Also in this issue:

- Technologies to Store Carbon Dioxide Underground
- Models Reveal the Fate of Radionuclides
- A New Approach for Solgel Chemistry
This year marks the 100th anniversary of the “miraculous year” in physics—when Albert Einstein published four important papers that continue to influence physics research to this day. To honor this anniversary, the U.S. Congress, the United Nations, and physics organizations worldwide have designated 2005 the World Year of Physics. As part of that celebration, S&TR is publishing a four-part series examining the foundation that Einstein’s discoveries set for the Laboratory’s research. The first article in this series, which begins on p. 4, discusses the theories of special and general relativity and their importance to Livermore’s astrophysics and computational research. On the cover, a 1947 photograph of Einstein is superimposed on the handwritten manuscript of one 1905 paper. (Reprinted courtesy of Albert Einstein Archives, the Jewish National and University Library, the Hebrew University of Jerusalem, Israel.)

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Einstein’s Legacy Alive at Livermore
Commentary by Michael R. Anastasio

Applying Einstein’s Theories of Relativity
In their efforts to understand the cosmos, Livermore physicists must account for the relativistic effects postulated by Albert Einstein.

Locked in Rock: Sequestering Carbon Dioxide Underground
Livermore scientists are examining technologies to reduce atmospheric concentrations of carbon dioxide by burying it deep underground.

Modeling the Subsurface Movement of Radionuclides
Using data from past underground nuclear tests, a Livermore team is modeling radionuclide migration at the Nevada Test Site.

Novel Materials from Solgel Chemistry
Livermore chemists are developing a method for fabricating solgels to better control the physical properties of the new materials.

The Laboratory in the News
Patents and Awards
Abstracts
Device can stop a bomb on wheels

Laboratory researchers recently demonstrated their latest version of a truck-stopping device. Operated by remote control, the shoebox-size instrument is designed to protect sensitive buildings and facilities, such as power plants, that are potential targets for a terrorist attack. For example, at a facility’s inspection point, tamper-resistant devices could be mounted on a truck before the vehicle is allowed on site and removed before the vehicle leaves. If a driver then tried to crash a truck into a building, security personnel could push a remote-control button to set off that vehicle’s air-brake valves.

The Livermore team has also developed a control system that uses antennas placed around a site’s buildings. In the event a runaway truck tries to crash through the gates, the antennas, operating on a continuous signal, will activate the truck’s air brakes as the vehicle passes by. The antenna system is designed to eliminate interference from other radio frequencies, such as from a cell phone, to prevent hackers from interrupting signals or circumventing the system. To have such devices automatically equipped on all commercial transportation vehicles would require legislation.

Livermore’s work on truck-stopping technology receives funding from the California Highway Patrol and the California Energy Commission.
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Telescope to peer into deep sky

The National Aeronautics and Space Administration (NASA) has approved a collaborative study to build and launch the Nuclear Spectroscopic Telescope Array (NuSTAR). Led by the California Institute of Technology, the collaboration also includes researchers from Lawrence Livermore, Columbia University, the Danish Space Research Institute, Jet Propulsion Laboratory, and several other institutions.

Laboratory scientists will use the pioneering telescope to understand how stars explode and produce elements such as calcium. With NuSTAR, scientists will for the first time be able to obtain a high-energy (hard) x-ray map of the sky in extraordinary resolution. The telescope can be used to study supernovae phenomena and the accretion of matter by black holes. NuSTAR technologies may also have applications in homeland security because hard x rays are a key method for detecting and identifying nuclear material.

Telescopes have taken images of the deep sky in the optical, infrared, and low-energy (soft) x-ray bands. However, most black holes are obscured by dust and cannot be seen in images of those bands. Hard x-ray telescopes can penetrate this dust to detect even the most obscured supermassive black holes. NuSTAR will be hundreds of times more sensitive than any previous hard x-ray instrument, which will greatly improve the image resolution.

Scientists are particularly interested in the information hard x-ray imaging will provide on the deepest layers of exploding stars and the new chemical elements they produce. For example, titanium-44 is an interesting tracer element for studying what happened in a supernova. Also, when titanium-44 decays, it is dispersed throughout the universe in the form of calcium, which eventually winds up in human bones and teeth.

NASA will review the project in early 2006 to grant an initial confirmation for launch.
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Researchers study the transformation of neutrinos

As part of the international team working on the Main Injector Neutrino Oscillation Search (MINOS) experiment, Livermore scientists hope to study in detail the transformation of neutrinos from one type to another. Neutrinos are relatively massless particles with no electric charge, but they are fundamental to the makeup of the universe. To explore the mysterious nature and properties of neutrinos, the MINOS researchers will use two giant detectors—one at Fermi National Accelerator Laboratory (Fermilab) and a 6,000-ton detector lying in a historic iron mine at Soudan, Minnesota.

One goal of the MINOS experiment is to discover the rate at which neutrinos “change flavors,” or oscillate from one type to another. Neutrinos are difficult to detect because they rarely interact with anything. Although they can easily pass through a planet or solid walls, they seldom leave a trace of their existence.

In the MINOS experiment, a narrow beam of neutrinos is generated and characterized by the near detector at Fermilab. The beam is aimed at a far detector, located in the Soudan Underground Laboratory in Minnesota. The neutrino beam energy is chosen so that the distance between the two detectors corresponds to an expected maximum in the probability that a neutrino produced at Fermilab will oscillate to another flavor. Studying the elusive neutrino will help scientists better understand particle physics, specifically the role of neutrinos in the formation of the universe and their relationship to dark matter.

Dedication ceremonies for the MINOS detectors were held at Fermilab on March 4, 2005. Livermore’s MINOS research is funded by the Laboratory Directed Research and Development and Physical Data Research programs. The MINOS experiment as a whole is funded by the Department of Energy’s Office of Science.
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Commentary by Michael R. Anastasio

Einstein’s Legacy
Alive at Livermore

In March 1905, a little-known patent examiner in the Swiss patent office published a paper about the properties of light in the German physics journal, *Annalen der Physik*. The examiner was 26-year-old Albert Einstein, and his paper, “Concerning an Heuristic Point of View toward the Emission and Transmission of Light,” marked the beginning of a surge of human creativity nearly unprecedented in science. In seven months, Einstein published four papers and a thesis that together had far-reaching effects on physics, technology, and our understanding of the universe.

In celebration of Einstein’s extraordinary accomplishments, the U.S. Congress, the United Nations, and various governments and nongovernmental bodies have declared 2005 the World Year of Physics. As part of Lawrence Livermore’s participation in this yearlong celebration, *Science and Technology Review* (*S&TR*) is publishing a four-part series, examining how Einstein’s discoveries form the basis for much of the Laboratory’s physics research.

Beginning on p. 4, the first article in this series discusses Einstein’s most famous 1905 paper, “On the Electrodynamics of Moving Bodies,” which introduced the revolutionary concept of relativity. Special and general relativity play an important role in Livermore physics research, especially our research into the physics of astronomical events such as gamma-ray bursts, black holes, and supernovae. In like manner, our supercomputer codes that model these events must account for relativity. Many of our astrophysics codes were adapted from versions developed originally for nuclear weapons research, which are based on concepts outlined in another Einstein paper. Finally, our work with machines that accelerate ions close to the speed of light would not be possible without incorporating the tenets of relativity.

In June, *S&TR* will discuss Einstein’s first paper of 1905, “Concerning an Heuristic Point of View toward the Emission and Transmission of Light.” In this paper, he explained some puzzling properties of light as a consequence of its particulate nature. Einstein called light’s discrete packets quanta; we now call them photons. This paper is the foundation for the Laboratory’s research in quantum physics, ionizing radiation, lasers, and advanced optical-imaging techniques.

The July/August *S&TR* will examine Einstein’s third 1905 paper, “Investigations on the Theory of the Brownian Movement.”

In this paper, he explained the random motion of microscopic particles suspended in a liquid, and he used a branch of physics known as statistical mechanics to estimate the size of molecules. This work helped confirm the atomic theory of matter and is the basis for much of the Laboratory’s work in molecular dynamics, Monte Carlo statistical techniques, and physical chemistry.

In September, *S&TR* will finish the series with a discussion of Einstein’s fourth 1905 paper, “Does the Inertia of a Body Depend upon Its Energy-Content?” In this paper, which appeared in the September 1905 edition of *Annalen der Physik*, Einstein reported that, as a consequence of special relativity, matter and energy are interchangeable. This work led to the famous equation \( E = mc^2 \). Thirty years later, physicists discovered fission and fusion, which demonstrate the conversion of mass into large amounts of energy. This work made possible the nuclear weapons research done at Lawrence Livermore and Los Alamos national laboratories. It also paved the way for Livermore research efforts in peaceful nuclear power, such as magnetic fusion energy and inertial confinement fusion, as well as the Laboratory’s nuclear and particle physics experiments, in which matter and energy are interchanged.

Einstein’s work in 1905 was such an amazing burst of creativity that it has been called the annus mirabilis, or miraculous year. A measure of the lasting effects of Einstein’s achievements is the way in which they still form the basis of work in pure and applied physics. In that respect, one of our goals in publishing this series is to show how Einstein’s legacy is alive and well at Lawrence Livermore. We pride ourselves on forming teams of specialists to attack challenging science and technology problems in national security. Einstein showed us how much one person can accomplish.

