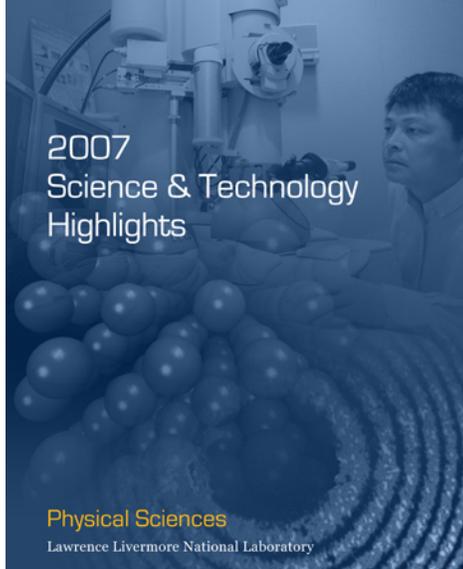




2007 Science & Technology Highlights

Physical Sciences

Lawrence Livermore National Laboratory



About the Cover

On the front cover—Top: Zurong Dai from the Institute of Geophysics and Planetary Physics using the scanning transmission electron microscope (SuperSTEM) to take high-resolution images of the cometary particles that were collected and returned to Earth by NASA's Stardust spacecraft. Livermore researchers are using the Laboratory's unique analytical tools to determine the mineralogy, and the chemical and isotopic composition of these particles (see p. 5). Bottom right: A coherent diffraction pattern encoding the shape and temporal evolution of an object illuminated by an ultra-short x-ray laser pulse. The pattern is from an experiment, in which Livermore researchers demonstrated a holographic imaging technique for observing the x-ray-induced explosion of nanometer-scale objects (see p. 12). Bottom left: An image showing the atomic structure of solid sodium at high pressure. The positions of the atoms (depicted by the balls) were taken from first-principles molecular dynamic simulations of body-centered-cubic sodium at a pressure of 40 gigapascals. The results of the simulations, done on the world-class, high-performance computers at Livermore, elucidate the unusual melting behavior of dense sodium (see p. 14).

On the back cover—Top: A time-integrated photograph shows the blow-off plasma and parts of the experimental apparatus, as a strong laser-produced shock was applied to a pre-compressed sample of helium in a diamond anvil cell. Livermore scientists are designing experiments for the National Ignition Facility that will use this technique to characterize materials at the extreme densities and pressures typical of the deep interiors of giant planets (see p. 2). Bottom: The two-stage gas gun at the Joint Actinide Shock Physics Experimental Research (JASPER) Facility at the Nevada Test Site. Livermore researchers are using JASPER to measure the equation of state of shock-compressed plutonium. Recent experiments played a key role in explaining the effects of radiation-induced changes in the physical properties of plutonium and its alloys (see p. 7).

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About this Report

This document highlights the outstanding research and development activities in the Physical Sciences Directorate that made news in 2007. It also summarizes the awards and recognition received by members of the Directorate in 2007.

About Physical Sciences

The Physical Sciences Directorate applies frontier physics and technology to grand challenges in national security. Our highly integrated and multidisciplinary research program involves collaborations throughout Lawrence Livermore National Laboratory, the National Nuclear Security Administration, the Department of Energy, and with academic and industrial partners. The Directorate has a budget of approximately \$150 million, and a staff of approximately 350 employees. Our scientists provide expertise in condensed matter and high-pressure physics, plasma physics, high-energy-density science, fusion energy science and technology, nuclear and particle physics, accelerator physics, radiation detection, optical science, biotechnology, and astrophysics.

About Our New Name

Effective October 1, 2007, Lawrence Livermore National Security LLC (LLNS) manages and operates the Laboratory for the Department of Energy. LLNS is a partnership of five world-class organizations: Bechtel National, University of California, BWX Technologies, Washington Group International, and Battelle. As part of this organizational change, the name of the Directorate changed from Physics and Advanced Technologies to Physical Sciences.

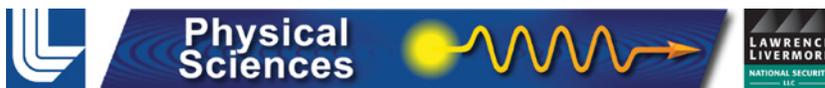
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Research in the News

*Advancing science and technology
in the national interest*

A new laboratory capability to probe a planet's deep interior

The National Ignition Facility (NIF), a 192-beam laser being completed at Livermore, will help improve scientists' understanding of material behavior at ultrahigh densities, which is highly uncertain even for a simple element such as hydrogen. Theoretical research indicates that deep within a planet's interior, materials could exhibit unusual characteristics such as high-temperature superconductivity. Yet, without high-fidelity experimental data, such predictions cannot be verified. Livermore scientists are designing experiments for NIF that will characterize materials at the extreme densities and pressures typical of the deep interiors of solar and extrasolar giant planets.

The first high-pressure experiments planned for NIF will explore planet formation and structure. In collaboration with researchers from the University of California at Berkeley, Princeton University, the Carnegie Institution for Science, Washington State University, and Université Pierre et Marie Curie in France, the Livermore team plans to study the phase state (fluid or solid) of hydrogen at extreme density and pressure. To create and observe these phase states, the scientists plan to stage a series of ramp-wave-compression (RWC) experiments. RWC experiments increase the pressure applied to a sample without inducing a shock wave. By precisely shaping the pressure pulse, the team will be able to compress the sample up to 2,500 gigapascals (or 25 megabars). With the RWC technique, the sample will remain relatively cool and solid with nearly constant entropy, even under very high pressure. The results from an RWC experiment on aluminum were published in the February 9, 2007, issue of *Physical Review Letters*.

