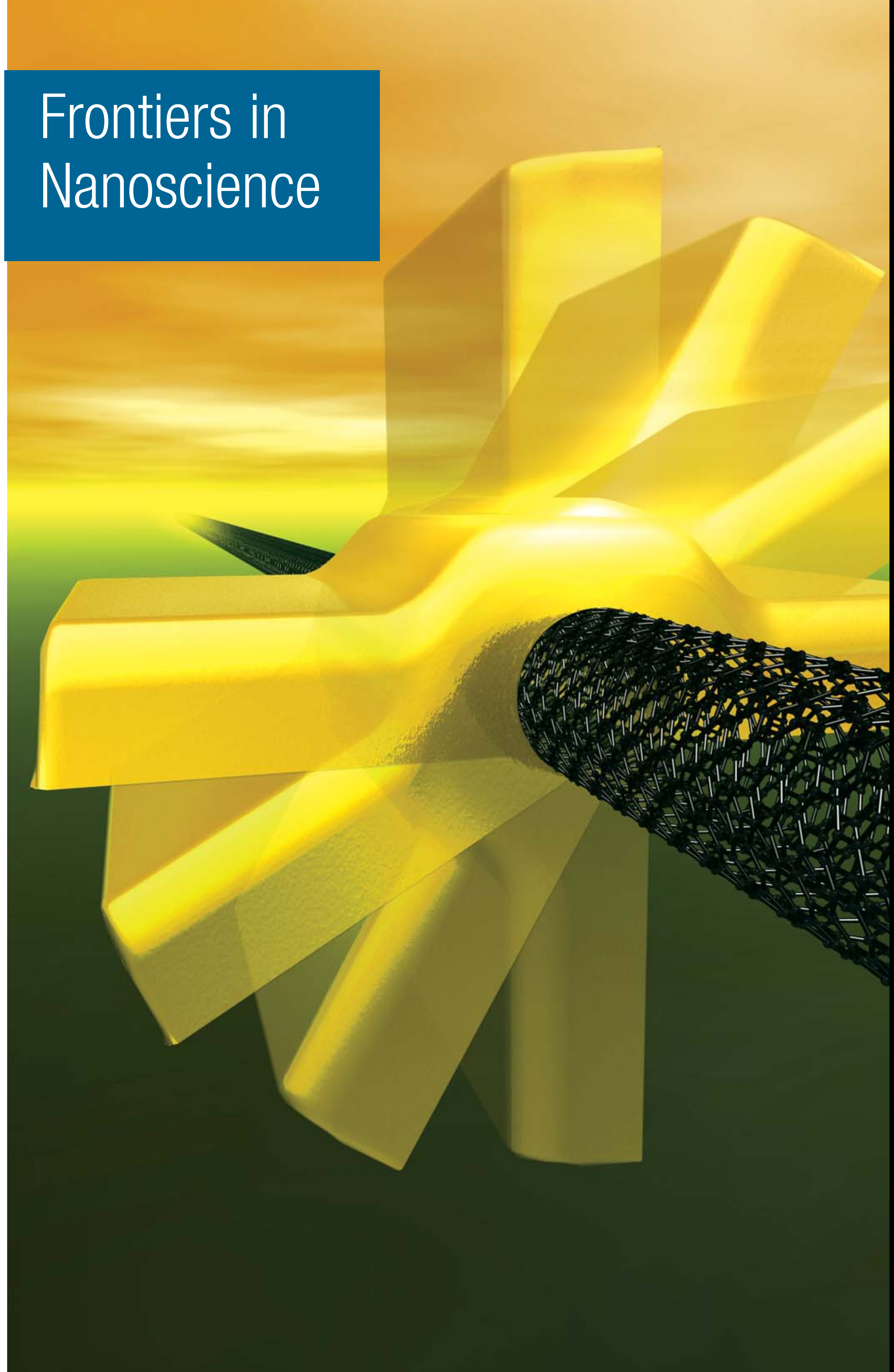
Engineering a Nano Revolution

It's been said that what a society can achieve depends on what it can make. Through nanoscience, which promises the ability to build machines and create materials atom by atom, what we can make is limited only by the power of our imagination. Nanoscience is no longer the stuff of science fiction. Economists predict a trillion dollar global market for nanoproducts within the next ten years, and the Federal government is investing hundreds of millions of dollars in nanoresearch. Berkeley Lab researchers have been at the vanguard of the nano revolution; this position of leadership is about to be substantially enhanced with the addition of the Molecular Foundry.

One of five nanoscience centers being established by the U.S. Department of Energy's Office of Science, Berkeley Lab's Molecular Foundry will provide the nanoscience community with the knowledge and tools needed to create technology that operates within the nanometer length of scale. (A nanometer is one billionth of a meter, one thousandth the size of the micrometer scale of today's electronic technology.) It will house facilities for the development of inorganic and organic nanomaterials, nanofabrication techniques, biological nanostructures, and nanotools. The Foundry will be adjacent to the National Center for Electron Microscopy (NCEM), which features electron microscopes capable of imaging even the tiniest features on nanosized structures.

The list of advancements in nanoscience already achieved by Berkeley Lab researchers is lengthy. Scientists here were the first to grow nanocrystals in a variety of shapes, rather than the simple spheres everyone else had produced. They were the first to fashion insulated nanowires, buckyball wires sheathed in a boron nitride coating, and created the world's first nanowire nanolasers, measuring just under 100 nanometers in diameter (about one ten-millionth of an inch). With the opening of the Molecular Foundry, Berkeley Lab researchers expect this list of accomplishments to grow.

Frontiers in Nanoscience



ABOUT THE IMAGE

World's Smallest Synthetic Motor

A team of scientists led by physicist Alex Zettl, who holds a joint appointment with Berkeley Lab's Materials Sciences Division and the UC Berkeley Physics Department, succeeded in creating the world's smallest synthetic motor.

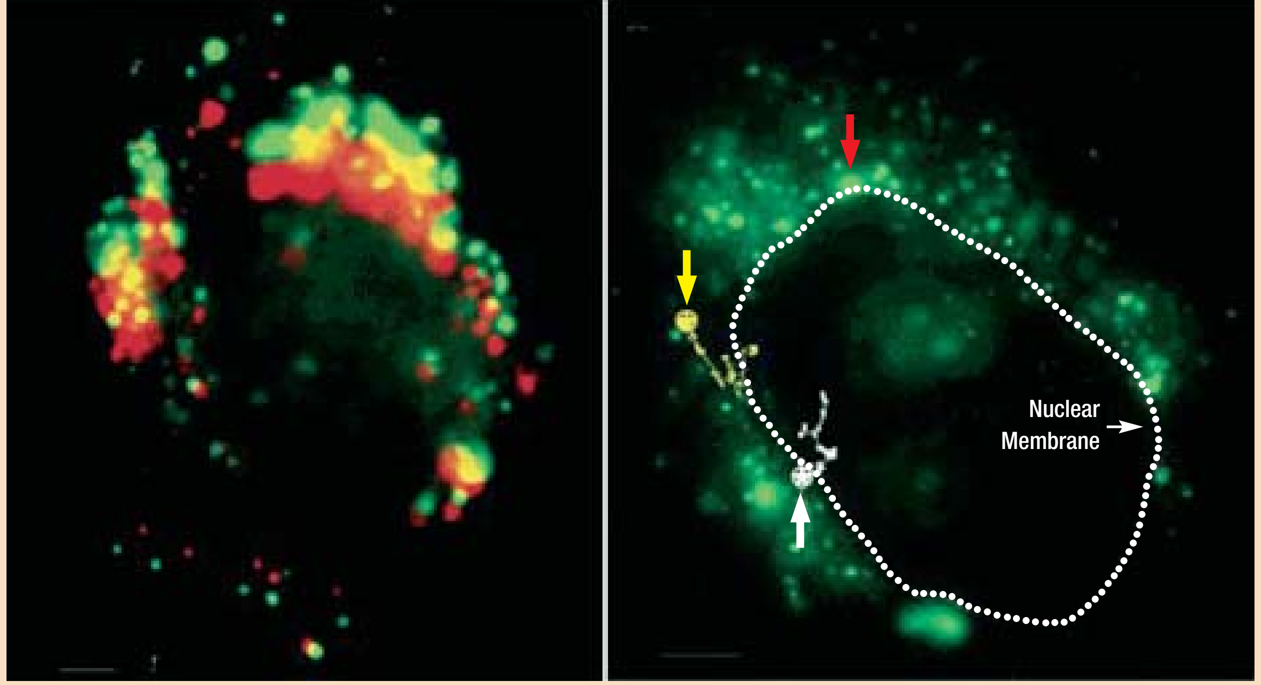
Called a synthetic rotational nanomotor, this device consisted of a gold paddle-shaped rotor blade, measuring between 100 and 300 nanometers in length, that was connected to a carbon nanotube shaft less than 10 nanometers thick. While the first version of the Berkeley nanomotor was about 300 times smaller than the diameter of a human hair, the technology behind it allows for future versions to be made even smaller — perhaps as much as five times smaller. For their accomplishment, Zettl and his colleagues received a 2004 R&D 100 Award, which is given by R&D Magazine in recognition of the "100 most technologically significant new products and advancements over the past year." The R&D 100 Awards have been called the "Oscars of Technology."

The synthetic rotational nanomotor has been clocked at 33,000 cycles per second and is believed capable of speeds approaching one billion rotations per second. Because the carbon-carbon bonds connecting the rotor blade to the shaft are practically frictionless, the motor can run indefinitely without wearing down. It is also rugged enough to withstand the harshest of environmental conditions, including extreme temperatures and radiation.

Potential applications of the synthetic rotational nanomotor technology include biological and environmental sensors, cell phones, optics, airbags, tire sensors, digital pens, blood pressure monitors, extremely smart subwoofers and antenna alignment. The technology should also find a broad range of applications in the field of cosmology for the exploration of deep space.

"This was the first nanosized device where you can put external wires on it and have something rotating that you can control," Zettl said, when the invention was announced. "There are biological motors that are slightly smaller in size, but ours can operate in a vacuum and over wide frequency and temperature ranges." ■

Image created by Noah Bodzin

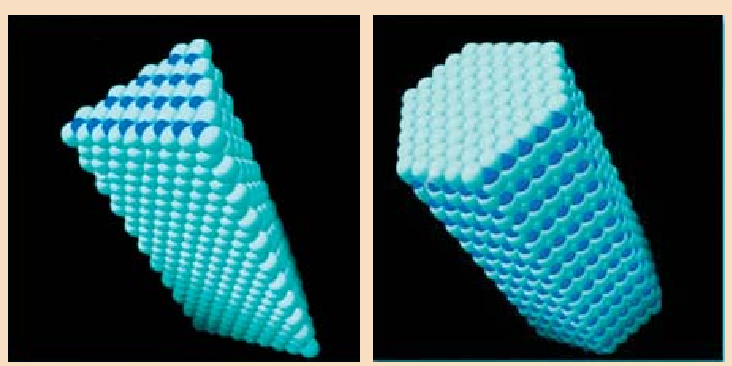


Biologists may soon use nanotechnology to watch the inner workings of a living cell and track the effectiveness of disease-fighting drugs. These two images portray the movement of nanosized probes, called quantum dots, as they pass through a cell's membrane.