Michael R. Anastasio is director of Lawrence Livermore National Laboratory.

Lawrence Livermore National Laboratory
Applying Einstein’s

Albert Einstein’s theories of relativity play an essential role in many Livermore research projects.
In 1905, Albert Einstein wrote four papers that revolutionized the field of physics. The impact of his work helped launch quantum mechanics, deepened scientific knowledge about how molecules behave, and advanced understanding of astronomical objects and cosmology. Technologies such as solar power, global positioning systems, and digital equipment from computers to cameras stem from his insights into light, radiation, velocity, and gravity. Researchers at Lawrence Livermore and throughout the world continue to benefit from this legacy.

When he was a young man, Einstein is said to have asked himself what he would see if he could travel on a beam of light. He thought that if such an adventure were possible, he would see an oscillating electromagnetic field. In 1905, these reflections led Einstein to formulate what is now known as the theory of special relativity.

Light travels as a wave of oscillating electric and magnetic fields that are produced by the acceleration of electrically charged particles. In 1861, James Maxwell’s research explained the relationship between electricity and magnetism. By the end of the 19th century, scientists discovered that all electromagnetic radiation travels at the same velocity—about 300,000 kilometers per second. This velocity is called the speed of light because light is a form of electromagnetic radiation, and it remains the same, regardless of the velocity of the emitting source or the receiver.

**Speed of Light as a Constant**

Because speed is the ratio of distance over time, Einstein reasoned that, if the speed of light is constant, measures of time and distance must vary from one observer to another, depending on their relative motion. Einstein wrote one of his 1905 papers, “On the Electrodynamics of Moving Bodies,” to reconcile the difference in observed space and time between frames of reference with different velocities.

For example, the explanation for the force between a moving, electrically charged particle and a wire carrying an electrical current is different if given from the viewpoint of an observer moving along with the particle than it is if given from that of someone watching at rest. For someone watching at rest, the force acting on the moving particle is due entirely to the magnetic field produced by the current in the wire. But for an observer who is moving with the particle, no force is produced by the wire’s magnetic field. Rather, the wire appears to be charged, and the force is caused entirely by the wire’s electric field. The magnitude of the force is the same for both observers.

Einstein showed how to reconcile the disparity between the descriptions of observers moving and those at rest. Special relativity is based on two premises. First, light has the same speed for all observers regardless of their relative motion. Light velocity provides an upper limit for the speed of all forces, effects, and material objects. Second, the equations of physics are the same for observers moving at different relative speeds. A surprising consequence of these premises is that an observer’s measurements of an object’s characteristics—such as its size, mass,
Einstein’s Theories of Relativity

and rate of time—depend on the relative velocity of the observer and the object. To an observer viewing an object as it approaches the speed of light, a clock traveling with the object appears to slow—almost to a stop—and the length of the object seems to shrink along the direction of travel.

Physicists categorize objects with velocities close to the speed of light as relativistic, and objects with velocities much less than the speed of light as nonrelativistic. Adding velocities is not as simple as mere arithmetic. For nonrelativistic speeds, the intuitive result is almost precisely correct. However, at relativistic speeds, it is not. For example, suppose an observer at rest sees a second observer traveling at a velocity of 0.8c (where c equals the speed of light). The second observer emits an object in the same direction and measures its speed as 0.7c. The first observer will not measure 1.5c as the object’s speed. Because of the way in which velocities add according to special relativity, the observer will find 0.96c as the object’s velocity.

**Simulating the Big Bang**

The relativistic change of mass and the apparent spatial length are important factors in studies of matter in high-energy physics. For example, researchers are attempting to simulate the first microseconds after the big bang so they can explore new high-energy forms of matter and their origins. In a collaboration involving 40 institutions and 300 physicists from around the world, Livermore scientists are using the Relativistic Heavy-Ion Collider (RHIC) at Brookhaven National Laboratory to accelerate gold ions to within 99.995 percent of the speed of light. (See S&TR, January/February 2003, pp. 4–9.) In RHIC, about 1 million ion collisions occur each second. Because a particle moving with extreme speed has much higher energy than a slow-moving particle, the nuclei shatter and are transformed into a plasma of their constituent quarks and gluons.

Scientists believe that quarks are the basic particles making up protons and neutrons. Additional particles called gluons mediate the strong force that holds quarks together and keeps the protons and neutrons in atomic nuclei. Quarks and gluons possess a type of charge called color, which is the source of the powerful forces that bind the quarks together.

Quantum chromodynamics—the theory of the strong interaction, or color forces—states that quarks and gluons can be liberated only under high-temperature conditions similar to those in the very early universe. At that time, in the first moments of the big bang, quarks and gluons are free as part of a quark–gluon plasma.

The collisions between two nuclei at RHIC are highly explosive, releasing more than a trillion electronvolts of energy in a volume the size of an atomic nucleus. At these high speeds, a special relativistic effect, called Lorentz contraction, is noticeable. The nuclei appear flat rather than spherical. (See the figure at left.)

“Einstein’s theory of special relativity is ingrained in the design of particle accelerators,” says Livermore physicist Ron Soltz. “As the nuclei attain more energy, the velocity of the ions gets closer to the speed of light, but without ever reaching it. If we didn’t have relativity, the way in which we use accelerators would be very different.”

Soltz’s team, which includes Livermore physicists Mike Heffner, Jennifer Klay, David Brown, and Ed Hartouni and postdoctoral researchers Jason Newby and Akitomo Enokizono, is running RHIC experiments with gold because the element has a heavy nucleus, from which it is easy to generate ions. The team has used lead, another element with a heavy nucleus. Next, they plan to experiment with copper, which has a lighter nucleus. Soltz explains, “The heavier the nucleus of an element is, the more particles there are to participate in the interaction. Because of our success with gold-to-gold collisions, we are trying a lighter element to determine if we will see similar plasma results.”

**Observing Celestial Fireworks**

Einstein’s theories on the speed of light and frames of reference also enable astrophysicists to understand celestial objects such as gamma-ray bursts (GRBs), supernovae, black holes, and neutron stars.

GRBs were discovered serendipitously in the late 1960s when U.S. military satellites were launched to ensure compliance with the Atmospheric Nuclear Test Ban Treaty. GRBs are short-lived, lasting from a few milliseconds to several minutes, and they release gamma-ray photons. The leading model to explain the events surrounding a GRB is the collapsing star, or collapsar, model. According to this model, a GRB arises when a dying, rotating star is too massive to successfully explode as a supernova. Instead, the iron core of the massive star collapses into a black hole surrounded by a dense accretion disk, thus emitting gamma rays with energies exceeding 100,000 electronvolts. (See S&TR, March 2005, pp. 24–26.)

Gamma rays are a very energetic part of the electromagnetic spectrum, which

In studies at Brookhaven National Laboratory’s Relativistic Heavy-Ion Collider, gold ions accelerated to relativistic speeds appear flat rather than spherical.
ranges from radio waves at the lowest energies through visible optical light at higher energies to gamma rays. The extreme energies released during GRBs make them the brightest source of gamma-ray photons in the observable universe, about a million trillion times as bright as the Sun. Gamma rays can be detected only from space because Earth’s atmosphere absorbs them.

GRBs originate from deep space, some more than 8-billion light years away. They exhibit strong relativistic behaviors, including special relativistic aberration, in which light emitted is not uniformly distributed but rather is beamed to 1 percent of the sky in the direction of the jet’s motion. From Earth, this emission appears as a jet of material that is ejected and accelerated toward the direction of the jet. Because of relativistic effects, the jet’s material moving directly toward an observer is seen to evolve more quickly than matter moving at an angle. Scientists refer to the directionality of a GRB’s jet emission as relativistic beaming.

Only a few stars in a million produce GRBs when they die. On average, at least one GRB is observed every day somewhere in the universe. However, the number of events may be up to 500 times greater because only the GRBs that are beamed toward Earth can be observed. In November 2004, the National Aeronautics and Space Administration (NASA) launched the SWIFT telescope to conduct the most comprehensive study of GRBs to date.

Measuring a GRB’s Afterglow

Researchers can predict a relationship between the brightness, temperature, and duration of a GRB by studying its jet. Following the release of gamma rays, the ejected material continues to move away from the exploding collapsar and, like a snowplow, gathers material from interstellar space. As the energetic shell sweeps up material, it slows down and cools, emitting progressively lower energies of the electromagnetic spectrum, from x rays through radio waves. This effect, called the afterglow, fades over time, lasting from a few days to several years. However, because the afterglow lasts substantially longer than the GRB, astrophysicists can study it to glean information about the nature of the surrounding environment.

Livermore astrophysicist Jay Salmonson says, “One feature we look for is how the material cools in a burst. As material cools, it forms a light curve with a characteristic decay slope. At some point, the curve breaks and becomes steeper. This change indicates that the shock is slowing, and beaming becomes less pronounced. We can then see more of the shock area, which allows us to determine the jet’s size and energy as well as what caused it.”