Another technique for examining materials under extreme densities is to launch strong shocks in materials that are already compressed to an initial state of high pressure and density. This pre-compressed state is achieved in a diamond anvil cell (DAC). Pre-compression allows researchers

to tune the sample's initial density, and thus the final thermodynamic states that can be achieved with strong shocks. By applying a strong shock to a pre-compressed sample, scientists will be able to produce in the laboratory conditions that exist in the deep interior of solar and extrasolar giant planets.

In a DAC, a support structure holds two diamonds that squeeze the sample contained inside a washer. The diamond on one side of the target is thin, so the laser-produced shock remains strong and planar as it transits through the diamond. The diamond's thickness determines the initial pressure of the pre-compressed sample. Because NIF will have outstanding pulse-shaping capability and produce so much energy, the diamond on the drive side can be much thicker than those used in previous experiments on lower-energy lasers. As a result, scientists will be able to use NIF to study samples with unprecedented initial density and pressure. In the experiments, an ultrafast diagnostic called VISAR (Velocity Interferometer System for Any Reflector) will measure the shock velocity of the sample and a reference material. From these data, the researchers will extract the density and pressure of the shocked pre-compressed sample. They will also measure the optical emission from the shock front to deduce the shock temperature.

The planned high-pressure NIF experiments on planetary materials were featured in the July/August 2007 issue of *Science & Technology Review* (<https://www.llnl.gov/str/JulAug07/Celliers.html>).

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Understanding heavy-ion induced desorption of gas from metals

A research collaboration involving Lawrence Livermore, Lawrence Berkeley, and several particle accelerator laboratories in Europe has led to an improved understanding of desorption of molecular gases from stainless steel induced by heavy ion

bombardment. In experiments conducted at Lawrence Livermore and the Institute for Heavy Ion Research (GSI) in Darmstadt, Germany, the team investigated the dependence of desorption on the energy and angle of incidence of the bombarding ions. The researchers found that the energy dependence of the yield scales with roughly the second power of the electronic energy loss, as found in many electronic sputtering studies. However, the dependence of desorption on the angle of incidence, θ , is significantly less than $1/\cos \theta$, in contrast with previous results.

The team measured desorption yields in two energy regimes. In the first, low-energy regime below 1000 kiloelectronvolts (keV), the yield increases with the energy of the bombarding ions. Nuclear slowing dominates at energies below 250 keV, and electronic energy loss (EEL) dominates above 250 keV. In the second, high-energy regime, the incident ion energies were well above the energy where EEL has a maximum. In this regime, EEL decreases with increasing energy.

To explore the low-energy regime, the team used a beam of potassium ions produced by the Ion Source Test Stand at Livermore. The energy of the incident ions varied between 70 and 400 keV, and the angle of incidence varied between 80° and 89° . In these experiments, the researchers measured between 1,000 and 10,000 desorbed molecules per incident ion. They found that the yield increased by only a factor of 1.5 as the angle of incidence changed from 81.5° to 89° (near grazing incidence). This increase is much smaller than that observed for electronic desorption and sputtering from thick layers. They also found that the yield increased with increasing incident ion energy, following the trend in EEL.

To study the high-energy regime, the team used highly charged uranium ions (U^{73+}) with energies between 15 and 100 mega-electronvolts, available at GSI in Darmstadt. In these experiments, the ions hit the stainless steel target at perpendicular incidence ($\theta=0^\circ$). As found for low energies, the yield of desorbed molecules followed the trend in EEL, both decreasing with increasing incident

ion energy.

The results of this research, which appeared in an article published in the February 9, 2007, issue of *Physical Review Letters*, are relevant to the operation of ion accelerators. In these devices, the copious gas desorption that results from lost heavy ions striking the walls of the vacuum chambers leads to dynamic pressure rises, which limit the intensity of the ion beam.

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Early light curves of type 1a supernovae

Three Livermore astrophysicists were part of an international collaboration that reported light curves—luminosity as a function of time—for eleven type 1a supernovae (SNe Ia) in galaxies behind the Large Magellanic Cloud (LMC). Supernovae are stellar explosions that create extremely luminous objects. The luminosity rapidly increases after the explosion, reaching a maximum in a few days, and then decreases over weeks or months. The light curves reported by the collaboration represent some of the earliest pre-maximum observations of SNe Ia to date. These observations are significant because the time from the explosion to maximum brightness and the shape of the rising light curve can be used to test competing models of the SN Ia explosion mechanism.

The supernovae were discovered by the SuperMACHO project—a five-year optical survey of the LMC aimed at detecting microlensing of stars. The primary scientific goal of the survey was to better constrain the fraction of Massive Compact Halo Objects (MACHOs) in the Galactic halo. The survey was conducted on the Cerro Tololo Inter-American Observatory (CTIO) Blanco 4-meter telescope using a custom broadband filter and a wide-field Charge-Coupled Device (CCD) camera. The SuperMACHO project surveyed 50 million astronomical sources. The team used an

image-differencing technique to identify those sources whose brightness exhibited changes with time. These sources included microlensed stars and a wide range of variable astronomical objects including supernovae.