In the growing world of nanosized particles, structures and devices, one of the most compelling stories has been that of quantum dots, semiconductor nanocrystals that light up like neon in a rainbow of sharp colors when bathed in ultraviolet light. Qdots, as they are known, have already fueled several startup high-tech companies, including one spun off from Berkeley Lab. Paul Alivisatos, a Berkeley Lab-UC Berkeley chemist who directs the Materials Sciences Division, is Associate Laboratory Director and one of the founders of quantum dot technology. He and his research team recently added an important new chapter to this unfolding story when they combined quantum dots with segmented nanorods to produce an extensive new array of multi-branched nanostructures.

Furthermore, they learned to tune the separate components of these nanostructures and calculate the electronic interactions of their branches in three dimensions. This makes it possible to create electronic devices tailored to a variety of applications, ranging from quantum computing to artificial photosynthesis.

In another study, quantum dots were used by a Berkeley Lab and Lawrence Livermore National Laboratory team as nanosized probes for looking inside the nuclei of biological cells. The cell nucleus has been called one of the best known but least understood of all cell organelles, a knowledge gap that stems from the lack of a way to image long-term phenomena within the nuclei. Berkeley's Fanqing Chen and Livermore's Daniele Gerion found a way to transport silica-coated quantum dots inside cell nuclei. To slip their quantum dots past the membrane that guards entrance to the nucleus, Chen and Gerion stole a trick from the SV40 virus, which gets through the barrier with the help of a protein that binds to a cell's nuclear trafficking mechanism. The researchers obtained a portion of this protein and attached it to their quantum dot, creating a hybrid, part biological molecule and part nanosized semiconductor, small enough to slide through the nuclear membrane's pores, and believable enough to fool its defenses. They've been able to introduce and retain quantum dots in nuclei for up to a week without harming the cell. The dots fluoresce for days at sufficient resolution to detect biological events carried out by single molecules. This



A Lab and UC research team achieved a breakthrough by growing nanowires out of the highly prized semiconductor gallium nitride and then controling the direction in which the nanowires grew. Gallium nitride nanowires are triangular in cross section when grown on a substrate of lithium aluminum oxide but hexagonal when grown on a magnesium oxide substrate. Growth direction is critical to determining a nanowire's electrical and thermal conductivity and other important properties.

2010

GOAL FOR NANOTECHNOLOGY

Transfer Nanophotovoltaic Systems to Industry and Initiate Commercial Use.

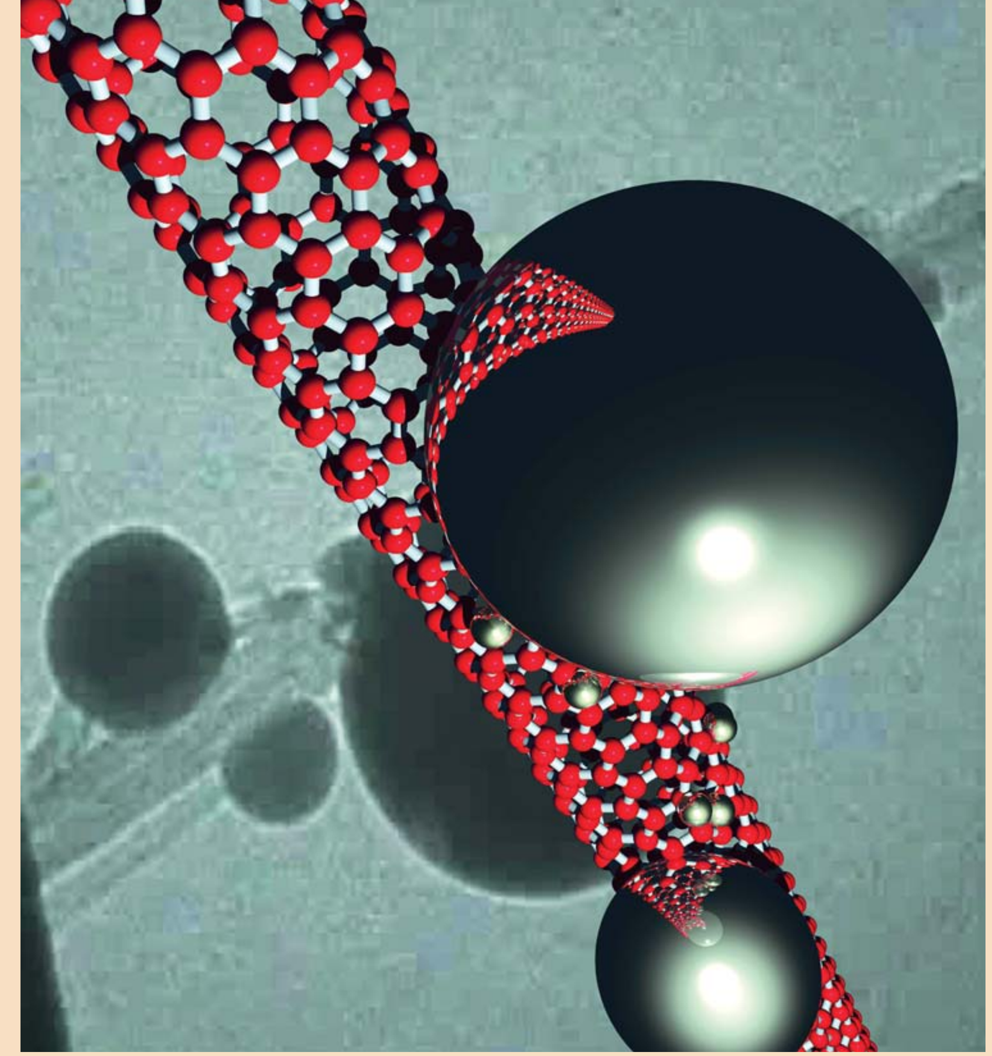


Image courtesy of Zettl Research Group

In a development that brings the promise of mass production to nanoscale devices, Berkeley Lab scientists have transformed carbon nanotubes into conveyor belts capable of ferrying atom-sized particles to microscopic worksites. Someday, a nanoscale conveyor belt such as the one shown in this simulation could expedite the atom-by-atom construction of the world's smallest devices.

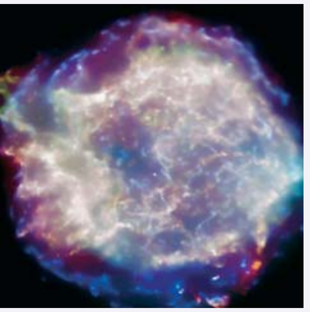
should allow scientists to track specific chemical reactions inside nuclei, such as how proteins help repair damaged DNA.

Just as the Microtechnology Age was built upon the introduction of impurities into crystals of semiconductor materials, so too will crystalline doping be the bedrock upon which the Nanotechnology Age is built. Another Alivisatos-led team showed just what happens to nanosized crystals under the various forms of crystalline doping.

They demonstrated that for nanocrystals, the doping process in which one type of positively charged atom, or cation, is exchanged for another takes place at a much faster rate than for microsized crystals, and is fully reversible, something that is virtually forbidden in the larger crystals under the same environmental conditions. This should accelerate the process of developing doped nanocrystals.

Another breakthrough was achieved by a Berkeley Lab-UC Berkeley team led by chemist Peidong Yang, who grew nanowires out of the highly prized semiconductor gallium nitride, and controlled the direction in which these nanowires grew. Growth direction is critical to determining a nanowire's electrical and thermal conductivity and other important properties. Nanotechnologists are eager to tap into the enormous potential of gallium nitride for use in high-power, high-performance optoelectronic devices. With further development, the technology of Yang and his colleagues should make it possible for gallium nitride nanowires to be integrated with thin films of various compositions to produce light-emitting diodes, transistors, biochemical sensors and ultraviolet-wavelength nanolasers.

Yet another development brings the promise of mass production to nanoscale devices. A team of Berkeley Lab and UC Berkeley researchers led by physicist Alex Zettl has been able to transform carbon nanotubes into conveyor belts capable of ferrying atom-sized particles to microscopic worksites. By applying a small electrical current to a carbon nanotube, the team was able to move individual atoms of indium along the tube, like auto parts on an assembly line. In a series of tests, the indium was repeatedly moved back and forth along the nanotube without losing a single atom. This research lays the groundwork for the high-throughput construction of the atomic-scale optical, electronic, and mechanical components from which future nanodevices will be fabricated.



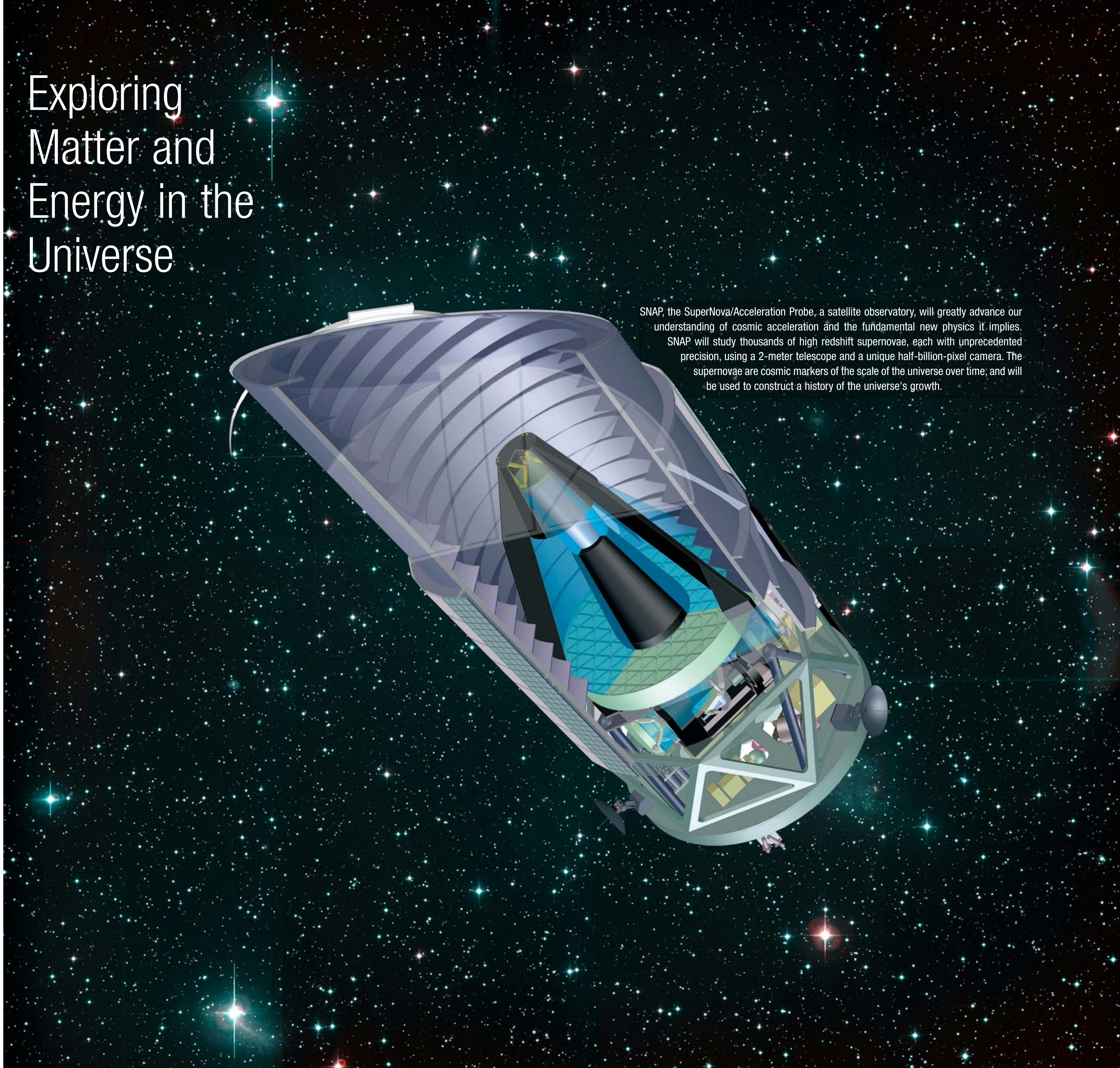
Can We Coax the Cosmos to Reveal its Secrets?