Salmonson has developed a model to study possible afterglow shapes at various viewing angles. Called AfterglowView, the program calculates what an observer at a specific orientation relative to the jet’s axis would see from a GRB. By comparing predictions with observations, his team hopes to gain clues as to the shape and size of afterglows. The studies require detailed accounting of relativistic motions of material through space–time. Salmonson says, “So far, we’ve inferred the angular size of a jet to be 5 to 10 degrees. One surprising result of our studies is that most bursts appear to have the same amount of energy, although they presumably originated from a range of stellar progenitors.”

Adding Gravity to the Equation

In 1907, Einstein began work on an extension to special relativity. Called the theory of general relativity, it described gravitation and its relation to the other forces of nature. Isaac Newton’s theory of gravitation states that masses experience an attractive force between them. This force, which acts at a distance, accelerates masses toward each other. The strength of the force depends on the size of the masses and is inversely proportional to the square of the distance between them. In Newton’s universe, space existed independent of the matter contained within it.

Newtonian physics explains how to calculate forces that are caused by the mass of a body, but it does not explain why matter causes gravity. Einstein proposed that matter bent space and time, and this distortion is what is perceived as gravity. The more massive an object is in space, the larger the space and time distortion around it and, hence, the stronger its gravity.

The theory of general relativity states that bodies, regardless of their mass, fall freely in a uniform gravitational field with the same acceleration. Thus, the effects of gravity are equivalent to the effect of an accelerated frame of reference without gravity. Einstein proposed that, without a frame of reference, no one can distinguish...
between acceleration and gravitation. This idea is known as the principle of equivalence. Several predictions result from this theory: that light and all forms of electromagnetic radiation are deflected or bent by gravitational force, that a clock on the surface of a massive object will run slower than a clock in open space, and that gravitational waves radiate at the speed of light from large masses that are accelerating.

**Codes to Model the Universe**

With Einstein’s theories of special and general relativity, researchers can model the forces in the universe to study its origins, determine how celestial objects influence one another, and then predict the evolution of these objects. Unfortunately, the equations of general relativity are complex and difficult to solve. Advances in computing methods and technologies have been essential to understanding cosmological models, the universe, and astrophysical processes within them, by allowing researchers to solve the relativistic equations on computers.

In 1968, Laboratory physicist Jim Wilson began work in numerical relativity, which explores the computational aspects of general relativity and its applications for cosmology, astrophysics, and gravitational-wave physics. Beginning with one-dimensional codes and later working with two- and three-dimensional codes, Wilson applied Einstein’s complex, nonlinear partial differential equations to advance understanding in astrophysics. Over the last three decades, he has developed several codes that work on Livermore’s supercomputers to model a variety of phenomena. His research has explored heavy-ion collisions, supernova explosions, black-hole accretion and encounters, energy extraction from magnetic black holes, black-hole formation in neutron-star binaries, thermonuclear initiation from white dwarfs, and GRB production in neutron-star binaries.

Wilson is collaborating with Livermore physicist Dave Dearborn and Grant Matthews from the University of Notre Dame to study how stars are destroyed by a black hole at the center of the galaxy. Their research indicates that stars known as white dwarfs become unstable when they are subjected to the strong gravitational field near a black hole. If a white dwarf passes too closely to a black hole, carbon and oxygen in the star’s center are squeezed, initiating a runaway thermonuclear burn that blows the star apart. To better understand these phenomena, Wilson and his collaborators are modeling such events using both a general relativity code and the Djehuty stellar evolution code. (See *S&TR*, May 2002, pp. 4–10.)

**Modeling Whirling Black Holes**

The application of numerical relativity is being continued in the COSMOS code. In 2001, Livermore astrophysicist Peter Anninos completed the code, which can calculate relativistic problems. One of the first applications of COSMOS was to model astrophysical events having special relativistic effects, such as first-order cosmological phase transitions occurring in the first frictions of a second after the big bang. These simulations allowed researchers to investigate the stability of quark–hadron phase boundaries and the possibility of generating primordial perturbations in hadronic matter that could grow to become galaxies. (See *S&TR*, March 2003, pp. 4–11.)

In 2004, Anninos added magnetic fields and adaptive, or moving, meshes to the COSMOS code. He and astrophysicist Chris Fragile began modeling astrophysical events for which general relativistic effects are significant. The mesh enhancement allows the team to follow the way gas flows behave near black holes—in particular, the pancake-shaped distribution of matter outside a black hole known as an accretion disk. The team models such characteristics as black-hole spin and the
tilt and sound speed of the accretion disk to determine the range of possible effects, including the relativistic effect known as frame dragging.

Any object with mass warps the space and time around it, but a rotating object distorts space–time more radically, twisting it like a pinwheel around the object. Earth’s rotation is sufficient to cause satellites to be dragged by 2 meters every year. Near a spinning black hole, frame dragging changes the shape of the accretion disk and affects how much gas can be captured by the black hole.

Livermore is the first to simulate frame-dragging effects on generic gas flows with no assumed space–time symmetries. The team is also simulating GRB systems, black hole–neutron star binaries, and magnetized jet outflows from black-hole accretion disks. The researchers have examined tilted disks around rapidly rotating black holes and are now including magnetic fields in the simulations. They also are exploring oscillation modes in black-hole accretion disks. Astronomers have observed periodic oscillations in the x-ray light curves of accreting black holes. One possible explanation is that the accretion disk, which emits x rays, is oscillating, producing an effect similar to sounding a note on a musical instrument.

A Place Light Can’t Escape

The greater the mass of an object, the stronger is its gravitational pull. If a star is sufficiently massive, its gravitational pull crushes atoms. Electrons combine with protons in the atomic nuclei to form neutrons. The nuclei are crushed together, which reduces the star to a huge conglomerate of neutrons, called a neutron star.

Perhaps the most extraordinary prediction of general relativity is that sometimes a neutron star becomes a black hole. A black hole is a mass so concentrated, and thus its gravitational hold so powerful, that an object’s velocity would have to exceed the speed of light to escape the hole’s surface, or event horizon.

Black holes are described by two parameters: mass and angular momentum.

![Simulation](image)

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Lawrence Livermore National Laboratory
Scientists determine these parameters by studying the region surrounding the event horizon and knowing the stellar progenitor of a black hole. When a spinning neutron star collapses into a black hole, the hole also spins to conserve angular momentum. In 1916, Karl Schwarzschild solved gravitational field equations for a nonspinning black hole, but it was not until 1963 that Roy Kerr discovered a solution for a spinning black hole.

Although a black hole emits no light, matter from nearby stars can be captured by its gravitational field, creating an accretion disk. Matter in the disk gradually spirals inward, converting gravitational potential energy into kinetic energy, thermal energy, and light. As this matter approaches the event horizon, it reaches relativistic velocities. Because black holes have a small angular size, or observational angle, scientists cannot yet image these environments directly. Instead, they study the radiation emitted from a black hole’s accretion disk, much of which emerges as X-rays.

**Measuring Relativistic Effects**

In collaboration with researchers at the Massachusetts Institute of Technology and the Harvard-Smithsonian Center for Astrophysics, Laboratory astrophysicists Duane Liedahl and Christopher Mauche are developing computer codes to model the complex physics associated with X-ray spectral emission from an accreting black hole.

The COMPASS code (computer models of the physics of accretion disk structure and spectra) was developed by the collaborative group in the 1990s. It can model the temperature, density, ionization state, and velocity of matter in the accretion disk. COMPASS incorporates HULLAC (Hebrew University and Lawrence Livermore atomic code), a code originally developed in the 1980s. HULLAC generates atomic models to determine the heating and cooling of the accretion disk and the spectrum of the emitted light. A Monte Carlo–based photon propagator has also been developed to track individual photons during their path through space–time.

Accretion disks are made up of common elements such as hydrogen, helium, oxygen, and iron. These elements are ionized by the photoelectric effect, which results when an ion absorbs a high-energy photon and, in turn, ejects an electron. Left in a state of high excitation, the ion can return to its lowest energy level by emitting a photon, which for iron has an energy of 6.4 kiloelectronvolts. In the X-ray spectrum, this energy normally appears as a narrow line on top of a radiation continuum. However, for a black-hole accretion disk, the lines are highly distorted by several classical and relativistic effects.

One such effect, called the Doppler effect, accounts for the change in the frequency of electromagnetic waves as an object moves toward or away from an observer. The Doppler effect alters the energy or color of light. For example, light from a star moving toward an observer appears bluer, but light from a star moving away from the observer appears redder.

In an accretion disk, the Doppler effect broadens iron’s narrow energy line into a...
double-horned profile, which for the high velocities (150,000 kilometers per second or half the speed of light) near a black hole, extends from 0.5 to 1.5 times the original energy of the line. Relativistic effects, such as time dilation and the beaming of the radiation in the direction of motion, further distort the line, dimming the red horn of the profile and brightening the blue horn. Finally, the emitted photons lose a significant fraction of their energy as they climb out of the gravitational well that surrounds a black hole, leading to a net redshift of the line profile. The resulting broad, skewed, and redshifted lines observed from Earth are the unmistakable signature of black-hole accretion disks.

Liedahl and Mauche's computer models account for all these effects, allowing the team to calculate x-ray spectra as a function of black-hole spin and the angle of observation. These data are then compared to spectra collected from satellites such as NASA's Chandra X-Ray Observatory and the European Space Agency's XMM-Newton. X-ray satellites to be deployed in the next decade, such as NASA's Constellation-X Observatory, are expected to provide about 100 times the sensitivity of current satellites, allowing scientists to study in even more detail the extreme environments surrounding accreting black holes.