As a result of frequent and deep imaging of sources in a given portion of the sky, the collaboration was able to obtain a uniform set of SNe 1a light curves that were densely sampled in time before the luminosity reached the maximum. The light curves were fitted to a functional model from the time of the explosion to 60 days afterwards. The team used an expanding fireball model to describe the light curve immediately following the explosion, but constrained it to smoothly join the observed light curve at later times. Using the best fit to this model of the light curve, the team found the time between the explosion and the observed maximum brightness to be 17.6 rest-frame days.

This research was published in the February 2007 issue of the *Astronomical Journal*.

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New routes to high temperatures and pressures

Livermore researchers have developed an approach to study the properties of materials at high temperatures and pressures under experimental conditions that are not constrained to a single thermodynamic path. Their technique uses multilayered, functionally graded material (FGM) impactors (also called graded density impactors) in gas-gun experiments to simulate conditions that were previously inaccessible in controlled laboratory environments. Impactors are the projectiles a gas gun launches toward its target. With FGM impactors, data obtained for a set of continuously varying thermodynamic conditions can be used to create models of material behavior, which previously would have required extrapolated data from several experiments conducted at disparate pressures and temperatures.

More than 20 years ago, gas-gun experiments designed to achieve quasi-isentropic compression

used impactors composed of several layers of different materials with increasing density. Experiments with these impactors created a modest shock in the target followed by a series of small step-like pressure increases. The FGM impactors designed by the Livermore team are discs with as many as 100 or more layers, each less than 30 micrometers thick. As the number of layers increases and the thickness of any particular layer decreases, the induced pressure profile changes from step-like to continuous. By carefully selecting the different layers for an FGM impactor, an experimenter can design the pressure profile for each experiment. For example, a series of impactor layers with increasing density imparts a compressive force, while a series of layers with decreasing density creates a controlled release of pressure. An abrupt increase in density from one layer to the next generates a shock wave. An FGM impactor with up to 100 different layers provides an unprecedented level of control of the temperature and pressure conditions. Thus, researchers can combine a powerful shock, quasi-isentropic compression, controlled pressure release, and periods of continuous pressure, all in one experiment.

These impactors are rapidly fabricated using advanced powder-processing techniques such as tape casting. In this process, individual layers are prepared from powdered metals such as copper, magnesium, and tungsten. The metal powders are mixed with an organic solvent, plasticizers, and binders to form a slurry, which is then cast onto a Mylar film. After drying, the tapes are smooth and flexible. The tapes' composition is tailored to provide specific properties. To fabricate an FGM impactor, circular discs punched from different rolls of tape are stacked in the precise order required for an experiment. The stacked discs are laminated together, heated to remove the organic plasticizers and binders, and hot pressed to increase the density of the metal powders.

In the past six years, the team has conducted more than 125 experiments using the FGM impactors on Livermore's gas guns. The researchers have analyzed the performance of the impactors, obtained the equation of state (EOS) of tantalum and aluminum, probed the strength

of solid aluminum and the strain-rate effects of twinning in copper, examined liquid-to-solid-phase transitions in bismuth and water, and made novel materials. They have extended the technique to the Joint Actinide Shock Physics Experimental Research (JASPER) Facility at the Nevada Test Site. Experiments with the JASPER gas gun will improve scientific interpretations of EOS measurements and predictions of phase behavior and strength in materials of interest to the Stockpile Stewardship Program.

This research was featured in the March 2007 issue of **Science & Technology Review** (<https://www.llnl.gov/str/March07/Nguyen.html>) and published in the July 15, 2007, issue of the **Journal of Applied Physics**.

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Stardust results challenge astronomical convention

Livermore scientists are continuing their intense efforts to analyze material retrieved from a comet by the National Aeronautics and Space Administration's (NASA's) Stardust spacecraft. In 2004, Stardust flew through the tail of Comet Wild 2 as it neared the orbit of Mars. As it approached the 4.5-kilometer-diameter comet, the spacecraft briefly extended a collector filled with lightweight aerogel glass foam to capture thousands of tiny particles. With its collector stowed, the spacecraft then sped close to Earth and on January 15, 2006, ejected its sample return capsule that safely landed on the desert southwest of Salt Lake City.

For the past two years, the Livermore team has used a wide array of state-of-the-art analytical instruments at the Laboratory to study the mostly nanoscale particles painstakingly harvested from the spacecraft's aerogel collectors. The team's results, along with those obtained by the other members of the multi-institutional Stardust collaboration, are providing new and sometimes startling insights into the makeup of comets and suggest that the early solar system was far more active than previously believed. Comet Wild 2

contains an impressive assortment of materials, many unexpected. In particular, the comet contains an abundance of high-temperature minerals that appear to have formed in the inner regions of the solar nebula. Their unexpected presence strongly suggests that the formation of the solar system included mixing over radial distances much greater than has been generally accepted by scientists in the past. The December 15, 2006, issue of **Science** featured seven articles detailing the preliminary findings from the Stardust mission. The Livermore team's contributions were featured in the April 2007 issue of **Science & Technology Review** (<https://www.llnl.gov/str/April07/Bradley.html>).