Entering the 21st century, we have discovered that we don't know what 95 percent of our universe is made of. The urge to find out is rooted in the human longing to understand where we come from and where we're going. Knowledge may have practical implications, too, yet we can no more guess at these than could Einstein when he proposed, just 100 years ago, that matter and energy are equivalent and mediated by the speed of light. Dark matter and dark energy are real, but facts are few.

Berkeley Lab researchers are no strangers to studies of the cosmos. Physicists here pioneered the measurement of minute temperature differences in the cosmic microwave background radiation, and it was here that the Supernova Cosmology Project developed methods for measuring the expansion of the universe with distant supernovae, leading directly to the discovery of accelerating expansion and the existence of dark energy.

While the questions may be cosmic, the answers are intertwined with our understanding at the highest energy and smallest length scales. In the tradition of Ernest Lawrence, teams of Berkeley Lab scientists and engineers, through collaborations with many institutions in many nations, are leaders in the design of novel accelerator systems and detectors worldwide. Their contributions are crucial to the ATLAS detector at the Large Hadron Collider at CERN. Digital Optical Modules devised here are being sunk in the South Polar ice for the IceCube neutrino telescope. The GRETINA detector and the VENUS superconducting heavy ion source created here are prototype components for a potential Rare Isotope Accelerator; farther in the future will come detectors and damping rings for the International Linear Collider. Electron beams accelerated by laser-driven wakefields through plasma channels have demonstrated a new principle of "tabletop" acceleration.

Exploring Matter and Energy in the Universe



SNAP, the SuperNova/Acceleration Probe, a satellite observatory, will greatly advance our understanding of cosmic acceleration and the fundamental new physics it implies. SNAP will study thousands of high redshift supernovae, each with unprecedented precision, using a 2-meter telescope and a unique half-billion-pixel camera. The supernovae are cosmic markers of the scale of the universe over time, and will be used to construct a history of the universe's growth.

Superbright, uniform Type Ia supernovae are the best standard candles in the astronomical toolkit, measuring cosmic distances to a few percent accuracy. In 1998, after comparing the distances and redshifts of 42 painstakingly collected Type Ia supernovae, the international Supernova Cosmology Project led by Berkeley Lab's Saul Perlmutter announced the accelerating expansion of the universe — driven by an exotic something comprising two-thirds the universe's density and quickly christened "dark energy."

Candidates for dark energy include the quantum-mechanical energy of the vacuum; fields dubbed "quintessence" whose strength varies with time; discontinuities in the fabric of space-time created in the Big Bang; or even extra-spatial dimensions. To distinguish among them, the expanding universe must be probed to greater distances and earlier times.

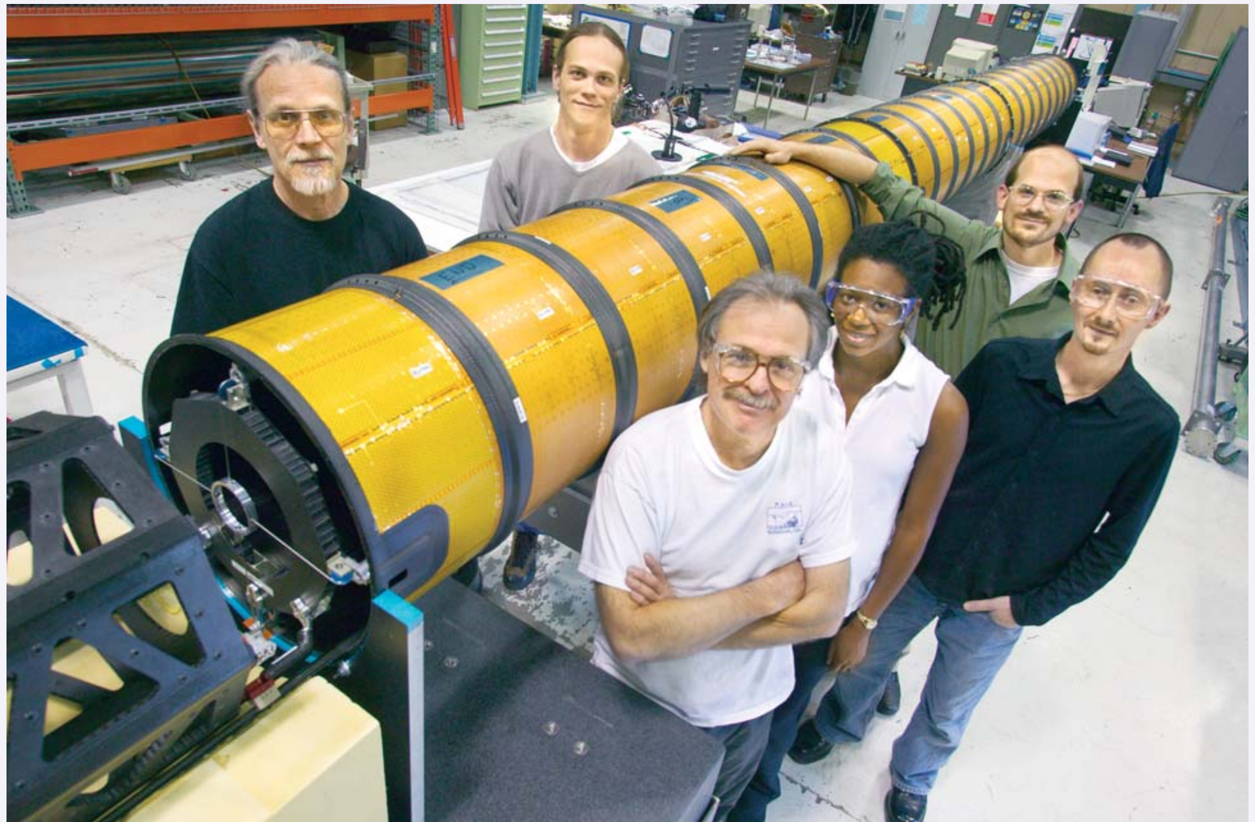
Lab scientists are attacking the problem from many angles. The international Nearby Supernova Factory based here will reduce the remaining uncertainties in Type Ia measurements through advanced spectroscopy of hundreds of supernovae only tens of millions of light-years distant, found by an automated sky search.

The SuperNova/Acceleration Probe, SNAP, is a collaboration of over 100 individuals from 15 academic and government institutions in the U.S., France, and Sweden, based at Berkeley Lab. Designed to measure thousands of distant supernovae in unprecedented detail, SNAP is the inspiration and a leading candidate for the Joint Dark Energy Mission announced by NASA and DOE in 2003, which ranks among the highest of DOE's priority scientific facilities for the future.

SNAP has been described as "a camera with a telescope attached" — a two-meter reflector focusing a square degree of sky on a half-billion-pixel imager, hundreds of times the Hubble Space Telescope's field of view. The imager's most critical component is a rugged, radiation-resistant charge-coupled device (CCD) with extraordinary sensitivity to long wavelengths.

SNAP's astronomical CCD is a descendant of the silicon vertex detectors built by Berkeley Lab for some of the world's most important high-energy physics experiments, among them the CDF experiment at Fermilab, used to find and measure the top quark; the BaBar experiment at SLAC, which measures the asymmetric decay of B mesons; and the innermost pixel detector of the giant ATLAS experiment at the Large Hadron Collider (LHC), now under construction at CERN. ATLAS is hoping to find the Higgs Boson, from which all other particles derive their mass — and search beyond the Higgs for supersymmetric particles, extra dimensions of space, and even miniature black holes.

Team members of the ATLAS project (left to right) Jon Wirth, Tom Johnson, Mario Cepeda, Alexis Smith, Neal Hartman, and Eric Andersson are pictured with the support structure for ATLAS' Pixel Detector. When completed, ATLAS's mission will include searching for the Higgs Boson, from which all other particles derive their mass.



2010

GOAL FOR MATTER AND ENERGY IN THE UNIVERSE

Complete the Detector Assembly for the Dark Energy Mission, Supporting a NASA Satellite Launch by 2014.

(Left) IceTop, a surface cosmic-ray detector array that forms part of the IceCube experiment, is being installed at the South Pole. (Above) IceCube is designed to detect several neutrinos from a single gamma-ray burst of the kind that probably occurred in the supernova remnant W49B, located about 35,000 light-years from Earth and shown in a composite image from NASA's Chandra X-ray Observatory.

The Lab's expertise in silicon detectors is matched by experience with another kind of detector invented here, the time projection chamber (TPC). At the heart of the STAR experiment at Brookhaven's Relativistic Heavy Ion Collider, seeking the quark-gluon plasma that characterized one of the earliest phases of the universe, is a TPC built by Berkeley Lab. Both technologies will contribute to the detectors of the International Linear Collider, designed to complement CERN's LHC by using lepton collisions to study high-energy events with more precision.

Some of the most elusive of fundamental particles are wispy, chargeless neutrinos. Luckily their reluctance to interact with matter is matched by their abundance, enough that a handful of the trillions upon trillions of neutrinos that pass through a reservoir of heavy water or mineral oil, or a cubic kilometer of transparent Antarctic ice, will betray their presence with flashes of pale Cherenkov radiation — perhaps a dozen interesting interactions a day, perhaps only a dozen a year, depending on their energy.