**Bewildering But Essential**

To many, Einstein's theories of special and general relativity seem bewildering and violate common sense. However, to scientists, the theories are essential to understanding the universe. Einstein began by wondering what he would see if he traveled on a beam of light. One hundred years later, many researchers, including those at Livermore, are applying his theories to accelerate particles to almost the speed of light, model various astronomical and cosmological events, and gain insight into mathematical and physics properties to help in areas such as stockpile stewardship. Einstein left a rich legacy from that miracle year of physics in 1905, and his legacy continues to influence physics research to this day.

—Gabriele Rennie

**Key Words:** AfterglowView, Albert Einstein, COMPASS (computer models of the physics of accretion disk structure and spectra) code, COSMOS code, HULLAC (Hebrew University and Lawrence Livermore atomic code), Relativistic Heavy-Ion Collider (RHIC), speed of light, theory of general relativity, theory of special relativity.

*For information on Lawrence Livermore's activities for the World Year of Physics, see www.llnl.gov/pao/WYOP.*
For more than a century, scientists have measured a steady buildup of greenhouse gases in the atmosphere as a result of burning fossil fuels. The accumulation of these gases in the upper atmosphere traps solar radiation, which then increases Earth’s atmospheric and oceanic temperatures. Many research studies indicate that this continued rise in temperatures will adversely affect Earth’s climate, which could lead to dramatic—even catastrophic—changes in weather patterns around the world.

By far, the most abundant greenhouse gas is carbon dioxide (CO₂). Many climate research studies focus on developing technologies to greatly reduce the atmospheric levels of CO₂. One approach being considered to help mitigate CO₂ concentrations is geologic carbon sequestration. With this technique, CO₂ emissions are captured from sources such as power plants and refineries and injected into underground formations—for example, old oil or gas fields or deep,
briny aquifers—where the gas can be permanently isolated.

Lawrence Livermore research on geologic sequestration combines fieldwork, laboratory experiments, and modeling and includes scientists and engineers from the Laboratory’s Energy and Environment (E&E), Engineering, Chemistry and Materials Science, and Computation directorates. For example, one project is developing methods to capture CO$_2$ at smokestacks. Another project is helping monitor CO$_2$ movement after the gas has been injected underground. Laboratory scientists are also studying the safety of carbon sequestration and how CO$_2$ injection affects a formation’s geophysical and geochemical properties. Computer simulations of sequestration techniques will also help decision makers evaluate potential storage sites across the nation.

The carbon sequestration effort receives funding from various sources, including Livermore’s Laboratory Directed Research and Development
Conservation Is Not Enough

“Reducing energy consumption would help cut CO₂ emissions, but not nearly to the degree we need,” says Livermore scientist Julio Friedmann, who leads the Carbon Storage Initiative for the E&E Directorate. “For the foreseeable future, the U.S. and the world will remain dependent on burning fossil fuels.” Given this assumption, many scientists believe that safe storage of CO₂ in benign form is a more realistic approach to limit the amount of emissions.

Friedmann and Thomas Homer-Dixon, program director of the Trudeau Centre for Peace and Conflict Studies at the University of Toronto, analyzed the problem in the November/December 2004 issue of Foreign Affairs. In that paper, they compared the accumulation of greenhouse gases to the problems cities faced with trash and sewage a hundred years ago. “Like trash, carbon dioxide can be sequestered. Trees and plants already do it: they absorb the gas and turn it into leaves, wood, and roots. But to make a dent in global warming, massive amounts of carbon need to be stored away for a long time—at least a few hundred years—and trees and plants are not up to the task.” [Foreign Affairs 83(6), pp. 78–79.]

Each year, human activities emit 25-billion tons of CO₂ into the atmosphere. About 2- to 3-billion tons of this annual output is absorbed by forests. Another 7-billion tons is absorbed by the ocean, which could conceivably store even larger amounts of CO₂. (See S&TR, May 2004, pp. 20–22.) However, CO₂ can make water acidic, prompting concerns about its long-term effect on marine life.

Preliminary estimates indicate that geologic formations could store many decades’ worth of CO₂ emissions safely. “By 2050, nations could be burying 5- to 10-billion tons of CO₂ every year,” says Friedmann. “We think Earth’s crust could handle that.”

CO₂ Already Captured, Stored

Friedmann points out that scientists already know how to capture CO₂ and inject it underground. Since the 1930s, manufacturers have extracted CO₂ from factory emissions and used it to process food and make dry ice. For the past three decades, U.S. oil companies have also injected CO₂ underground to increase production from oil and natural gas wells, a process called enhanced oil recovery. Indeed, the U.S. leads the world in enhanced oil recovery technology, using about 32-million tons of CO₂ per year for this purpose. In addition, Friedmann says, “Enhanced oil recovery represents an opportunity to sequester carbon at a lower cost, compared with storing it in geologic repositories that do not contain fossil fuels. Sales of the recovered oil and gas would generate revenues to help offset the expenses of sequestration.”

For safe, long-term storage, CO₂ must be injected more than 800 meters below Earth’s surface. At that depth, CO₂ becomes a supercritical fluid, in which it is neither liquid nor gas. Supercritical CO₂ is more dense than CO₂ gas and thus would require less storage volume. Supercritical CO₂ is also less mobile and has a higher solubility underground, which would make sequestration more effective.

Once injected, the supercritical CO₂ begins to displace the oil, brine, or other fluids in underground formations. After several weeks, some of it dissolves into natural gas or oil or becomes trapped in tiny rock pores. One concern is that CO₂ injection changes the pressure in an underground reservoir. If the pressure increases too much, it could reactivate faults or fracture the overlying rock layer, or caprock. These events could lead to CO₂ leakage, compromising the storage effectiveness and possibly posing risks to the environment and human health.

“We know how to capture CO₂ and put it underground, but we also want to understand how carbon injection on a massive scale might affect the geology of an area,” says Friedmann. Livermore’s focus is on characterizing and quantifying these risks. To do that, researchers must conduct experiments and simulations at several measurement scales, from examining rock pores in microscopic detail to modeling geologic reservoirs many kilometers wide and deep.

Capture Comes First

Before CO₂ can be sequestered, it must be captured from a waste stream, typically a smokestack at a factory or power plant. One economic barrier is the high cost of technologies for the capture process. Developing techniques that can be used at existing power plants is especially challenging because the new processes must be easily integrated with old equipment.

Livermore researchers are pursuing capture techniques that do not create a secondary waste stream and will minimize costs. For example, an LDRD project led by engineer Kevin O’Brien is developing polymeric membrane technology, which is a spin-off from the precision techniques developed to fabricate laser targets for the National Ignition Facility at Livermore. The process, called SLIP (for solventless vapor deposition combined with in situ polymerization), uses nanotechnology to engineer membranes by aligning and polymerizing individual molecules on membrane surfaces. It produces uniform, ultrathin-film membranes that require significantly less separation power and exhibit much greater selectivity than conventional membranes. The Livermore team is collaborating with a consortium...
Geologic Carbon Sequestration

A Long-Term Investment for a Healthy Future

The Department of Energy (DOE) is leading the nation’s effort to better understand the geochemical and geomechanical forces underlying carbon sequestration and to develop technologies for long-term carbon storage on a large scale. DOE has created a network of seven public- and private-sector Carbon Sequestration Regional Partnerships to determine which approaches are best suited for different regions of the country. In announcing the initiative in 2002, DOE Secretary Spencer Abraham called the partnerships “the centerpiece of our sequestration program.” The partnerships include more than 150 organizations in 40 states, 3 Indian nations, and 4 Canadian provinces.

Lawrence Livermore is a member of the West Coast Regional Carbon Sequestration Partnership, which is led by the California Energy Commission and includes representative organizations from Alaska, Arizona, California, Nevada, Oregon, and Washington. Livermore researchers are helping to investigate potential geologic storage sites in the western U.S.

DOE’s Teapot Dome oil field in Wyoming, which is also known as Naval Petroleum Reserve No. 3, will serve as a field laboratory for carbon dioxide (CO₂) storage and monitoring experiments. As part of the project, CO₂ gas will be injected into Teapot Dome fields to boost oil production, and researchers will evaluate technologies for both sequestration and enhanced oil recovery. Livermore geologist Julio Friedmann is the program’s senior scientific coordinator, and several Laboratory investigators are developing measurement, monitoring, and verification techniques for the project.

With a potential surface area spanning 130 square kilometers, the Teapot Dome project could grow to be one of the largest sequestration demonstrations in the world. Anadarko Petroleum Corporation has built a 200-kilometer pipeline that moves by-product gas from a natural gas processing plant at Shute Creek in western Wyoming to the Teapot Dome site. Anadarko plans to inject about 7,200 tons a day of CO₂ gas into the declining, century-old Salt Creek field, which amounts to an annual output of about 2.6-million tons of CO₂ that would otherwise be vented into the atmosphere. The CO₂ pumped into the ground will push an additional 30,000 barrels of oil to the surface each day—totaling six times the current production level from the Salt Creek field. Carbon dioxide injection began in 2005 and will continue for several years.

Another DOE project is evaluating sequestration in the Frio formation in the South Liberty field near Houston, Texas. Livermore is collaborating with many institutions on the Frio Brine Pilot Test, which is led by the University of Texas.