The researchers are characterizing particles extracted from both aerogel and the aluminum foil that surrounded the aerogel with highly specialized instruments such as the super scanning transmission electron microscope (SuperSTEM), nanometer-scale secondary-ion mass spectrometer (NanoSIMS), scanning electron microscope (SEM), and nuclear microprobe. The ability to carry out correlated studies on individual micrometer-size grains using multiple analytic tools is a unique strength of the Livermore effort. The scientists also use the infrared microspectroscopy beam line at the Advanced Light Source at Lawrence Berkeley and the x-ray microprobe at the Stanford Synchrotron Radiation Laboratory. The highest spatial resolution work is being done using SuperSTEM, the world's most powerful, aberration-corrected electron microscope that has already demonstrated sub-angstrom spatial resolution and 100 millielectronvolts energy resolution. The capabilities of this instrument were highlighted in the November 2007 issue of **Science & Technology Review** (<https://www.llnl.gov/str/Nov07/bradley.html>).

The particles studied so far are full of surprises. One surprise is the scarcity of presolar material, the interstellar grains produced around other stars that existed before the Sun and solar system formed. Except for a single 250-nanometer-diameter grain highly enriched in oxygen-17, the mineral grains have isotopic compositions similar to typical solar system material. Another surprise is that although comets were formed a long distance from the Sun,

far beyond the orbit of Neptune, Wild 2 appears to be full of material from the inner solar system and from close to the Sun. For example, a calcium-aluminum-rich inclusion has been identified. It is believed that this inclusion formed in the hottest, innermost regions of the gas and dust disk that created the Sun and planets. This type of inclusion is also found in meteorites formed in the asteroid belt. Other high-temperature minerals include olivine and pyroxene (magnesium iron silicates), both associated with igneous rocks on Earth. Olivine is the most common crystalline mineral in the galaxy.

Many of the particles contain organic compounds that are surprisingly diverse. The comet's organic materials appear to be more primitive than those seen in meteorites and might have formed in clouds between the stars or in the disk-shaped cloud of gas and dust from which the solar system formed. They may represent a new class of organic compounds not previously observed in other extraterrestrial samples, including meteorites and interstellar dust particles. The presence of organic material in comets is of particular interest to astrobiologists because the precursors of life on Earth may have come from a comet.

Stardust is part of NASA's Discovery missions and is managed by the Jet Propulsion Laboratory. Other members of the Stardust collaboration include the University of Washington, Lockheed Martin Space Systems, the Boeing Company, Max Planck Institute for Extraterrestrial Physics, NASA Ames Research Center, and the University of Chicago.

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Precise measurement of energy splitting in the thorium nucleus

Livermore scientists have measured the energy splitting (difference) of the ground state doublet of the 229-isotope of thorium (^{229}Th) and found it to be significantly greater than earlier measurements. They used the NASA Goddard Space Flight

Center's microcalorimeter x-ray spectrometer (XRS), installed at Livermore's Electron Beam Ion Trap (EBIT), to measure the energies of the gamma rays produced following the alpha decay of the 233-isotope of uranium. The alpha decays populate many excited states of thorium including the 71.82 kiloelectronvolt state, which decays by gamma ray emission populating both members of the ground state doublet. The Livermore experiment used a superior differencing scheme based on the difference of the total gamma energies from the decay to each of the ground states. They obtained 7.6 ± 0.5 electronvolts (eV) for the energy splitting of the ground state doublet. This value is two times larger than the previously accepted result, which explains why prior direct observations were unsuccessful. The precision of the Livermore result was made possible by the superior energy resolution of the XRS (26 eV) compared to that of the germanium detectors used previously (> 200 eV).

These findings, published in the April 6, 2007, issue of *Physical Review Letters*, are important because ^{229}Th is considered the premier candidate for using atomic probes such as table-top lasers to exploit atomic-nuclear couplings. The ability to manipulate a nuclear system "at will" with a laser offers a myriad of intriguing possibilities, such as a clock with unparalleled precision for general relativity tests and measuring the variability of physical constants, creating a superb qubit for quantum computing, and studying the effects of the chemical environment on nuclear decay rates.

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Quantum simulations help the development of new technologies

Livermore scientists are continuing to use computer simulations, run on some of the world's fastest computers, to investigate the thermodynamic, electronic, and optical properties of materials at the nanoscale (at distances 1 to 100 nanometers). Previous research focused on basic but poorly understood phenomena such

as the behavior of water and the melt curve of hydrogen at extremely high pressures. More recently, the scientists have begun working on simulations for a diverse group of materials that are relevant to the development of new technologies.

Accurate descriptions of nanoscale materials must account for the behavior of individual atoms and electrons. Modeling dynamics at the atomic level requires computer codes based on first principles—that is, with no laws other than quantum mechanics characterizing the system being studied. The Livermore Quantum Simulations group is using codes based on density functional theory and the quantum Monte Carlo method to evaluate and optimize nanoscale materials for specific technological applications.

One example is research on thermoelectric materials that could be used to cool portable devices used by the military. A highly efficient thermoelectric material, suitable for such an application, must exhibit a combination of properties that do not coexist in conventional materials. It must have the high thermoelectric power of semiconductors, the high electrical conductivity of metals, and the low thermal conductivity of insulators. Semiconductor nanowires exhibit these required characteristics. Nanowires are so thin that they are often considered to have only one macroscopic dimension because of the quantum confinement of the electrons in the transverse directions.