Berkeley Lab scientists and engineers designed and built the support structure for the 10,000 photomultiplier tubes of the Sudbury Neutrino Observatory (SNO), buried two kilometers deep in Ontario, Canada and designed to study neutrinos created in our sun. KamLAND, the Kamioka Liquid-scintillator Anti-Neutrino Detector that studies low-energy neutrinos from Japanese nuclear power plants, employs electronics designed, built, and installed by Berkeley Lab collaborators. At the heart of the IceCube astronomical observatory now under construction at the South Pole are the unique electronics of the digital optical modules (DOMs) designed here — eventually 80 strings of 60 DOMs each will dangle up to 2.5 kilometers under the ice, catching signals of high-energy cosmic neutrinos from the farthest reaches of space.

From the most elusive of Standard Model particles to yet-undiscovered particles, fields, and extra dimensions, Berkeley Lab physicists and engineers lead the cosmic search.

Faster X-ray Pulses Promise Breakthrough Science

Just as scientists strive to manipulate matter at ever-smaller scales, they also strive to observe matter using ever-faster pulses of light. Called ultrafast science, the need for lightning-quick x-ray flashes lies in the fact that chemistry starts with the movement of electrons, a motion that takes place in a matter of attoseconds, a timescale almost too small to comprehend. An attosecond is one billionth of a billionth of a second, and there are more attoseconds in one minute than there have been minutes in the history of the universe.

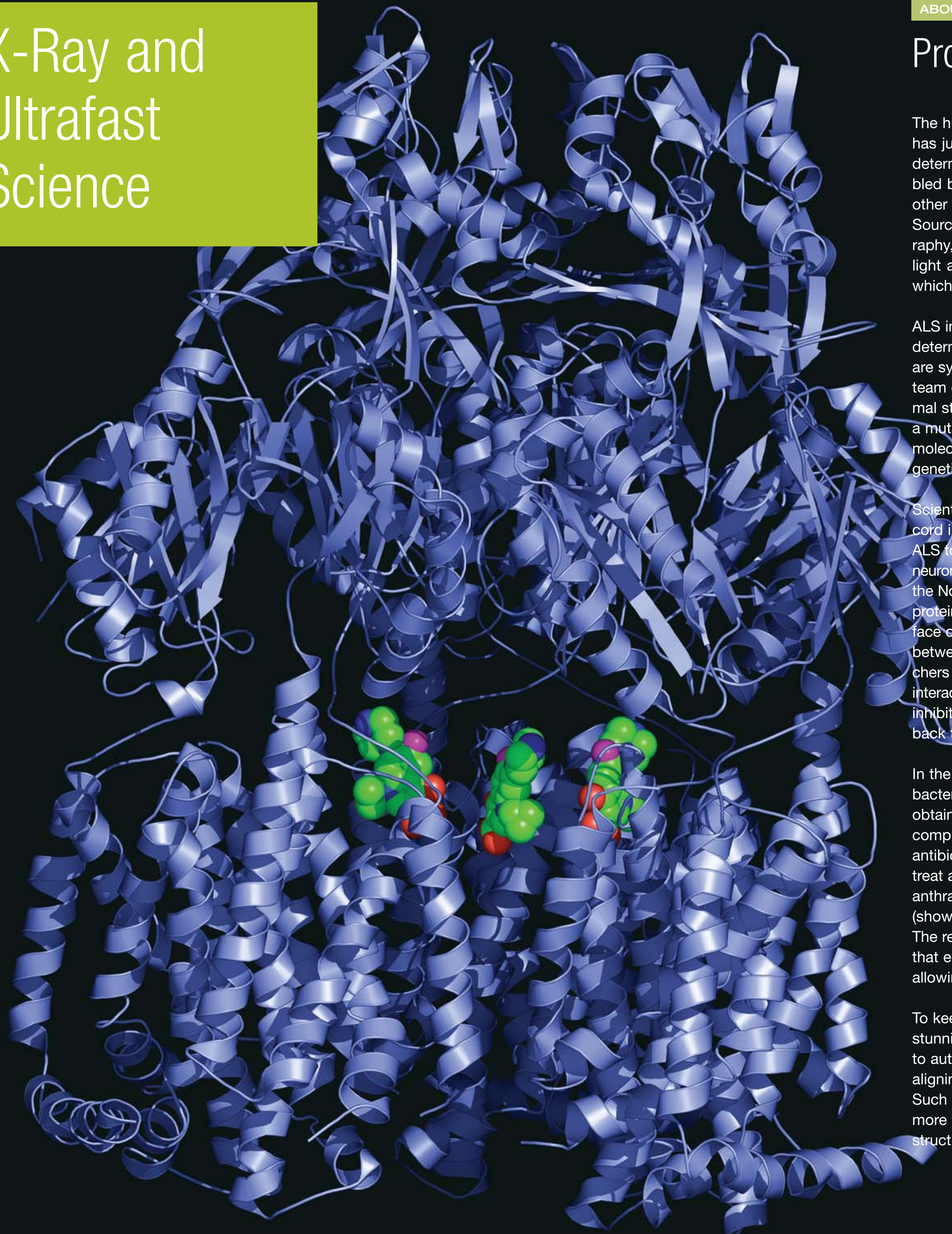
Berkeley Lab scientists are working to bring x-ray science into these ultrafast time domains. They are already pioneers in developing x-ray pulses at the femtosecond scale, which is three orders of magnitude slower than attoseconds, but still fast enough to study the motion of atoms in molecules during physical, chemical, and biological reactions. Now, Berkeley Lab scientists are working to ratchet down the duration of coherent pulses of x-ray light to the attosecond level, which will make the hidden world of electron movement visible for the first time — and herald a new age of fundamental materials science and biological research.

Another cornerstone of Berkeley Lab's x-ray science program is the Advanced Light Source (ALS), a national user facility that generates intense light for scientific and technological research. As the world's brightest source of ultraviolet and soft x-ray beams — and the world's first third-generation synchrotron light source in its energy range — the ALS makes previously impossible studies possible.

The ALS works by accelerating electrons to nearly the speed of light and bending them in a circular path by powerful magnets. At this speed, electrons emit extremely bright x-ray light that is directed along a beamline toward an object that researchers want to investigate at the atomic level, such as a crystallized protein. The pattern in which x-rays diffract off the protein reveals its structure. Ongoing research topics include investigating the electronic structure of matter, protein crystallography, ozone photochemistry, computer microchips, and optics testing.

Berkeley Lab scientists are also ensuring the ALS remains at the forefront of x-ray science.

X-Ray and Ultrafast Science



ABOUT THE IMAGE

Protein Crystallography

The human genome has been sequenced, but the work has just begun. One of the big challenges in science is determining the function of the 30,000 proteins assembled by the human genome, as well as the genomes of other organisms — which is where the Advanced Light Source comes in. It's a world leader in protein crystallography, a process in which extremely bright beams of light are used to elucidate a protein crystal's structure, which can then be used to determine its function.

ALS images helped a Berkeley Lab team make new determinations about the process by which proteins are synthesized from the genetic code. The research team compared images of ribosomes taken from normal strains of the bacterium *Escherichia coli* to those of a mutant, antibiotic-resistant strain. Ribosomes are the molecules in living cells responsible for translating the genetic code into proteins.

Scientists are also inching closer to a cure for spinal cord injuries, thanks to a research team that used the ALS to determine the structure of a protein that prevents neurons from repairing themselves. The protein is dubbed the Nogo receptor because it binds with several other proteins that block neural growth. It's found on the surface of thin fibers, called axons, which carry information between neurons in the brain and spinal cord. Researchers believe that if they can pharmaceutically block the interaction between the Nogo receptor and these growth-inhibiting proteins, then severed neurons may fuse back together, and paralyzed people might walk again.

In the race to stay one step ahead of drug-resistant bacteria, scientists from Berkeley Lab and UC Berkeley obtained high-resolution images of AcrB (left), a protein complex found in bacteria that repels a wide range of antibiotics. Even ciprofloxacin, an antibiotic used to treat a variety of bacterial infections including inhaled anthrax, is no match for AcrB—the green-colored drug (shown at left) is firmly ensnared in the protein's cavity. The research may inform the development of antibiotics that either evade or inhibit these protein complexes, allowing drugs to slip inside bacteria cells and kill them.

To keep pace with the ever-growing demand for these stunning images, Berkeley Lab scientists were the first to automate the painstaking process of mounting and aligning protein crystals for study at a synchrotron. Such improvements have allowed ALS users to screen more than 10,000 protein crystals and collect complete structural datasets on several hundred of them. ■

The secrets of chemical reactions reveal themselves in the blink of an eye. To glimpse these processes, Berkeley Lab physicists Alexander Zholents and William Fawley have an idea for creating intense bursts of x-rays in pulse lengths of about 100 attoseconds. How fast is that? In Niels Bohr's classic 1913 model of a hydrogen atom, it takes about 100 attoseconds for the electron to orbit the proton.

Using their technique, scientists may be able to directly observe phenomena such as an atom becoming ionized, or the bonding of two or more atoms into molecules, by using a flash of light to stimulate an electron, and attosecond x-ray flashes to follow its activities.

"What made our idea possible is the amazing work that has been done with lasers over the past five years," says Zholents. "Lasers can now provide the intense, few-cycle pulses that we can use to effectively slice attosecond soft x-rays from an ultrarelativistic electron beam."

Zholents and Fawley's proposal could be realized at a soon-to-be-completed center for ultrafast science. Berkeley Lab scientists are collaborating with the Stanford Linear Accelerator Center on the development of the Linac Coherent Light Source (LCLS), which will be the world's first x-ray free electron laser when it becomes operational in 2009. Pulses of laser light from the LCLS will be many orders of magnitude brighter and several orders of magnitude shorter than what can be produced by any other x-ray source. These characteristics will enable frontier science, such as probing new states of matter, following chemical reactions and biological processes in real time, imaging chemical and structural properties of materials on the nanoscale, and imaging noncrystalline biological materials at atomic resolution.

The venerable ALS is also well poised to lead x-ray-driven science for years to come. In the fall of 2001, the ALS underwent a retrofit, replacing three of its conventional storage-ring bend magnets with superconducting magnets or "superbends." This retrofit, the first ever to take place at an operating synchrotron radiation source, elevated the ALS from being the nation's premier source of low-energy or "soft" x-rays to also being an important source of high-energy or "hard" x-rays. Plans call for the

ALS Beamline 6.1.2 is a bend magnet beamline used for x-ray microscopy and tomography and 3-D imaging.