In addition, DOE is planning several geologic storage demonstrations. The largest and most ambitious of these is the FutureGen Initiative, whose goal is to build a 275-megawatt zero-emission power plant that generates electricity and hydrogen from coal. The plant, announced by President George W. Bush in 2003, will be designed to capture and store CO₂, making it the world’s first coal-fueled prototype power plant to incorporate carbon sequestration technologies. The projected cost of this project is $1 billion, but the plant’s location has yet to be determined. When operational, the prototype will be the cleanest fossil fuel–fired power plant in the world.

The U.S. is also cooperating with other nations to advance carbon sequestration technologies. In 2003, DOE, the U.S. State Department, and ministries from 16 nations formed the Carbon Sequestration Leadership Forum to discuss technical and policy issues relating to geologic and other forms of carbon sequestration.

Many nations, including Norway, Canada, Australia, Germany, and the Netherlands, are pursuing large sequestration projects, many of which are associated with the forum. Livermore researchers are also collaborating on some of these international projects. Friedmann, for example, serves as an advisor to a European Union sequestration project in Germany called CO₂ SINK.

The CO₂ Capture Project, an international effort funded by eight of the world’s leading energy companies, is addressing methods to reduce greenhouse-gas emissions in a manner that contributes to an environmentally acceptable and competitively priced energy supply for the world. Livermore researchers are supporting the project with advanced simulations.

Teapot Dome in Wyoming is a potential site for a large-scale sequestration demonstration that is part of the Department of Energy’s study on the effectiveness of storing carbon dioxide deep underground.
of other national laboratories, private industry, and universities to develop and deploy full-scale membrane systems based on SLIP and other technologies.

Another novel approach uses limestone as a CO$_2$ separation and sequestration strategy. This effort, which is led by chemist Greg Rau from the University of California at Santa Cruz, takes advantage of accelerated weathering of limestone (AWL). AWL treats waste CO$_2$ with water to produce a carbonic acid solution. The solution can then be neutralized with limestone, thereby converting the original CO$_2$ gas to bicarbonate.

AWL could be an ideal separation process for coastal power plants because bicarbonate can be safely injected into the ocean. Rau’s team is developing an AWL technique that uses the water coproduced with oil or natural gas. Because of the surface-water discharge restrictions associated with oil and gas production, this by-product water must be reinjected. If the AWL technique is successful, it would effectively treat both the water and the CO$_2$.

**Monitoring Sequestered CO$_2$**

Livermore researchers also have developed techniques to monitor the CO$_2$ injected underground and ascertain its location. “We need to show that the CO$_2$ goes down and stays down,” says Friedmann.

Physicist Barry Kirkendall has demonstrated crosswell electromagnetic (EM) imaging of CO$_2$ sequestration at the Lost Hills field in central California—an enhanced oil recovery site operated by Chevron USA. The project combines laboratory and field data to develop image interpretation techniques that discriminate between oil, CO$_2$, and water phases.

The technology, originally developed by researchers at Lawrence Livermore and Lawrence Berkeley national laboratories and scientists at Schlumberger Corporation, takes advantage of the differences in how EM fields are induced in various materials. A transmitter is deployed in one well and a receiver in a second well to measure the electrical resistivity or conductivity of geologic media between the two holes. The resulting data provide a detailed, two-dimensional map of the subsurface resistivity at multiple frequencies between the wells.

A related technology, called electrical resistivity tomography (ERT), works like the computed tomography scans used in medical diagnostics, but instead, it reconstructs the subsurface...
electrical resistivity distribution in three dimensions. Livermore engineers Bill Daily and Abe Ramirez originally developed ERT for environmental research—an effort initially funded by LDRD. Daily has now extended the technology to oil-field applications, such as monitoring sequestered CO₂.

One implementation of Daily’s concept used the steel casings of production wells as electrodes extending about 1,000 meters deep. In this approach, which is called long-electrode ERT, electrical current is driven between two of the casings, and the resulting voltage distribution is measured at the remaining casings. This process is then repeated using different wells as the electrode pairs, until the electrical properties of the entire subsurface have been sampled. Results from field trials conducted at oil fields in California, New Mexico, and Wyoming indicate that long-electrode ERT is an effective method for measuring the movements of oil, water, and gas.

Crosswell EM and ERT complement traditional seismic imaging, which uses sound waves to map underground geologic strata. Seismic imaging, however, has a limited capability in distinguishing oil from other fluids such as CO₂.

Livermore physicists Brian Bonner and Jim Berryman are investigating whether broadband seismometers, which can record the low-frequency data associated with fluid movement, could be used to map the migration of injected CO₂ over time.

Techniques are also needed to warn operations personnel should CO₂ begin to leak from a storage site. One approach, under investigation by geochemist Greg Nimz and physicist Bryant Hudson, uses noble gas isotopes dissolved in the CO₂ to trace its movement. Noble gases are chemically inert and environmentally safe, and they are persistent and stable in the environment. According to Nimz, xenon isotopes are particularly suitable for monitoring CO₂ storage operations. Batches of CO₂ with different concentrations of xenon isotopes could be injected at the same site, making each batch identifiable with a single xenon analysis.

Remote sensing is another technology that may be useful in detecting CO₂ leakage. For example, Laboratory physicist Bill Pickles has developed a technique using airplanes equipped with hyperspectral cameras, which provide more information than traditional remote-sensing units do. In analyzing images taken during flights over a study area, Pickles found evidence of plant stress caused by high concentrations of CO₂ in the soil. (See S&TR, May 2003, pp. 12-21.) He has applied this approach successfully at natural sites, such as Mammoth Lakes, California, and at CO₂ injection sites, such as oil fields in Rangely, Colorado. Ultimately, future space-based platforms might directly monitor CO₂ flux from the surface.

**Studying Sequestration Risks**

Scientists are concerned that even slow, small releases of CO₂ over many years could significantly reduce the efficacy of carbon storage and could even pose risks to the environment and human health. Studies indicate that faults in the caprock are the natural path for subsurface fluids to slowly escape to the surface, especially when a reservoir is overpressurized. According to Friedmann, the risks of CO₂ leakage are not serious. “Almost all of the risks associated with leakage can be prevented by carefully analyzing the site and downhole pressure data,” he says. In addition, any leaks are likely to be detected early by standard monitoring techniques and remediated.

The worst-case scenario is that CO₂ might escape from an injection well that was completely open to the surface, perhaps because the well’s seal failed. “A drilled well could be a faster conduit for CO₂ than tiny fissures,” says Friedmann.

To study the environmental risk from such an event, Livermore meteorologist Frank Gouveia and geologist Mackenzie Johnson collected field data at Crystal Geyser in Utah in October 2004. Crystal Geyser is an ideal site for evaluating CO₂ leakage because it mimics the worst-case scenario.

The geyser first erupted in 1936, when a wildcat well being drilled more than 800 meters deep intersected a CO₂-charged aquifer. Today, the geyser erupts...
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intermittently as a result of pressure changes in the aquifer. Because this is an artesian well—that is, water flowing into the well is driven by hydrostatic pressure in the aquifer—the CO$_2$-charged waters naturally flow to the surface. As the water rises in the well, the pressure decreases, and explosive degassing of dissolved CO$_2$ results. The process is repeated because the CO$_2$-charged waters continue to flow naturally to the surface.

For the field study, Gouveia and Johnson camped near the geyser for two days, collecting CO$_2$ samples at different distances from the geyser and recording meteorological data for the area. Five eruptions occurred during the 48-hour period, with eruptions lasting from a few minutes to more than two hours. Geochemist Roald Leif measured the samples when they were returned to Livermore. The results showed that, even just a few meters from the gushing geyser, CO$_2$ levels were well below human health and safety concerns. “Even very low winds are sufficient to mix the CO$_2$ quickly,” says Gouveia.

A larger team of Livermore researchers plans to return to Crystal Geyser to test various detection and monitoring technologies. The team also will collect data to construct vertical profiles of the CO$_2$ plume emitted by the geyser.

Simulations Lead the Way

Guiding much of the sequestration experiments and fieldwork are simulations designed by a team of computational scientists led by geochemist James W. Johnson. Johnson’s team has produced the first reactive transport models of CO$_2$ injection and sequestration within geologic formations. These simulations show how CO$_2$ moves through a geologic formation, displacing ambient water, with which it is largely unmixable, and rising relative to this water, owing to its lower density. As the CO$_2$ plume migrates, some of it precipitates as carbonates in a process called mineral trapping, and some dissolves in the underground water, called solubility trapping. Some CO$_2$ is eventually isolated within rock pores bound by the overlying caprock, which is typically composed of shale—a process called hydrodynamic trapping.

The Livermore team used these models to evaluate a sequestration operation for Norway’s state oil company, Statoil. Each year, Statoil injects about 1-million tons of CO$_2$ recovered from its offshore Sleipner site into a saline geologic formation under the North Sea. The amount of CO$_2$ being sequestered is equivalent to the output of a 150-megawatt coal-fired power plant. Statoil pursued the sequestration effort after Norway imposed a federal tax on atmospheric CO$_2$ emissions from combustion-based sources. The Sleipner site is the first and largest commercial CO$_2$ geologic sequestration facility in the world, and it is proving to be both environmentally and financially sound.