In a project supported by the Defense Advanced Research Projects Agency (DARPA), the researchers have used simulations to compare the growth direction, surface structure, and size of silicon nanowires to optimize the electrical conductivity. They studied silicon with lattices grown in directions known as [001], [011], and [111], and with symmetric, canted, and reconstructed surfaces. Starting with bulk silicon, they computationally constructed 1-, 2-, and 3-nanometer cylinders of silicon “terminated” with hydrogen on their surfaces and then optimized their atomic structure using a density functional code called QBox. The [011] growth direction showed the highest electrical conductivity and thermoelectric power. However, all the silicon

nanowires exhibited high thermal conductivity. To remedy this problem, the scientists have examined changes in the composition of the material used for the wires. The simulations indicate that a silicon-germanium (Si-Ge) combination will reduce lattice thermal conductivity by as much as five times without affecting electrical conductivity. Calculations are in progress to optimize the Si-Ge nanowires for thermoelectric applications.

This research, along with other quantum simulations of technologically relevant materials, was highlighted in the May 2007 issue of **Science & Technology Review** (<https://www.llnl.gov/str/May07/Williamson.html>).

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Advances in understanding the long-term behavior of plutonium metal

A multi-year research program, carried out jointly at Lawrence Livermore and Los Alamos national laboratories, has determined that the degradation of plutonium in the nation’s nuclear weapons will not affect warhead reliability for decades. One of the most important components of a nuclear weapon is the core, or pit, a sphere of plutonium-239 that is compressed by conventional explosives to create a nuclear chain reaction. The safety and reliability of the nation’s nuclear stockpile depend on confidence in the long-term stability of the pit and credible estimates for pit lifetimes. Using the results from an extensive set of coordinated experiments, simulations and metallurgical testing, the research teams determined that the minimum lifetime for most of the plutonium pits in the nation’s nuclear weapon stockpile is at least 85 years—25 to 40 years longer than scientists had previously estimated.

Researchers from the Physical Sciences (PhySci) Directorate have made significant contributions to this program. They used some of Livermore’s unique experimental capabilities to measure the physical properties of plutonium and its alloys, and to examine the effects of radiation induced changes in these properties. Theoretical studies

and advanced computer simulations helped design the experiments and provided key insights that complement the experimental results.

In one project, the researchers used the Joint Actinide Shock Physics Experimental Research (JASPER) Facility to simultaneously acquire the first dynamic compression data for naturally aged plutonium obtained from retired pits and newly produced plutonium. JASPER is a 30-meter-long, two-stage light-gas gun located at the Nevada Test Site. Designed to gather equation-of-state (EOS) data on plutonium, the gas gun hurls projectiles at speeds up to 8 kilometers per second at plutonium targets. The impact produces an extremely high-pressure shock wave (about 600 gigapascals (GPa)) in the target, raising its temperature to as high as 7,000 kelvins. For these experiments, targets were made of old plutonium pressed into a disk of new plutonium and machined extremely flat (to 1.5-micrometer variation). Nineteen pins placed in the two samples gathered shock velocity data. The results unequivocally showed no statistically significant difference in the Hugoniot EOS of the new and old plutonium.

Members of the PhySci team also conducted static high-pressure experiments on plutonium using diamond anvil cells (DACs) at the Advanced Photon Source (APS) at Argonne National Laboratory. In these experiments, a small mechanical press slowly squeezed a microgram or so of material between two small, flat-tipped diamonds, achieving pressures as high as 100 GPa. X-rays from APS, the brightest x-ray source in the world, were used to probe the crystal structure of the samples under pressure. The measurements were sensitive enough to reveal minute changes in material properties. Samples included material recently produced, artificially aged, and taken from retired pits up to 45 years old. The three samples of different ages were enclosed in the same DAC for side-by-side comparison. The assembly was heated either electrically or by a laser to several thousand kelvins. As pressure was slowly increased, the researchers tracked volume changes that occurred when samples transitioned from one phase to another.

The experiments revealed no significant differences among the plutonium samples of different ages and no sudden or unexpected changes in properties.

The team also used a transmission electron microscope (TEM) to directly image the accumulation of self-irradiation damage, which is critical to understanding the aging process. Plutonium-239 undergoes alpha-particle decay, forming uranium-235 and emitting a high-energy alpha particle (helium nucleus). Using Livermore's 300-kiloelectronvolt, field-emission TEM, the researchers observed spherically shaped helium bubbles, each about 1 nanometer in diameter. The bubbles form as helium-filled atomic vacancies migrate and coalesce. However, the scientists did not observe larger voids in aged specimens with the TEM. Although the number of helium bubbles grows over time, the bubble size appears to be limited.

Modeling and simulations have aided the plutonium imaging and experimental effort. The researchers studied whether the delta-phase plutonium-gallium alloy could eventually convert to a more stable phase, such as alpha, which is 25 percent more dense. The calculations showed that self-radiation damage is, surprisingly, a key factor in stabilizing delta-phase plutonium. The researchers have also used Livermore's Blue Gene/L supercomputer to simulate collision cascades of uranium-235 atoms created from the alpha decay of plutonium atoms. The simulated reactions have a volume of 30 cubic nanometers and occur over a span of 10 picoseconds. The simulations, which used 32,768 processors and required 30 hours of computational time, depicted an entire cascade of atomic collisions from one alpha decay. These and related simulations were published in the October 2007 issue of ***Journal of Computer-Aided Materials Design***, which was devoted, in its entirety, to plutonium science.