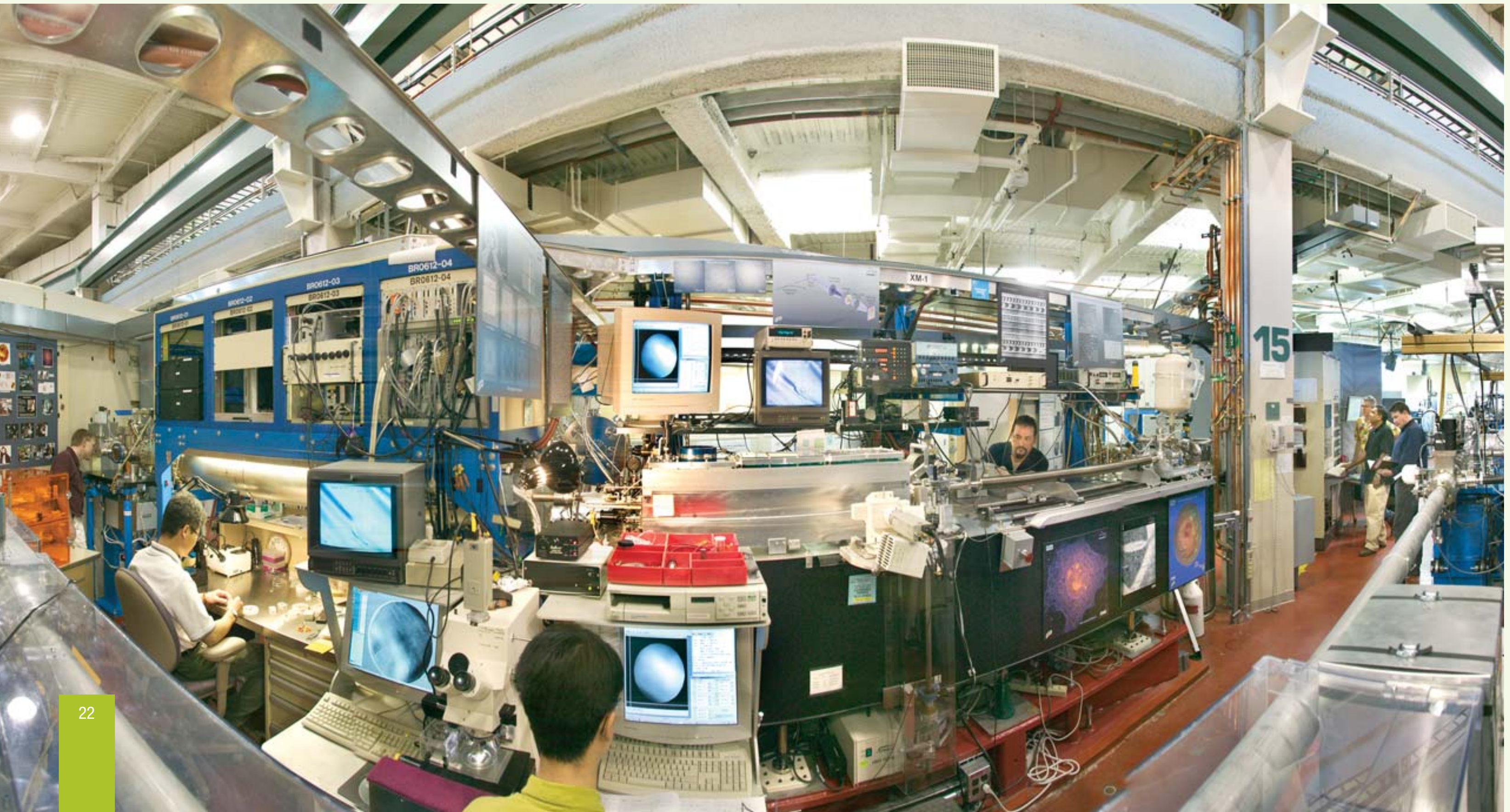
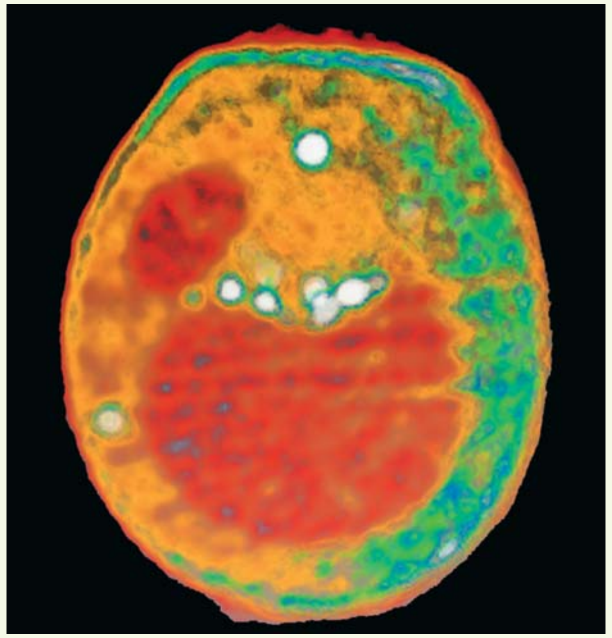


Image courtesy of Carolyn Larabell Group



This x-ray tomography image of a yeast cell was taken at ALS beamline 6.1.2. Internal organelles are color coded according to x-ray absorption, with the nucleus and large vacuole shown as red, lipid droplets as white, and other cytoplasmic structures as either orange or green.

ALS to be upgraded so that it operates in a "top-off" injection mode, meaning electrons are injected into the storage ring every half minute or so, which keeps the storage-ring current nearly constant. At present, when the ALS is in operation, the storage ring is filled once every eight hours. By operating in a top-off mode, the ALS is expected to undergo a twofold increase in beam brightness. Further increases in beam brightness at a modest cost will be achieved in the future as today's ALS insertion devices are replaced with superconducting devices.

Although the primary reason for retrofitting the ALS with superbends was to help meet the huge demand for protein crystallography research, the ALS also remains one of the world's best tools for state-of-the-art research in materials science, chemistry, physics, and the environmental sciences. For example, a team of scientists used the ALS to determine that carbon-containing aerosols remain in the atmosphere much longer than previously thought — meaning they have more time to influence the Earth's climate. The results, based on high-resolution images, will help climate scientists refine the computer models used to predict climate change. The images reveal that aerosol particles oxidize more slowly than earlier estimates indicated, which buys them more time to waft about in the atmosphere.

"Moore's Law," Gordon Moore's prediction that the density of circuit elements on microchips will double every 12 to 18 months, has held true for the past 30 years. But if it is to continue to be the law for computer chips, new fabrication techniques will be needed. At the ALS, a consortium of industry and government labs has constructed the first prototype machine for measuring (and even printing) test computer chips using extreme ultraviolet light. Microprocessors based on this technology will operate ten times faster than today's most powerful chips and are expected to come to market by 2007.

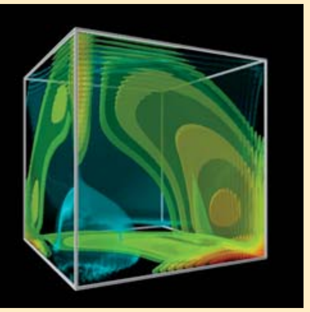
To learn how organisms work at the cellular level, a first-of-its-kind x-ray microscope built for the ALS holds forth the promise of "CT scans" for biological cells, and other unprecedented capabilities for cell and molecular biology studies. The new microscopy resource also promises a better understanding of human diseases at the molecular level and possibly new discoveries for treating those diseases.

In the quest to determine the chemical composition of solids with greater and greater accuracy, Berkeley Lab scientists are also using extremely short laser bursts that span one-quadrillionth of a second. These femtosecond-length laser bursts are used to zap a substance's surface and dislodge an aerosolized plume of particles that can be spectroscopically analyzed. The technique is much more sensitive than similar systems that rely on longer, nanosecond-length laser bursts, and may revolutionize scientists' ability to quickly and accurately analyze the chemical makeup of any solid—from nuclear material and hazardous waste to Martian rocks.

2010

GOAL FOR X-RAY AND ULTRAFAST SCIENCE

Conduct X-ray Probe Experiments in Reaction Dynamics at Subfemtosecond Resolution.



Tools for Scientific Discovery

When Japan's Earth Simulator debuted early in 2002, the scientific computing world got a wake-up call. Reaching 87 percent of its theoretical peak performance, running five times faster than the world's next-fastest machine, the Earth Simulator was a reminder of what supercomputers designed to do science could achieve.

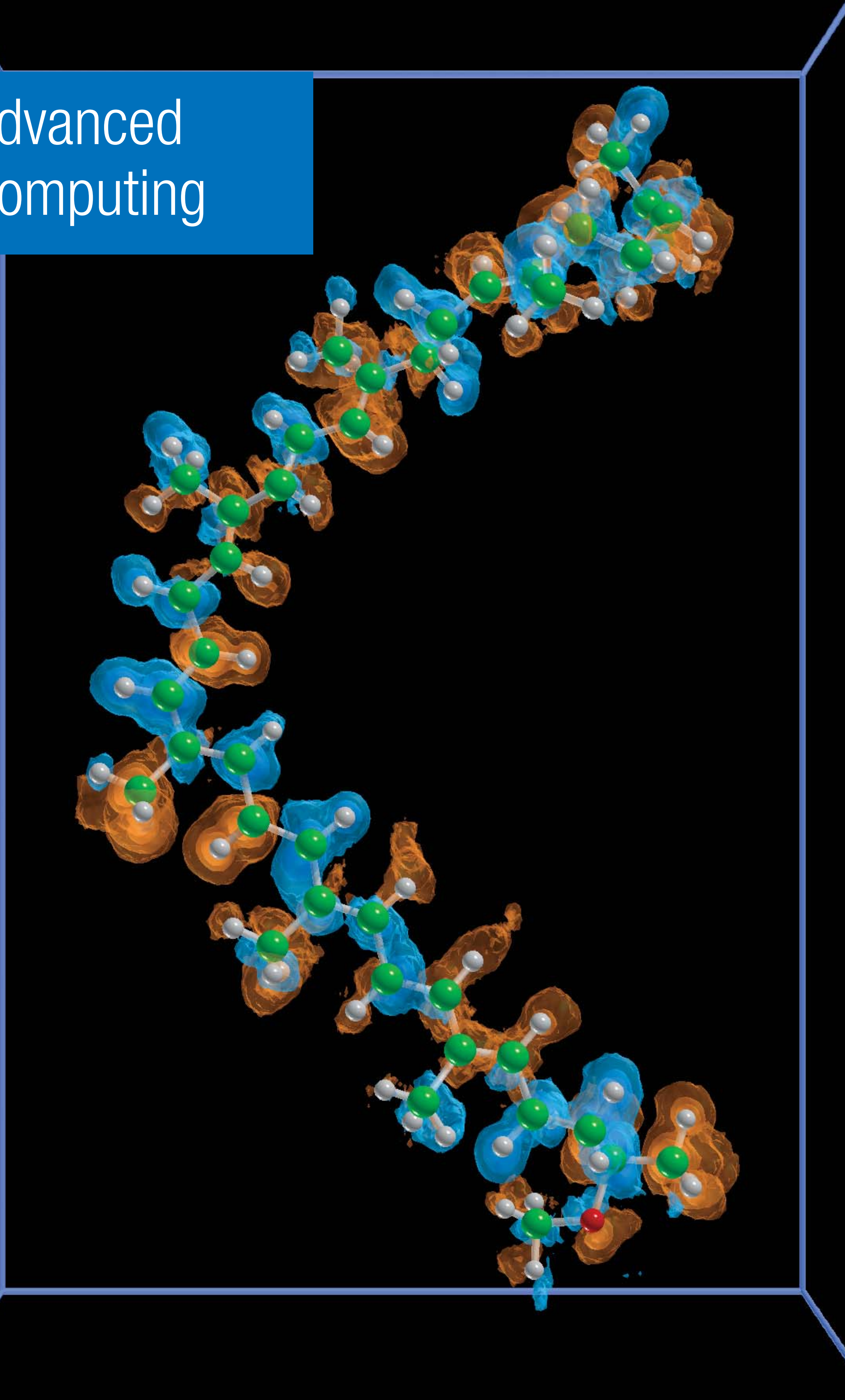
A government study concluded that one reason the U.S. had fallen behind was "the 1990s approach of building systems based on commercial off-the-shelf components." While the sophisticated processors used in personal computers are some of the most advanced microdevices in existence, a PC's applications don't access memory the way scientific applications do. When the same kinds of processors are clustered together to do science, they are incapable of reaching anything like their potential.