In analyzing the Sleipner site, Johnson’s team developed a suite of computational tools to identify the geochemical, hydrologic, and structural constraints for successful geologic CO$_2$ sequestration. (See S&TR, December 2000, pp. 20–21.) This modeling software includes NUFT, a reactive transport simulator developed by Livermore.
physicist John Nitao; GEMBOCHS, the supporting geochemical software and databases developed by Johnson; and LDEC, a geomechanical model developed by Laboratory physicist Joe Morris. Reactive transport modeling integrates the processes that characterize dynamic geologic systems, including chemical reactions, fluid flow, heat transfer, and mechanical stress and strain. Because these processes are interdependent, they must be modeled simultaneously for the simulations to show the true behavior of geologic systems.

“We learned a lot from studying the Sleipner site,” says Johnson. “It showed us how CO₂ moves underground, where and when it becomes trapped, and the relative effectiveness of distinct trapping mechanisms.” The team also studied the integrity of the caprock in a project funded by the energy industry–supported CO₂ Capture Project. “We discovered that two opposing processes—geochemical and geomechanical—act on microcracks in the caprock.” Geochemical processes, mainly the formation of carbonates when CO₂ reacts with minerals, help to seal caprock fractures. However, geomechanical processes work in the opposite direction, forcing some microcracks to widen as the injected CO₂ increases the pressure underground.

In an LDRD project, Johnson and Livermore geochemist Kevin Knauss are performing integrated laboratory and modeling experiments to verify key geochemical predictions of the Sleipner work. These experiments are expected to confirm that CO₂ interaction with typical shale caprock forms carbonates containing magnesium, iron, and calcium. The experiments are also investigating the potential importance of dawsonite—carbonate containing sodium and aluminum, which may precipitate through CO₂ interaction with typical sandstone reservoirs.

Johnson, Nitao, and others are expanding their simulation capabilities to model in three dimensions. Three-dimensional modeling will allow researchers to examine injection scenarios in detail, including those involving enhanced oil recovery, and to “test” monitoring tools in a virtual environment before expensive prototypes are built. So far, says Johnson, “Our simulation results have been very encouraging for carbon sequestration technology.”

**Sound Data for Decision Makers**

“The Earth’s crust is complex and heterogeneous, but we’re gaining a good understanding of what happens when we inject CO₂ deep underground,” says Friedmann. “The bottom line is that geologic storage appears to be a safe, reliable, and permanent means to help mitigate the buildup of greenhouse gases.” He acknowledges, however, that much more research is required to provide a sound basis for the U.S. and other governments to make important policy and economic decisions about carbon capture and sequestration.

Large-scale sequestration will require significant, long-term investments of governmental and industrial resources. National laboratories such as Lawrence Livermore play a vital role in providing the science and technology needed to support these investments. Livermore researchers are meeting the challenge—using their combined expertise in such diverse fields as geophysics, chemistry, engineering, and computer modeling to help mitigate the effects of greenhouse-gas emissions.

What they’re finding is that, for once, burying a problem might be a good solution.

—Arnie Heller

**Key Words:** carbon sequestration, Carbon Storage Initiative, climate change, crosswell electromagnetic (EM) imaging, electrical resistivity tomography (ERT), FutureGen Initiative, GEMBOCHS, global warming, hyperspectral cameras, LDEC, NUFT, reactive transport modeling, SLIP (solventless vapor deposition combined with in situ polymerization) process, Teapot Dome.

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In past decades, when underground nuclear tests were routinely conducted at the Nevada Test Site (NTS), scientists and engineers designed their experiments so that data could be recorded without releasing radioactive gases and materials to the atmosphere. Less attention was given to the fate of the radionuclides that remained underground.

But today, scientists know much more about the movement of fluids through geologic media, and they are paying greater attention to the issue of radioactive contamination of the groundwater near these old sites. In 1989, the Department of Energy (DOE), which operates NTS, created a multicontractor effort called the Underground Test Area (UGTA) Project to better understand the risks that past tests may still pose to human health and the environment.

Scientists in Livermore’s Energy and Environment (E&E) Directorate are supporting the UGTA Project by modeling in detail how radionuclides from specific underground tests enter the groundwater and migrate through geologic formations. Geologist Gayle Pawloski, who leads the team, says, “Our responsibility is to calculate the ‘hydrologic source term.’ That is, we determine what radionuclides were released into the groundwater and how they move.”

The Livermore models are designed to generate results at a resolution of 2 to 10 meters. These data then become the starting point, or input parameters, for computer models developed to examine large regions of NTS—up to hundreds of square kilometers in area.

**A Complex Problem**

DOE has established three overall goals for the UGTA Project: identify those areas where radiological contamination from past underground nuclear tests threatens the groundwater, predict the movement of potentially contaminated groundwater, and define the contaminant boundaries or the extent of radionuclide migration.

“It is not economically or technically feasible to clean up the groundwater at NTS,” adds Pawloski. “DOE and the Nevada Division of Environmental Protection agreed: the contamination at
NTS is deep and extensive. The project is focused on determining whether groundwater contamination poses a risk to human health or the environment. To that end, the project is developing 1,000-year models of the system, and DOE plans to monitor the site for 100 years or as long as needed.

An underground nuclear explosion is instantaneous, but its effects on a site’s geology and hydrology last for centuries. The detonation releases an immense amount of energy—heat and shock waves—vaporizing rock and the nearby groundwater and melting the rock that surrounds the device. Molten rock collects in the cavity formed by the explosion and eventually hardens into a glass puddle on the cavity’s floor. The cavity fills with falling rock, which forces the remaining vapor into the surrounding geologic media. The overlying rock continues to collapse, creating a rubble-filled column, or chimney, that may extend to the surface, where a crater forms.

Over time, temperatures cool and gas pressures dissipate, allowing groundwater to filter back into the area. Radionuclides are also moving through the subsurface. They leach out of the glass puddle, react with water and minerals, and continue to decay.

Simulating these complex interactions is not simple, nor is the geology of the NTS test areas—Pahute Mesa, Frenchman Flat, Yucca Flat, Climax Mine, Rainier Mesa, and Shoshone Mountain.

Livermore’s E&E Directorate provides the UGTA Project with expertise in containment science, site characterization, and the geology at NTS. Pawloski’s team includes Livermore scientists Andrew Tompson, Reed Maxwell, Steve Carle, and Dan Shumaker, who nearly a decade ago developed technologies to model groundwater contamination in complex environments. (See S&TR, November 2000, pp. 4–11.) The team also draws on the experience of Laboratory geochemists who worked on DOE’s Yucca Mountain Project.

Details Down Under

For the UGTA Project, NTS is divided into areas called corrective action units (CAUs). Pawloski’s team is modeling each CAU and, to date, has reported on its studies of Frenchman Flat and Pahute Mesa.

To set up the simulations, the team first chooses a representative test from each CAU. For example, at Pahute Mesa, the team focused on the Cheshire test, which was conducted on February 14, 1976. According to unclassified reports, Cheshire’s detonation point was 1,167 meters below the surface in fractured volcanic lava, and its announced yield was 200 to 500 kilotons.

The team’s overall approach is to first estimate the abundance, spatial distribution, and chemical state of radionuclides immediately following the experiment. To develop those estimates, Livermore geochemist Mavrik Zavarin included an averaged inventory of 43 radionuclides for underground tests at Pahute Mesa. He also used data from past NTS and international nuclear tests to distribute these radionuclides in the melt glass, the cavity, and the altered areas around the cavity.

Going with the Flow

“The legacy data give us a starting point for our calculations—the initial geologic settings and the radiologic source term,” says Pawloski. “Our next step is to develop detailed models of groundwater flow and incorporate the most important geochemical processes. Then we use reactive transport models to simulate radionuclide migration away from the test.”

The detonation of an underground nuclear device instantaneously releases an immense amount of energy. (a) In the first microseconds, heat and shock waves from the explosion vaporize rock and groundwater as the cavity grows to its maximum size. (b) Within milliseconds, molten rock begins to harden into a glass puddle on the cavity’s floor. (c) The cavity collapses within seconds to hours and fills with falling rock, which displaces the remaining vapor into the surrounding rock. (d) The overlying rock collapses, creating a rubble-filled column, or chimney, that may extend to the surface where a crater eventually forms.
To simulate groundwater flow, the team used Livermore’s NUFT code. NUFT is a flexible, three-dimensional (3D) code and can model how geothermal energy and residual test-related heat affect groundwater transport. Temperature data from the Cheshire test were included to improve the model’s calibration. Temperatures as high as 150°C had been measured in the melt glass nearly 5 months after the Cheshire test, and small temperature perturbations were observed in the upper part of a downward well 11 years later.

The flow model also accounted for the complex geology at Pahute Mesa. Hydraulic tests at the Cheshire site and a nearby water well showed that the permeability of the fractured lava varies as much as four orders of magnitude.

According to the results of the flow model, high temperatures following the Cheshire test may have dramatically increased the rate at which radionuclides were released from the melt glass. “In addition,” says Pawloski, “the simulations indicated the presence of a recirculating flow system that drove groundwater upward from the cavity and melt glass through the chimney and into adjacent undisturbed rock.”