As the result of this multi-year research program, scientists now have a much better understanding of several aspects of plutonium aging and, in turn, greater confidence in the reliability of the pits in the nation's nuclear weapon stockpile. Livermore's contributions to the program were featured in the

May 2007 issue of **Science & Technology Review** (<https://www.llnl.gov/str/May07/Schwartz.html>).

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Proton therapy made more accessible to cancer patients

Livermore's compact proton therapy system, which is being developed in collaboration with the University of California (UC) Davis Cancer Center, has been licensed to TomoTherapy, Inc., of Madison, Wisconsin. As part of a technology transfer pact announced in June 2007, TomoTherapy will fund development of the first clinical prototype, which will be tested on cancer patients at the UC Davis Cancer Center. If clinical testing is successful, TomoTherapy will bring the machines to market. These compact units are designed to fit in any major cancer center and cost one-fifth as much as the currently available, full-scale proton therapy machines. Proton therapy is the most advanced form of radiation therapy available. Unfortunately, the size and cost of the full-scale machines have limited the technology's use to only six cancer centers nationwide.

The key element of the compact proton therapy system is a dielectric-wall accelerator developed by Livermore, which uses a specially designed insulating pipe, or dielectric wall, to maintain vacuum while preventing the accelerator from short-circuiting. Livermore's dielectric insulator, which won an R&D 100 Award in 1997, consists of alternating layers of a conductor, such as stainless steel, and an insulator, such as polystyrene. Embedding thin metal layers within the insulator allows the system to withstand higher electric fields without electrical breakdown. To form the accelerator structure, the insulator rings are stacked to form a pipe. Transmission lines, stacked along the pipe's outside surface, are activated by fast switches to produce the electric field, which accelerates the proton beam inside the pipe. The electric field must be very strong for the beam to reach the energies

needed for cancer therapy in a relatively short distance (a few meters). The Livermore system is designed to achieve the required energies—from 70 megaelectronvolts (MeV) for eye tumors to 250 MeV for tumors deep in the body—with electric fields of up to 100 megavolts per meter. This design eliminates components such as bending magnets, which have large space requirements and generate unwanted radiation. It will also allow the clinician to vary the energy, intensity, and spot size of the proton beam used to treat tumors.

This technology was highlighted in the June 15, 2007, issue of **Newsline** (<http://publicaffairs.llnl.gov/employee/articles/2007/06-15-07-newsline.pdf>) and published in the August 2007 issue of **Nuclear Instruments and Methods in Physics Research, Section B**.

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A new geometry for tokamak divertors

A Livermore physicist has proposed a new magnetic configuration for the divertor region of tokamak devices that has the potential for significantly reducing the heat loads on the divertor walls of future tokamak fusion reactors. The main function of the divertor is to exhaust heat generated by fusion reactions in the plasma core. Since the divertor is the primary interface component between the plasma and material surfaces, it must tolerate high heat loads, which, in some designs, exceed the energy flux through the surface of the Sun. Reducing the heat load would improve the overall performance of tokamaks.

In a paper published in the June 2007 issue of **Physics of Plasmas**, the researcher showed that using just two divertor coils, properly positioned and with properly chosen currents, the poloidal plane can be divided into six regions, instead of four, as is the case with traditional (X-point) divertors. The resulting magnetic flux surfaces have a hexagonal shape reminiscent of a snowflake. Because the null (zero) of the poloidal

magnetic field is second order with respect to coordinate displacement from the location of the null point, the expansion of the magnetic flux controlling the scrape-off layer of the plasma near the null point is much stronger than in the traditional case. This suggests that the “snowflake” divertor may be useful in reducing the heat load in the divertor region.

A disadvantage of the snowflake configuration is its topological instability. A small change in the plasma (or divertor) current from its optimum value will change the overall structure of the divertor plasma substantially. To mitigate this effect, the researcher suggests operating at a divertor current five percent higher than what is optimum for the snowflake geometry. In this case, strong expansion of the magnetic flux surface still occurs, but minor variations in the plasma or divertor currents do not cause substantial changes in the plasma configuration.

While these conclusions were obtained from the analysis of a simple model for a tokamak, the researcher showed that the proposed scheme remains feasible in the toroidal geometry, and the results are applicable to strongly shaped plasmas. Further research, including three-dimensional simulation of the divertor region for realistic tokamak geometries will be required to verify the theoretical results.

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A new laboratory capability to study nucleosynthesis

When experiments begin at the National Ignition Facility (NIF), scientists will have a new tool to examine aspects of nucleosynthesis, which is the process that forms most of the elements in stars. With its 192 laser beams, NIF will generate 2 megajoules of laser energy—enough to create a miniature star. Scientists can use this scaled version of the stellar environment to better understand how stars create the elements. Livermore researchers are collaborating with colleagues at the University of California at Berkeley, Lawrence Berkeley National Laboratory, the Colorado School of

Mines, and Ohio University to design the initial NIF experiments for studying nuclear reactions pertinent to nucleosynthesis.

Nuclear fusion creates the elements in a young star. Two neutron-capture reactions, called the slow (s) and rapid (r) processes, occur as a star ages and dies, forming most of the elements heavier than iron. In the fusion reaction, nuclei of lightweight elements collide and fuse, releasing large amounts of energy and generating the nuclei of heavier elements. To date, accelerators have been the primary technology that scientists have used to study nuclear fusion reactions. However, it is difficult to operate an accelerator at the low energies relevant to stellar temperatures, and the particle fluxes generated by the accelerator at these energies would be too low to produce enough reactions to be measured.