Researchers in Berkeley Lab's computing divisions soon joined with counterparts at Argonne and the IBM Corporation to create a strategy for a new class of scientific computers. They came up with a conceptual design for a system that would enhance the architecture of IBM's Power series of processors.

Not all scientific problems are susceptible to the same mathematical approach or have the same needs for memory access and organization. The team identified specific problems like "memory contention" in IBM's existing multiprocessor design, severely affecting the performance of processors that share an interface with main memory. They devised Virtual Vector Architecture (ViVA), a way to create very-high-performance virtual vector processors from groups of individual processors in a node. IBM has incorporated the results in its new generation of microprocessors.

"The high-performance systems of the future have to be balanced in many ways" — neither off-the-shelf cluster machines nor expensive special-purpose machines will do — "since the scientific applications of the future will combine many different methods," the team concluded. Berkeley Lab's computer scientists and users are leading the way.

Advanced Computing



ABOUT THE IMAGE

Computer Visualization: Seeing the Unseeable

Some scientific questions can only be answered when data is visualized in three dimensions; with others, 3-D visualization helps researchers "see their data in a way they may not have seen it before," says Cristina Siegerist of the Computation Research Division's Visualization Group.

"Visualization begins when the researchers come to us with a box of data," Siegerist says. "I ask them, how did you write it? If I can read it, I know how to employ one of our standard programs or how to write my own."

For particle-accelerator simulations performed by Rob Ryne's group in the Accelerator and Fusion Research Group, with Andreas Adelmann of the Paul Scherrer Institute, Siegerist developed sophisticated electron-cloud visualizations using AVS/Express software; she also custom-made the PartView tool, whose simple interface allows the researchers access from their desktops.

In this way Siegerist and Visgroup leader Wes Bethel, John Shalf, and their colleagues help NERSC users, especially those pursuing SciDAC (Scientific Discovery through Advanced Computing) and INCITE (Innovative and Novel Computational Impact on Theory and Experiment) projects, to see what they want to see in their data — and also what they may be surprised to find.

"Sometimes the surprises may be as simple as errors that need correcting," Siegerist remarks, "like a bug in the code that assigns a particle the wrong charge." But visualization can also lead to fresh insight.

In his studies of carotenoids in photosynthesis (shown at left), William Lester of the Chemical Sciences Division used Quantum Monte Carlo calculations, which employ "random walkers" — in this case, 314 walkers, representing electrons — to feel out quantum-mechanical energies and wave functions. "Watching the walkers follow their trajectories was revealing, giving new perceptions about the molecules' electronic structures," Siegerist says.

Siegerist's background in physics and computer science, and her wide experience in academic and industrial settings in many countries, are typical of the broad reach and flexible approach the Visualization Group brings to its myriad challenges. ■

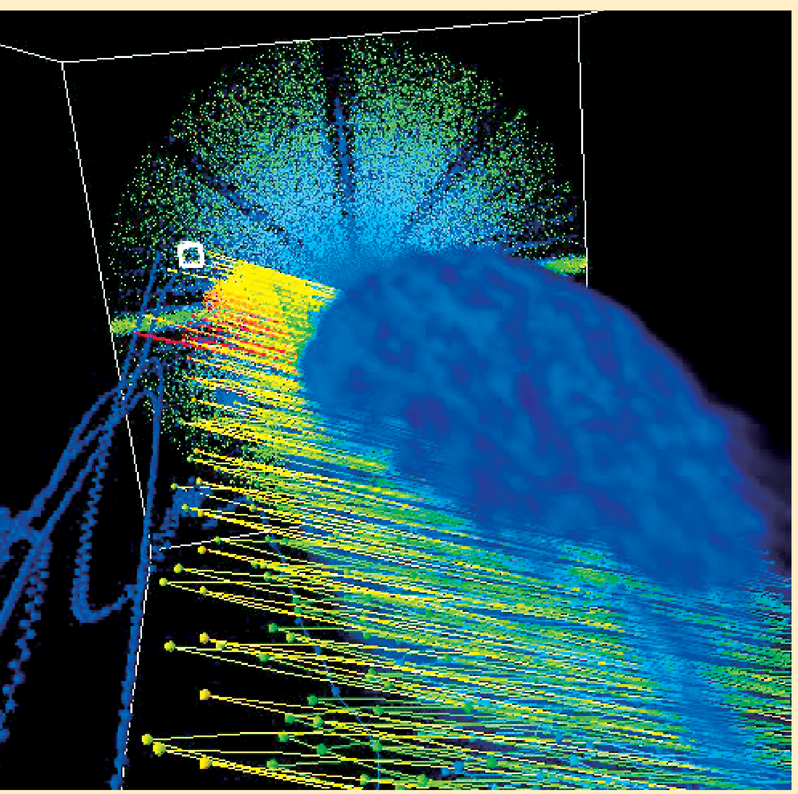
Advanced computing — a third mode of science, complementing both theory and experiment — has become indispensable to a wide range of disciplines. A few examples among many:

Molecules known as carotenoids are an organism's first line of defense against damage by free radicals. In humans, carotenoids protect the eyes from chemical reactions triggered by bright light. Plants are equally at risk from light that's too bright; during photosynthesis, carotenoids quench chlorophyll states that would otherwise generate low-energy oxygen molecules, which could damage or even kill the plant. Carotenoids play other important roles in regulating photosynthesis as well.

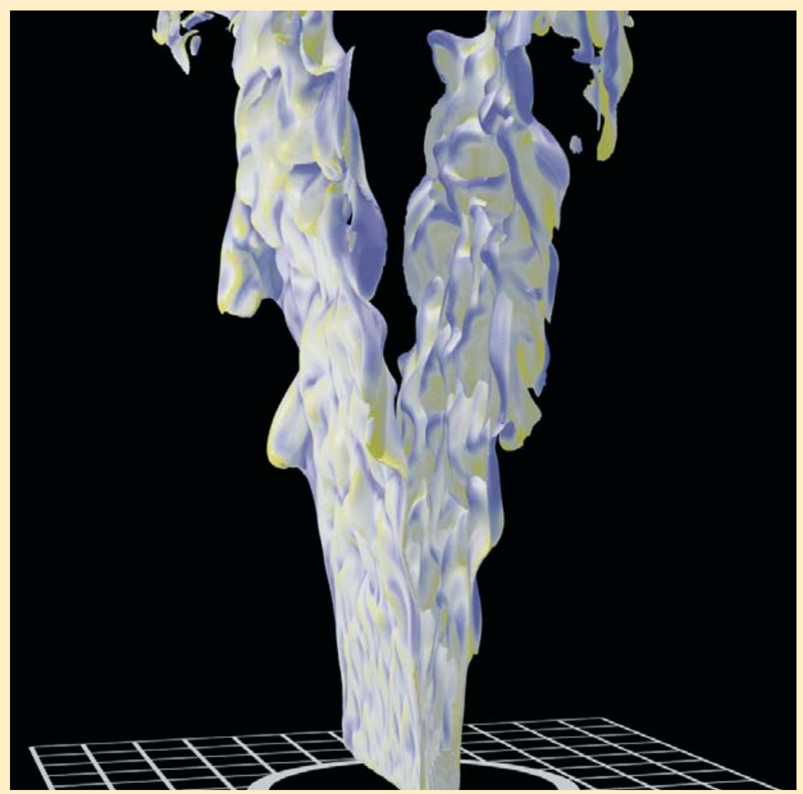
Exactly how they do it is a mystery. Carotenoid electronic structure is so complex it can't be studied by optical spectroscopy, but computing the excited states is a daunting task. One of the first three INCITE Awards from DOE's Office of Science went to William Lester, Jr., of the Chemical Sciences Division, and Graham Fleming, then director of the Physical Biosciences Division — a grant of a million hours of NERSC supercomputer time to study carotenoids in photosynthesis using a statistical method called Quantum Monte Carlo simulation.

These methods require enormous computing power — 80,000 NERSC hours for each electronic state, for each kind of carotenoid — but can produce results as accurate as those of an experiment. (No such experiments are possible, outside the computer.) Lester and Fleming expect the NERSC studies to clarify the carotenoid-chlorophyll interaction in photosynthesis, bringing the day closer when nature's clean, exquisitely efficient method of converting light to chemical energy can be reproduced synthetically.

A computing problem that could lead to more efficient turbines, furnaces, and incinerators is modeling turbulence in flames. The problem itself demands advanced



Visualizing a cloud of electrons in a beam enables engineers to fine-tune high-energy particle accelerators for optimum performance.

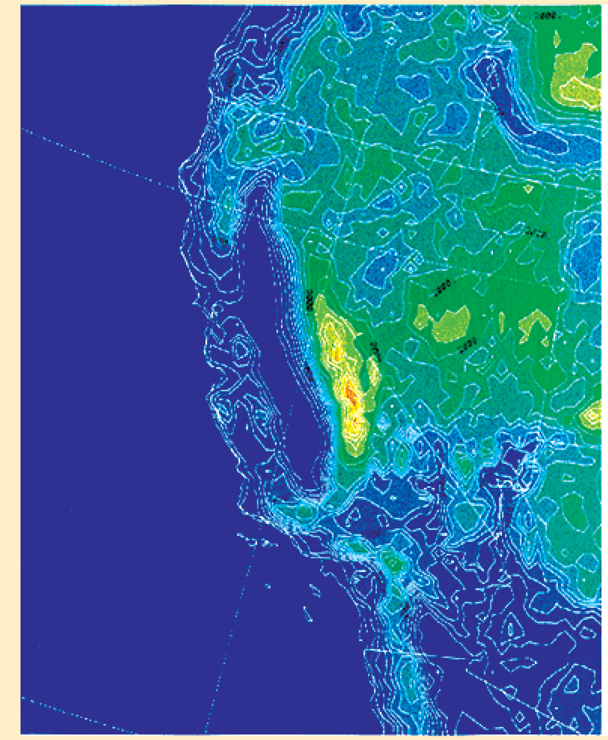


Using 3-D, time-dependent software, a team in the Lab's Center for Computational Sciences and Engineering has created the first detailed simulations of turbulent methane combustion. Flame modeling has applications for devices including power generators, heating systems, water heaters, stoves, and even clothes driers.