The Cheshire flow model also shows that heat convection through the highly permeable chimney ends about 25 years after the event. After about 100 years, the melt glass cools to background temperature, and groundwater flow returns to pretest conditions.

To model reactive transport after the Cheshire test, the team chose two methods: a GIMRT streamline-based model and a SLIM particle model. The GIMRT code performs one-dimensional simulations of transport along thousands of adjacent flow pathways, or streamlines. The SLIM code tracks motion of contaminant particles in the flow field. Both models used the same radionuclide inventories and distributions and were coupled to the NUFT groundwater flow simulations. “None of the codes available today can directly couple 3D hydrothermal flow and 3D reactive transport at the level of detail we require,” says Zavarin. “The streamline model helps us understand the changes to the site’s geochemistry. The particle model allows us to evaluate the data and process model uncertainties.”

The GIMRT model calculated several geochemical reactions, such as aqueous speciation, complexation, ion exchange, mineral dissolution and precipitation, radionuclide decay and ingrowth, and glass dissolution, to determine how radionuclides were released from the melt glass and how they interacted over time with the varied mineralogy along the flow path. This computationally demanding code ran between 4,500 and 6,300 streamlines over five time steps from 100 to 1,000 years. Such calculations would take several years to run on a desktop computer, but with Livermore’s clustered supercomputing system, run times were 10 to 100 times faster.

The particle-based model is more efficient than the streamline model, using simplified geochemical processes to simulate a flow scenario for the full 1,000 years. As a result, says Tompason, the team can complete hundreds of particle runs in the time needed to process one streamline model. Results from a single streamline model run compared well with the 100 particle-based runs in the 100- to 1,000-year time frame. These results, called the near-field hydrologic source term, then become the radionuclide source for regional models of Pahute Mesa.

One Piece of a Complicated Puzzle

“We’ve learned a great deal from modeling tests such as Cheshire,” says Pawloski. For example, in the Cheshire simulations, the team found that radionuclides moved up the highly permeable chimney and then migrated away from the test with the flow of the underground water—a process that was verified by field data. The longevity of high temperatures is another useful measure because it indicates the potential for groundwater flow through the cavity. The models also revealed that radionuclides are released from the melt glass slowly over a long time, regardless
of the geologic medium, and short-lived radionuclides decrease to relatively insignificant levels within 400 years of the test.

“NTS has a complex, underground flow system, with different groundwater flow rates and directions, a complicated heterogeneous geologic system, and a variety of radionuclides—all interacting in specific ways,” Pawloski says. “Here at Livermore, we’re doing our part by defining the hydrologic source term—which is just one piece of this very large jigsaw puzzle that is the UGTA Project. When the puzzle is complete, DOE and the people of Nevada will have a picture that allows them to predict the groundwater movement and help define boundaries for safe water use.”

—Ann Parker

Key Words: Cheshire test, environmental restoration, groundwater flow, hydrologic source term, Nevada Test Site, NUFT code, Pahute Mesa, radionuclides, underground nuclear testing, Underground Test Area (UGTA) Project.

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UGTA Web site: www.nv.doe.gov/programs/envmgmt/blackmtn/erundergroundtestarea(ugta).htm

(a) This snapshot from a GIMRT simulation of the Cheshire test shows the streamline locations along a 10-meter-wide zone used to calculate radionuclide transport for the 135- to 208-year time step. The differing permeabilities of the surrounding rock appear in the background, where lighter shading indicates higher permeability. (b) A cross section from a particle-based model provides another view of the Cheshire data, showing the concentration of aqueous americium 23.5 years after the event.
Novel Materials from Solgel Chemistry

Solgel chemistry is a remarkably versatile approach for fabricating materials. Scientists have used it to produce the world’s lightest materials and some of its toughest ceramics. Chemists in Livermore’s Advanced Materials Synthesis (AMS) Group are working to improve the solgel process so they can specify the properties in the materials they are designing.

In solgel chemistry, nanometer-sized particles form and then connect with one another to create a three-dimensional (3D) solid network. This technique allows scientists to change the composition and structure of materials on the nanometer (billionth-of-a-meter) scale. In addition, this process can be modified to produce solgel materials in different forms, such as powders, films, fibers, and freestanding pieces of material called monoliths. For example, a gel can be dried in a solgel process to make aerogels, a special class of ultralow-density materials. In fact, the Livermore group created an aerogel weighing only 1.0 milligram per cubic centimeter, which is listed in the Guinness Book of World Records 2005 as the lightest material on Earth.

But the AMS chemists do much more than create aerogels. With solgel chemistry, they can create a broad set of materials for applications such as optics coating, waste remediation, energy storage, ceramics, and nanoelectronics. To optimize the fabrication process for new materials, they are also developing a methodology to selectively control the physical properties of the resulting materials. Once it is refined, this capability will revolutionize the way these materials are prepared.

A Mastery of Solgel Chemistry

In the solgel process, simple molecular precursors are converted into nanometer-sized particles to form a colloidal suspension, or sol. The colloidal nanoparticles are then linked with one another in a 3D, liquid-filled solid network. This transformation to a gel can be initiated in several ways, but the most convenient approach is to change the pH of the reaction solution. Even the method used to remove liquid from a solid will affect the solgel’s properties. For example, to preserve a gel’s original 3D structure and produce low-density aerogels, chemists use a technique called supercritical drying. If, instead, the gel is dried slowly in a fluid-evaporation process, the gel’s structural network collapses, which creates a high-density material known as a xerogel. (See S&TR, October 2000, pp. 19–21.)

Alkoxides—compounds formed by the reaction of an alcohol and an alkali metal—are a common precursor in solgel chemistry. However, alkoxides can be very reactive and are commercially available for only a select number of elements, which limits the types of materials that can be prepared. In studying the mechanisms that drive the solgel process, the Livermore chemists found that organic epoxides would also initiate the reaction. With this approach, precursors that are more widely available can be used, thus increasing the number of potential materials that can be developed. In addition, the starting materials, solvents, and gelling agents used with epoxides are less expensive than those used with alkoxides. Reducing the production costs may increase commercial interest in the new solgel materials.
“That’s the beauty of working with epoxides,” says Livermore chemist Joe Satcher, who leads the AMS Group. “We can use readily available starting materials and simple benchtop chemistry techniques. Right now, we’re making new materials in a beaker, but this process is readily scalable.”

Because the group’s solgel process is so flexible, the chemists have been systematically going through the elements in the periodic table, creating materials composed of different metal oxides or of organic and inorganic elements. For example, they have developed solgels that are organic networks with an inorganic component and others that are inorganic networks with an organic component.

As a result of this systematic effort, the AMS Group has created a broad range of materials. For example, one composite has been designed to remove oil from water. This porous material is hydrophobic—it repels water—but absorbs organics such as oil. A similar aerogel composite is used to remove contaminants such as uranium, chromium, and arsenic from groundwater. The group also has developed an energetic composite—a material that stores energy chemically—by mixing an oxidizer and a fuel at the nanometer scale. The result is an energetic material that provides both high energy density and high power; that is, it will release an enormous amount of energy very quickly. Other new solgel materials include ultrathin films, which can be used to coat silicon wafers and protect optics, and solgel-derived powders, which can be used to produce ceramics with various properties.

The Livermore group is also working on a project in support of the Department of Energy’s (DOE’s) Centers of Excellence for exploratory research in hydrogen storage. This DOE effort is addressing a major technical barrier for hydrogen-powered vehicles, which is to store enough hydrogen on board so a vehicle can travel more than 300 miles without refueling and without reducing the cargo or passenger space. For this project, the AMS chemists are experimenting with a metal–carbon aerogel composite that can store, transport, and release hydrogen at reasonable operating temperatures and pressures.

**Observing the Process in Action**

According to Satcher, the next goal for the AMS chemists is to better understand the subtleties of their new method. For example, they want to determine what happens when different precursors or solvents are used in the colloidal solution and gelation stages and how different methods for extracting liquids will affect the drying stage. To meet this goal, they are examining the mechanisms by...
The AMS Group is expanding the number of materials that can be produced with the improved method. With each new material created, the group learns more about controlling the variables in the process. “Our goal is to replace chemical intuition with a systematic approach, so we can prepare a particular composition with well-defined chemical and physical properties,” says Satcher. “We’ve demonstrated this capability for some compositions, but we want to understand the solgel process so well that we can determine a material’s properties before we even start.”

By working methodically through the periodic table and using techniques such as NMR spectroscopy, the AMS Group is closer to achieving this goal.

**Solgel Materials of the Future**

For these experiments, the Livermore group is using nuclear magnetic resonance (NMR) spectroscopy to view the process as it happens, from sol formation to gelation to processing the composite material. NMR is ideal for this task. This nondestructive technique can be used to selectively track changes in the solution, gel, and solid phases. Details from the NMR experiments will help the chemists understand the relationship between the synthetic variables introduced in the process and the physical properties of the final material.

For example, in one experiment, the group is using NMR spectroscopy to monitor structure formation in two types of aluminum oxide aerogels. (See the figure above.) Changing a single variable—the precursor molecule—in the solgel reaction generates two different aerogels. Although the aerogels are composed of the same material, their morphologies—that is, their form and structure—and their mechanical properties are dramatically different. When the precursor is aluminum nitrate, the aluminum oxide foam has a random cluster morphology, and the resulting aerogel is opaque. Using aluminum chloride as the precursor produces an aerogel with fibrous morphology, which creates a stronger foam that is also translucent.