NIF will provide the experimental conditions needed to create a star-like thermal environment, with densities between 10^{23} and 10^{26} atoms per cubic centimeter and temperatures up to 10 kiloelectronvolts. The planned experiments will investigate the fusion of helium-3 and helium-4 to produce beryllium-7, a critical reaction in stellar hydrogen burning. The target capsules will contain a mixture of helium-3 and helium-4. NIF's laser beams will compress the capsules and produce beryllium-7 in the hot plasma at a rate that can be measured for the first time. The researchers estimate that one experiment will produce 300,000 beryllium-7 atoms. The researchers will use the results of these experiments to explain the role plasma electrons play in reducing (screening) the electrostatic repulsion between the two fusing helium nuclei. Theory predicts that electron screening increases the probability of the fusion reaction, but the effect has not been measured directly at collision energies relevant to stellar nucleosynthesis.

The other processes in nucleosynthesis are neutron capture reactions, in which the nucleus captures one or more neutrons to form another nucleus, which is either stable or susceptible to radioactive decay. The r-process occurs only when neutron densities and temperatures are extremely high, such as those in a supernova when a star collapses and explodes. In the r-process, a neutron

hits the nucleus, which captures it, but before the resulting nucleus can decay, even more neutrons bombard it, creating a highly unstable, neutron-heavy nucleus.

Unfortunately, accelerators cannot create these neutron-heavy nuclei so far from the region of stability, which prevents scientists from studying in the laboratory neutron closed-shell nuclei, which have a low probability of interacting with additional neutrons. However, some NIF experiments will produce extremely high neutron fluxes (about 10^{33} to 10^{34} neutrons per square centimeter per second) within about 10^{-10} seconds in a controlled laboratory environment. This short reaction time will allow researchers to study the neutron-rich nuclei created in the r-process. The resulting data will help improve the accuracy of models that simulate the brief, violent life of an exploding star.

The NIF experiments pertaining to nucleosynthesis were featured in the July/August 2007 issue of **Science & Technology Review** (<https://www.llnl.gov/str/JulAug07/Bernstein.html>).

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Unraveling the structure of light nuclei

Livermore researchers are continuing to investigate the properties of light nuclei using advances in nuclear structure theory and ab initio calculations. In research published in the July 27, 2007, issue of **Physical Review Letters**, they used two- and three-body nuclear interactions derived from chiral effective field theory in the no-core-shell computational framework, to calculate the properties of light nuclei including ${}^6\text{Li}$, ${}^{10,11}\text{B}$, and ${}^{12,13}\text{C}$.

The nuclear strong interaction has proven to be complicated and replete with ambiguities. However, chiral perturbation theory (ChPT) provides a promising bridge to the underlying fundamental theory of quantum chromodynamics that could remove ambiguities. The researchers used ChPT to determine the two- and three-body nuclear interaction potentials. They then used these potentials in the ab initio no-core-shell

computational model to evaluate the binding energies, excitation spectra, and other observable properties for nuclei with 6-13 nucleons. The derived nuclear potentials contain low-energy constants (LECs), all but two of which can be determined by requiring that the calculations reproduce the known properties of nuclei with only two nucleons. The remaining two constants that are associated with the three-body potential were constrained by the binding energies of nuclei with three nucleons ($A=3$).

To evaluate the efficacy of this approach, the researchers investigated the sensitivity of the calculated properties of nuclei with $A>3$ to the variation in one of the constrained three-body LECs, called c_D . While most of the properties (e.g., excitation spectra) are not very sensitive to variations of c_D , the scientists identified several observables that did demonstrate strong dependence on c_D . These included, for example, the quadrupole moment of ${}^6\text{Li}$ that changed sign depending on the choice of c_D . Generally, the researchers found that including the three-body interactions in the calculations significantly improved the theory in comparison with the experiment. This finding was especially well demonstrated for the lowest few excited states in nuclei with odd numbers of nucleons.

These ab initio calculations for light nuclei required substantial computational resources on massively parallel machines. They would not have been practical without the world-class capabilities of the high-performance computers at Lawrence Livermore.

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High-energy-density physics summer school

The Institute of Laser Science and Applications (ILSA), along with the Fusion Science Center (FSC) at University of Rochester co-sponsored the 2007 High-Energy-Density-Physics (HEDP) Summer School that was held at the University of California (UC), San Diego, July 29 to August 4, 2007. The Summer School (<http://hedpschool.ile.rochester>.

edu/), held every other year beginning in 2005, is designed for undergraduate seniors, graduate students, postdoctoral scientists, and other researchers who want to enter or advance their knowledge in HEDP. Other sponsors of the 2007 session included the Institute for Material Dynamics under Extreme Conditions at UC Berkeley, and the Center for Energy Research at UC San Diego. More than 50 scholarships covering meals, lodging, and travel expenses were available to the undergraduate seniors, graduate students, and postdoctoral participants.

The lecture topics included radiation transport and spectroscopy, hydrodynamics, materials properties under extreme conditions, laser-plasma interactions, and experimental techniques, along with other ongoing research activities in the area of HEDP. The Summer School also included student poster sessions as a unique opportunity for students to discuss their work in an informal and congenial setting not only with the experts, but with the other students in attendance, challenging each other to think more deeply, or perhaps along different lines, about their own research.