2010

GOAL FOR ADVANCED COMPUTNG

Provide NERSC With More Than 800 Teraflops of Computing Capacity.



Regional climate system models, like this one of California, can simulate the temporal and spatial precipitation and river flow of a local area at a resolution fine enough to aid researchers in accurately simulating specific local events, such as flood danger in a particular river valley.

visualization software, the kind that John Bell and Phillip Colella of the Computational Research Division delight in devising.

The two have developed software for adaptive mesh refinement, a technique that applies maximum computing power in a fine mesh to critical areas, but a coarse mesh to less important ones. Bell used the tools to create detailed 3-D simulations of turbulent methane combustion, involving more than 80 chemical reactions that must be computationally dissected as they occur.

Flame modeling belongs to the class of interface-dynamics problems, in which an instability arising at an interface between two fluids causes the interface to grow and change. In addition to turbulence, Bell and Colella's adaptive mesh refinement software has been applied to shock physics, astrophysics, fluid flow through porous media, and other studies — not least, climate modeling.

Making climate modeling predictive is a multiscalar challenge. Ferdinand Baer of the University of Maryland and Joseph Tribbia of the National Center for Atmospheric Research used NERSC to develop the Spectral Element Atmospheric Model to incorporate local mesh refinement within global climate models, long known for running at too coarse a resolution for meaningful prediction (modeling the Rocky Mountains as a single barrier, for example, while overlooking details like the Sierra Nevada). Their method increases resolution in dynamically significant areas like complex topographies, allowing regional resolution to enrich the global model.

The California Water Resources Research and Applications Center, whose lead scientist is Norman Miller of Berkeley Lab's Earth Sciences Division, models regional climate impacts on stream flow, water quality, and agriculture. The Regional Climate System Model pioneered by Miller and Jinwon Kim downscales global models to accurately simulate events on the local scale, such as flood danger in a particular river valley.

Understanding exchanges between land and atmosphere can improve models from the ground up. The Lab's Atmospheric Radiation Measurement program in the Great Plains, directed by the Earth Sciences Division's Margaret Torn, scales predictions of carbon, water, and energy flux — from individual land plots to entire regions. Torn is head of the Lab's Climate Change and Carbon Management Program, which coordinates climate research in the Earth Sciences, Engineering, Environmental Energy Technologies, and NERSC divisions. Under her initiative, the program designed the first regional climate and terrestrial ecosystem model coupling the land surface to the mesoscale; as a consequence, Berkeley Lab's climate-change simulations have achieved unprecedented fine resolution.

No matter how inaccessible, from the ionization of a helium atom to the thermonuclear explosion of a distant supernova, no scientific problem that can be well characterized is impossible to compute.

Operations Overview

Outstanding Science for Each Taxpayer Dollar

Scientific achievement depends upon the dedication of first-rate staff working to rigorous standards and procedures, using state-of-the-art tools and facilities. Operations and business management require a strategy to continuously improve and enhance the research support services that keep Berkeley Lab running.

A number of initiatives and improvements are envisioned during the coming years to insure that science excellence is being delivered with maximum efficiency and at the lowest possible cost, justifying its public support through a comprehensive assurance process and performance metrics.

The Management Priorities

Safety continues to be the number one priority for operations at Berkeley Lab. In FY04, the Lab posted the best safety record of the 10 Office of Science national laboratories, slashing by more than 50 percent both its injury rate and the number of accidents resulting in lost workdays among its full-time employees. In July of 2004, Berkeley Lab's self-assessment program was the first of its kind to be certified by the DOE, and its Integrated Safety Management program was among the first to achieve DOE validation.

When Director Chu arrived in August of 2004, he delivered the same urgent message that his predecessor, Chuck Shank, had emphasized. He initiated a campaign to reduce even further the number of incidents and accidents that jeopardized worker safety. Chu said his goal is to drive accident and injury rates as close to zero as humanly possible. Thus he will implement a five-year roadmap for continuous improvement in the area of environment, safety and health. Included will be a project to consolidate and integrate incident reporting, investigation, corrective actions, and lessons-learned processes.

The backbone of the modern laboratory — information management — will undergo a major assessment and overhaul, as Berkeley Lab moves toward standardizing and centralizing workstations through equipment and software upgrades. The savings over five years that will result from lower lifecycle costs, data protection, and strengthened cybersecurity is estimated at $5.8 million. Implementation in 2004 of the Berkeley Lab Information System (BLIS), a one-stop-shopping Internet control panel for employees, was an important first step.

Along with information technology, sound financial management is a priority at Berkeley Lab. A new supply-chain management system — including an electronic ordering system, pre-approved vendors, bulk pricing contracts, and streamlined source-to-payment processes — is expected to save the Lab $30 million over five years. And that means more money for science and less time spent on product acquisition by researchers. Its financial systems received significant upgrades in 2004, thanks in part to the hiring of Chief Financial Officer (CFO) Jeffrey Fernandez and additional key talent in the budget administration area. A primary goal of the Office of the CFO is to develop a Laboratory-wide budgeting and planning system, allowing the divisions to more accurately forecast and price out financial plans and budgets. This will also enable more stability in the institutional budgeting and rate-setting efforts.

The construction site at the Molecular Foundry displays a vivid reminder to put safety first.

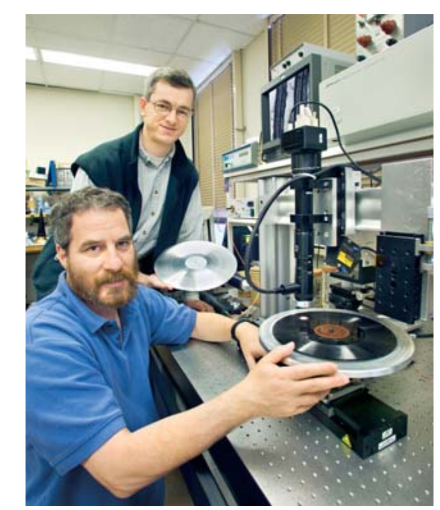
Scientific success in the future will be heavily dependent upon having modern facilities, and a 74-year-old laboratory faces additional challenges brought by aging and outdated buildings. Facilities management will get a boost through the implementation of the "Integrated Facilities Condition Management System" by the end of 2007. Once deployed, it will be the first of its kind in the DOE complex and will enable the integration of all relevant data so that intelligent and strategic investments in facilities can be made.

The system uses an engineered process to determine building conditions, deferred maintenance, replacement values, a condition index, renewal forecasts, prioritized deficiencies, and ongoing maintenance plans. A DOE Office of Science validation team, in reviewing the program late last year, pronounced it a "best practice" for integrating all the critical components of facilities assessment, planning and maintenance.

In most well-run businesses, institutional assurance and assessment are key factors to ensuring efficient and productive operations. At Berkeley Lab, a new assurance system has been established to develop, apply and track metrics of management functions, resulting in timely, accountable, and strong central control of performance. The new Office of Institutional Assurance — charged with ensuring that the Lab's contract compliance, scientific excellence, best management practices, and continuous improvement are achieved — has its first Director. Veteran project manager Jim Krupnick, who is currently overseeing the construction of the Molecular Foundry, will direct the assurance function and serve as the Laboratory's Project Management Officer. The Office of Institutional Assurance that Krupnick will manage, established as part of the new management contract with UC, includes two offices — contract assurance, headed by John Chernowski, and project management, a role that Krupnick will fulfill. This internal oversight will validate that performance targets are achieved. The objectives? A culture that will aim towards zero accidents and environmental incidents, and 100 percent customer satisfaction.

One of the tools that will be used is a "balanced scorecard," which will track performance evaluation measures in areas such as customer service, budget control, process reliability, compliance with rules and laws, and employee satisfaction. In operation since 1999, the scorecard will be expanded to include lab leadership and science and technology.

In concert with DOE commitments to small business contracting, Berkeley Lab intends to meet and exceed the goal of 50 percent of all subcontracts being allocated to small businesses for scientific and operations work. A new Small Business Program Office has been established to significantly expand both outreach and inreach activities, especially targeted to disadvantaged, underrepresented and women-owned businesses.



By adapting methods for measuring particle tracks in high-energy physics experiments, Lab researchers Carl Haber (left) and Vitaliy Fadeyev created a noncontact method for restoring damaged and fragile mechanical recordings. Archivists estimate that 40 percent of the millions of recordings in the world's major sound archives could benefit from restoration with the Berkeley Lab technology.

Knowledge Transfer: Good for Technology, Good for the Community

Berkeley Lab is a center of innovation and discovery, its work either contributing to the solutions to national problems or leading directly to benefits in the marketplace. It is also one of the laboratory's top priorities to grow this rapid transfer of technologies so that industry can incorporate them into programs that improve the nation's welfare.

The Lab has an impressive record in technology transfer; those innovations already in the marketplace include low-emissivity, coated windows; electronic ballasts for compact fluorescent lights; and advanced lipid protein tests for diagnosis of heart disease. More than 188 inventions have been transferred to industry in the last five years.

Also, more than 20 new companies that have spun off from Berkeley Lab research — including Symyx, Nanosys, Quantum Dot, Berkeley HeartLab, Nanomix, and Aeroseal — are responsible for nearly $2 billion in market capitalization and 800 new jobs in the Bay Area.

We have come a long way since our technology transfer office was established 15 years ago, but we can go still further. Through strengthening the technology transfer culture at the Lab, scientists will be transforming industries like biotechnology, information technology, and nanotechnology with exciting new processes and products. The dividends from such research accrue to the taxpayers, whose investments will be yielding tangible improvements in life and health, and for the scientists, who realize a fair return from their inventions to pursue more and better science.

Licensing revenue has grown by 20 percent a year over the last five years. And that total is likely to grow, thanks to tools like the Virtual Software Shop, a new central web site at the Lab with organized searchable access to open-source and other software. And, thanks also to an aggressive marketing strategy that matches the Lab community's discoveries with private-sector interests and needs.

Educating Future Scientists and Engineers

No less important for the future of the nation is the role Berkeley Lab plays in the education of future scientists and engineers. Just as technology transfer enables improvements and advances in industry, so the Lab's Center for Science and Engineering Education transfers critical knowledge, experience and real-world science to students from elementary grades through their undergraduate years. Teachers, too, are offered opportunities in front-line research that they may never have enjoyed in their career preparation.

Most agree that to encourage more students — in particular, women and underrepresented minorities — to pursue science as a career, one has to tap into the "pipeline." From grade school through college, promising young people need to be tracked and guided into research situations like those Berkeley Lab provides. And it is working. The Lab now gets 1,500 graduate and postdoctoral students each year to work in its programs, an increase of 56 percent over the past five years. In 2004, these students comprised 21 percent of the Lab's staff.