**Key Words:** aerogel, gelation, polymerization, solgel chemistry, supercritical drying, xerogel.

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Aerogel properties can be changed by adding different precursor molecules. For example, (a) an aluminum oxide foam prepared from aluminum nitrate has a cluster morphology that results in (b) an opaque aerogel. (c) Using aluminum chloride as the precursor produces an aerogel with fibrous morphology, resulting in (d) a stronger foam that is also translucent.
Each month in this space, we report on the patents issued to and/or the awards received by Laboratory employees. Our goal is to showcase the distinguished scientific and technical achievements of our employees as well as to indicate the scale and scope of the work done at the Laboratory.

**Patents**

**Solid State Laser Disk Amplifier Architecture: The Normal-Incidence Stack**
C. Brent Dane, Georg F. Albrecht, Mark D. Rotter
U.S. Patent 6,847,673 B2
January 25, 2005
Normal-incidence stack architecture coupled with diode-array pumping enables the power and energy per disk to be increased and reduces beam distortions by orders of magnitude. The beam propagation is no longer restricted to only one direction of polarization, and the laser becomes more amenable to robust packaging.

**Performance Analysis of Distributed Applications Using Automatic Classification of Communication Inefficiencies**
Jeffrey S. Vetter
U.S. Patent 6,850,920 B2
February 1, 2005
This system presents a technique for performance analysis that helps users understand the communication behavior of their message-passing applications. The system automatically classifies individual communications operations and reveals the cause of communication inefficiencies in an application. This classification allows the developer to quickly focus on the culprits of inefficient behavior, rather than manually foraging through massive amounts of performance data. Specifically, the system traces the message operations of message-passing interface applications and then classifies each event using a supervised learning technique called decision-tree classification. The decision tree may be trained using benchmarks that demonstrate both efficient and inefficient communication. The system can adapt to the target system’s configuration by using these benchmarks and thus can simultaneously automate the performance analysis process and improve classification accuracy. The system may improve the accuracy of performance analysis and dramatically reduce the amount of data that users must encounter.

**Halbach Array Generator/Motor Having an Automatically Regulated Output Voltage and Mechanical Power Output**
Richard F. Post
U.S. Patent 6,858,962 B2
February 22, 2005
The stationary portion, or the stator, of this motor–generator is positioned concentrically within the rotatable element, or the rotor, along its axis of rotation. The rotor includes a Halbach array. The stator windings are switched or commutated to provide a direct-current (dc) motor–generator much the same as in a conventional dc motor–generator. The voltage and power are automatically regulated by using centrifugal force to change the diameter of the rotor and thus vary the radial gap between the stator and the rotating Halbach array, as a function of the rotor’s angular velocity.

**Electro-Optic Modulator Material**
John J. Adams, Chris A. Ebbers
U.S. Patent 6,859,467 B2
February 22, 2005
This electro-optic device, designed for use with a laser beam, has a crystal with a first and second face. Applying a voltage across the crystal results in a net phase retardation on the polarization of a laser beam when the beam is passed through the crystal. In one configuration, the crystal is composed of a compound having the chemical formula ReAc_{46}(BO_{3})_{3}, where Re consists of one or more of the elements lanthanum, cerium, praseodymium, neodymium, samarium, europium, gadolinium, terbium, dysprosium, holmium, erbium, thulium, and ytterbium plus yttrium and scandium; and Ae is calcium, strontium, or barium.

**Using Histograms to Introduce Randomization in the Generation of Ensembles of Decision Trees**
Chandrika Kamath, Erick Cantu-Paz, David Littau
U.S. Patent 6,859,804 B2
February 22, 2005
This system uses modules to create decision-tree ensembles. The system has steps to read the data, create a histogram, and evaluate a potential split according to some criterion using the histogram. It will then select a split point randomly in an interval around the best split, split the data, and combine multiple decision trees in ensembles.

**Automated Macromolecular Crystallization Screening**
Brent W. Segelke, Bernhard Rupp, Heike I. Krupka
U.S. Patent 6,860,940 B2
March 1, 2005
This automated macromolecular crystallization screening system produces a multiplicity of reagent mixes. Analysis plates produced by combining the reagent mixes with a sample are incubated to promote crystal growth. Images of the crystals are analyzed to determine whether the crystals are suitable for analysis by x-ray crystallography. The design of reagent mixes is then based on the expected suitability of the crystals for analysis. A second multiplicity of reagent mixes produced from this design is used for a second round of automated macromolecular crystallization screening. In one embodiment, the multiplicity of reagent mixes is determined by a random selection of reagent components.

**Hybrid Heat Capacity-Moving Slab Solid-State Laser**
Eddy A. Stappaerts
U.S. Patent 6,862,308 B2
March 1, 2005
Laser material is pumped and its stored energy is extracted in a heat-capacity laser mode at a high duty factor. When the laser material reaches a maximum temperature, it is removed from the lasing region. A subsequent volume of laser material is positioned into the lasing region to repeat the lasing process. The heated laser material is cooled passively or actively outside the lasing region.
Stepped Electrophoresis for Movement and Concentration of DNA
Robin R. Miles, Amy Wei-Yun Wang, Raymond P. Mariella, Jr.
U.S. Patent 6,866,759 B2
March 15, 2005
A fluidic channel patterned with a series of thin-film electrodes makes it possible to move and concentrate DNA in a fluid passing through the channel. The DNA has an inherent negative charge, and applying a voltage between adjacent electrodes causes the DNA to move. When a series of electrodes is used, if one electrode voltage or charge is made negative with respect to the adjacent electrodes, the DNA is repelled from this electrode and attaches to a positive-charge electrode in the series. The DNA can be moved to and concentrated over the remaining positive electrodes by sequentially making the next electrode of the series negative.

Laser Driven Compact Ion Accelerator
Toshiki Tajima
U.S. Patent 6,867,419 B2
March 15, 2005
A laser-driven compact ion source includes a light source that produces an energy pulse. A light source guide directs the energy pulse to a target and produces an ion beam that can be transported to a desired destination.

Portable Apparatus and Method for Assisting in the Removal and Emplacement of Pipe Strings in Boreholes
Brian R. Mitchell
U.S. Patent 6,868,923 B2
March 22, 2005
This portable support apparatus can be used to install and remove a series of connectable pipe strings from a ground-level borehole. The support apparatus has a base, an upright extending from the base, and in one configuration, a pair of catch arms extending from the upright to define a catch platform. The catch arms hold the upper connector end of a pipe string by releasably catching the underside of a pipe coupler connecting two pipe strings in the series. The connector end is thus positioned at the proper elevation for an operator to stand upright while coupling and uncoupling the pipe strings. Processes are also included for using this support apparatus to install and remove a series of pipe strings.
Applying Einstein’s Theories of Relativity

In 1905, Albert Einstein wrote four papers that revolutionized the field of physics. One paper, titled “On the Electrodynamics of Moving Bodies,” introduced the theory of special relativity, which says that the speed of light is the same for all observers—there is no preferred reference frame. All forces and effects as well as the speed of objects are limited to the speed of light. In 1907, Einstein began work on an extension of special relativity to include the effects of gravity. The result was his theory of general relativity, in which gravity is described as a force that distorts the shape of space and the flow of time. Special and general relativity provide the foundation for much of Livermore’s research in high-energy physics and astrophysics. For example, Laboratory scientists are participating in experiments at Brookhaven National Laboratory’s Relativistic Heavy-Ion Collider to simulate the physics of the first milliseconds after the big bang. Relativity also provides the basis for understanding celestial objects, such as gamma-ray bursts, supernovae, black holes, and neutron stars. In addition, during the last three decades, Livermore has developed numerical physics codes to account for the relativistic effects postulated by Einstein, allowing researchers to model various phenomena.

World Year of Physics events at Livermore: www.llnl.gov/pao/WYOP.

Locked in Rock: Sequestering Carbon Dioxide Underground

The accumulation of exhaust gases, particularly carbon dioxide (CO₂), in the upper atmosphere traps solar radiation, which then increases the Earth’s atmospheric and oceanic temperatures. Many scientists believe that stabilizing concentrations of CO₂ in the atmosphere will require geologic carbon sequestration. Livermore’s Carbon Storage Initiative combines fieldwork, laboratory experiments, and modeling. For example, one project is developing methods to capture CO₂ at smokestacks. Another project will help monitor CO₂ movement after the gas has been injected underground. Laboratory scientists are also studying the safety of carbon sequestration and how CO₂ injection affects a formation’s geophysics and geochemistry. Computer simulations of sequestration techniques will also help decision makers evaluate potential storage sites across the nation. The Livermore initiative is part of the Department of Energy’s effort to further scientific understanding of carbon sequestration and develop technologies for carbon sequestration on a large scale.

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New software applications are helping researchers understand how genes are regulated.

Also in June
• The Laboratory’s laser research is based on Einstein’s description of the quantization of light.

• A Livermore-designed gamma-ray spectrometer was launched with the MESSENGER spacecraft to help scientists determine the contents of Mercury’s crust.

• Speckle imaging, a technique used to take the twinkle out of stars, also helps sharpen the images obtained in long-range surveillance.