Beamline scientist Michael Martin (left) works with student Christopher Taylor at the Advanced Light Source. Each year Berkeley Lab hosts hundreds of students, from 4th grade to graduate level, as part of its commitment to promoting and mentoring science.

Intervention can come up and down the pipeline — in K-12, where the Lab runs a program of tours, workshops, and summer work experiences; at the undergraduate college level, with jobs and internships; and with graduate students and post-docs. Once they are here, it's up to the mentors at Berkeley Lab — over 100-strong at any one time — to teach and to share their excitement about the profession.

Berkeley Lab intends to expand its student tracking system and hold its divisions accountable for pipeline recruitment success through the Director's Annual Work Force Review. A database developed by the Physical Biosciences Division will serve as a model for web-based tracking and mentoring.

One of the tangible illustrations of Berkeley Lab's commitment to local schools came in 2005 in the form of an offer to help the cash-strapped Berkeley city schools in their students' preparation for standardized state tests. With little money or time available for science instruction, the district welcomed volunteer Lab instructors as they visited all fifth graders in 11 schools and taught lessons geared toward the physical and earth sciences.

Information transfer isn't just limited to those in school. Berkeley Lab maintains an active community relations program, including its open-membership "Friends of Science" organization that sponsors public scientific talks for the layman, both on and off-site. The "Friends" roster grew to over 400 in 2004, reflective of a continuing hunger for knowledge about science.

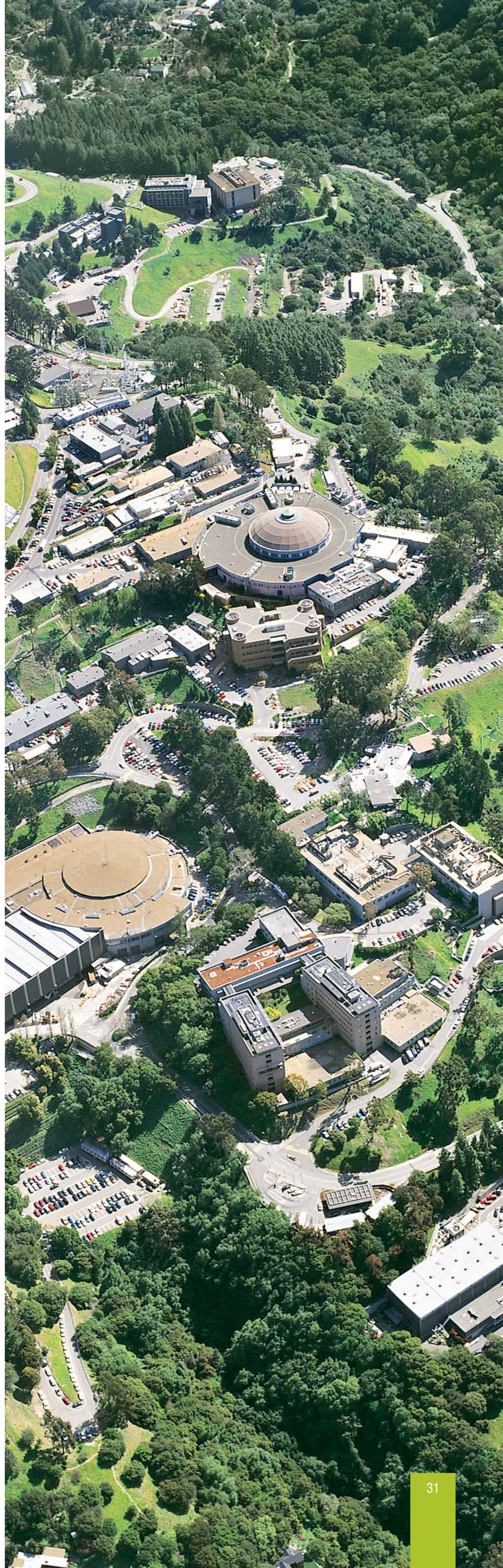
About the Lab

The Lawrence Berkeley National Laboratory (Berkeley Lab) was founded in 1931 by Ernest O. Lawrence, who won the Nobel Prize in physics in 1939 for his invention of the cyclotron. Lawrence's invention led to a Golden Age of particle physics and revolutionary discoveries about the nature of the universe. Under the stewardship of the University of California, which manages the Lab for the Department of Energy, Berkeley Lab has evolved from the birthplace of nuclear science and medicine into a multidisciplinary research facility advancing the forefront of scientific knowledge and addressing problems of national and global concern. Today, Berkeley Lab performs research in nanoscience and advanced materials, the life sciences, computing, energy and earth sciences, physics and cosmology. The Lab also operates a Homeland Security office dedicated to leveraging fundamental scientific research to develop methods for ensuring homeland safety.

Since its inception, Berkeley Lab's location on the hillside above the University of California at Berkeley has offered a unique opportunity for scientific and academic partnerships and has helped to foster the academic excellence that is the hallmark of the Lab's scientific endeavors. Of Berkeley Lab's staff of approximately 4,000, more than 250 faculty/scientists hold joint appointments with UC Berkeley and other UC campuses. In addition, nearly 800 students and postdoctoral fellows are employed each year, along with more than 3,000 participating guests from institutions around the world.

With an annual budget of more than $500 million, Berkeley Lab has a sizable regional economic impact as one of the 15 largest employers in the area. The Lab interacts with the private sector in a growing number of collaborative research projects intended to transfer research know-how into the national economy. A number of corporations supply both funding and expertise for many joint projects that range from building the next generation of semiconductors to developing new tests for heart disease risk.

In addition to its fundamental research, Berkeley Lab's research centers and user facilities provide intellectual resources, services, infrastructure and unique experimental facilities not found anywhere else in the world. They include the Advanced Light Source, the National Energy Research Scientific Computing Center, the Energy Sciences Network, the National Center for Electron Microscopy and the Joint Genome Institute.



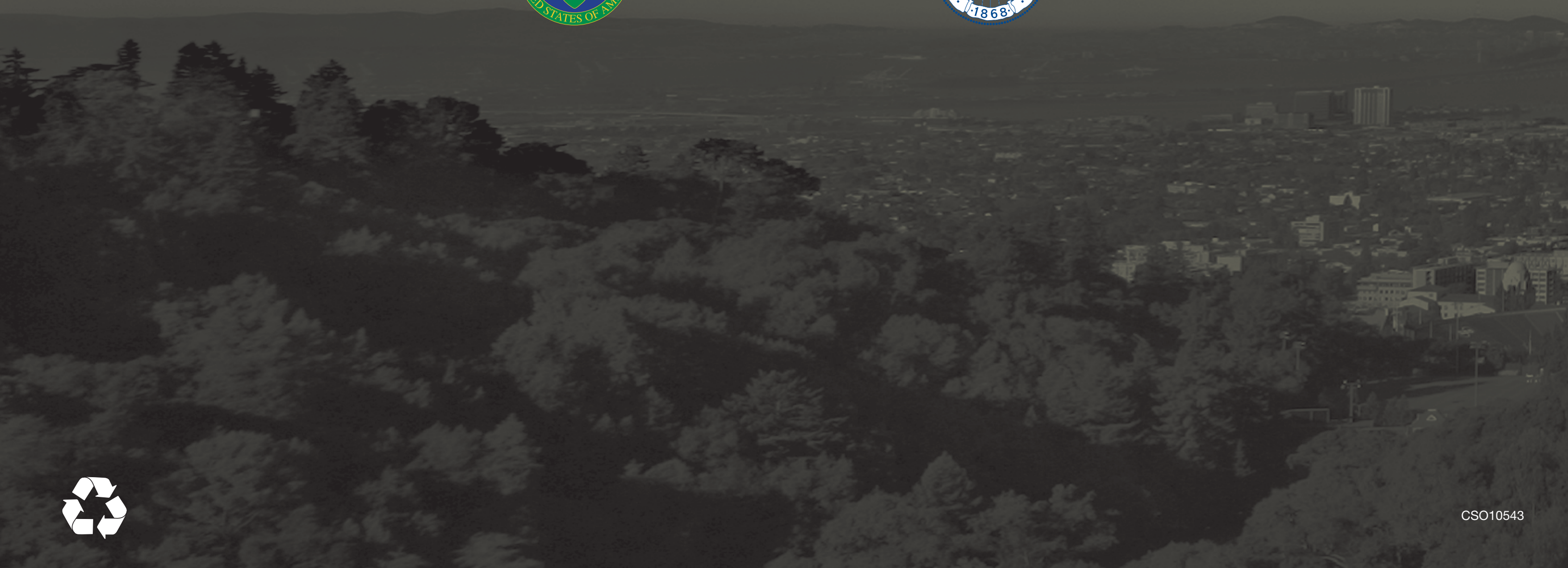
75 Years of Nobel Prize-Winning Science

It all began humbly enough. In the summer of 1928, a 27-year-old physics professor named Ernest O. Lawrence was wooed from his faculty position at Yale University to a job at the University of California's Berkeley campus. He had planned to continue his work on photoelectricity, but his research took a turn when he read a paper from Norwegian engineer Rolf Wideroe on a method for accelerating particles, a goal long sought after by physicists. With the help of his graduate student, M. Stanley Livingston, Lawrence invented a unique particle accelerator that became known as the cyclotron. The first cyclotron was an unimpressive looking contraption made of glass, sealing wax and bronze, not much bigger than the palm of Lawrence's hand, but it would eventually prove his hypothesis: whirling charged particles around to boost their energies, then casting them toward a target is an effective way to smash atomic nuclei. The cyclotron would go on to win Lawrence the 1939 Nobel Prize in physics and usher in a new era in the study of subatomic particles.

Lawrence also launched the modern era of multidisciplinary, team science. When he came to Berkeley, the traditional practice for scientists was to work within their own specialized field, seldom sharing information or collaborating outside of their departments. But in August of 1931, when he created his Radiation Laboratory in a modest building on the Berkeley campus, Lawrence began recruiting a brilliant circle of colleagues from physics, chemistry, biology, engineering and medicine, whose groundbreaking teamwork would be critical to the laboratory's legendary success. The Rad Lab was the forerunner of the present Lawrence Berkeley National Laboratory. When Lawrence's plans for bigger and better atom-smashing cyclotrons required more room, he moved his laboratory off campus and up to its present location in the Berkeley hills, overlooking the San Francisco Bay.

Today, Berkeley Lab continues the tradition of multidisciplinary scientific teams working together to solve global problems in human health, technology, energy, and the environment. Ten Nobelists have worked here, including the Lab's present director Steve Chu. And countless other researchers have contributed to the Lab's success as an institution for furthering our nation's scientific endeavors, whether in fundamental research, science education, or technology transfer. The year 2006 will mark the 75th anniversary of the founding of Lawrence's laboratory and his grand idea for multidisciplinary team science, truly a cause for celebration.

Lawrence Berkeley National Laboratory
University of California
Berkeley, California 94720
www.lbl.gov



CSO10543