The proceedings from both the 2007 and 2005 HEDP Summer Schools, along with background information about HED science, are available from the Fusion Science Center web site (<http://fsc.lle.rochester.edu/>). Opportunities for postdoctoral researchers who are interested in working with any of the FSC participants in HEDP, including ILSA at Livermore, can be found at <http://fsc.lle.rochester.edu/jobs.html>.

The mission of ILSA (<http://ilsa.llnl.gov>) is to foster and strengthen interactions between Lawrence Livermore and the academic community in the field of HEDP research involving high-intensity, high-power lasers. As part of this mission, ILSA oversees access for students and faculty to existing experimental facilities at Livermore in order to facilitate training and research in HEDP and advanced laser technologies. The next few years will see the completion of the National Ignition Facility at Livermore (<http://lasers.llnl.gov>) leading to ignition and a broad range of HED science experiments. Currently, the academic use of the Jupiter Laser Facility (<http://jlf.llnl.gov>), managed by ILSA, provides a bridge to future

experiments by academic researchers at NIF. In 2007, this program involved seven universities and 11 faculty members in 13 projects, with at least one graduate student or postdoctoral researcher per project.

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Ultrafast x-ray holography probes explosion of microscopic objects

Livermore researchers, collaborating with colleagues at several American and European institutions, have demonstrated a technique for observing the x-ray-induced explosion of microscopic objects. In an experiment using FLASH, the soft x-ray free-electron laser in Hamburg, Germany, the researchers placed an x-ray mirror a short distance behind a spherical plastic target. A very short x-ray laser pulse traversed the target, triggering its explosion. The x-ray pulse then reflected from the mirror back onto the target probing the explosion. The incident and reflected pulses interfered, with the time delay encoded in the resulting diffraction pattern to an accuracy of one femtosecond. The structural change in the exploding target was holographically recorded with high resolution. The scientists observed that the x-ray-induced explosion of the target occurred well after the initial pulse. These results support the notion that ultrafast x-ray imaging can be used to study biological samples beyond radiation damage limits with high resolution.

The design of the experiment, published in the August 9, 2007, issue of *Nature*, was motivated by Sir Isaac Newton's dusty mirror experiment, in which Newton made one of the earliest observations of optical interference. The researchers placed 140-nanometer-diameter spherical polystyrene particles on a 20-nanometer-thick silicon nitride membrane that was mounted with a thin spacer in front of a multilayer mirror. Another plane mirror angled at 45° reflected the x-rays onto a charge-coupled device-based detector, which recorded the interference patterns. Unlike the static conditions of Newton's experiment,

in the FLASH experiment, the object is ultimately vaporized by the incident, 25-femtosecond, x-ray pulse, and the object's size changes in the brief time that the pulse takes to reflect back to the object. The resulting interference pattern is an x-ray hologram, caused by the interference of a reference beam scattered from the 'known' sphere on the first pass, and then scattered again from the 'unknown object' (the exploding sphere) on the second pass. This hologram encodes both the time delay and the structural change.

The researchers varied the delay time between the pumping and probing of the sphere by changing its distance from the backing mirror. The distance was varied between 30 and 1,200 millimeters, corresponding to time delays between 200 femtoseconds and 8 picoseconds. The scientists found that at a delay of 500 femtoseconds, the spheres had not expanded by more than 20 percent of their transverse diameter, or 30 nanometers. At a delay of 350 femtoseconds, the expansion was about 6 nanometers. Extrapolation to the end of the incident x-ray pulse yields an expansion of no more than 0.4 nanometers. Thus, it appears feasible to overcome conventional radiation damage limits in soft-x-ray microscopy of cells with sufficiently short and intense x-ray laser pulses.

This research demonstrated that time-delay holography, inspired by Newton's experiment, provides a simple method to achieve extremely high spatial and temporal resolution in a single image. The method is well suited to a wide range of short-pulse x-ray sources and offers a way to examine the time evolution of complex geometries to study shocks and crack formation, ablation, melting, plasma formation, ultrafast phase transitions, and nonlinear optical effects.

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Spin transition zone in Earth's lower mantle

Mineral properties in Earth's lower mantle are affected by the electronic states of iron, but these states have not yet been probed in the laboratory

at the relevant pressures and temperatures until now. Livermore scientists, in collaboration with colleagues at several institutions in the U.S. and Europe, measured the spin states of iron in the mineral ferropericlase up to 95 gigapascals (GPa) and 2,000 kelvins. The team found that a gradual spin transition of iron occurs over a pressure-temperature range that corresponds to a zone in the lower mantle from about 1,000 kilometers in depth and 1,900 kelvin to 2,200 kilometers and 2,300 kelvins. Because low-spin ferropericlase exhibits higher density and faster sound velocity relative to the high-spin form, the observed increase in the low-spin mineral at these conditions would manifest itself seismically in Earth's lower-mantle as a spin transition zone characterized by a steeper-than-normal density gradient.

The experiments were conducted at the GeoSoilEnviro Consortium for Advanced Radiation Sources (GSECARS) sector of the Advanced Photon Source at Argonne National Laboratory. The samples had a composition of $(\text{Mg}_{0.75}\text{Fe}_{0.25})\text{O}$ and measured ~ 12 micrometers thick and 70 micrometers in diameter. Samples were loaded into diamond anvil cells (DACs) with beryllium gaskets. Dried sodium chloride layers acted as thermal insulators between the sample and diamond anvils, as well as the pressure medium and the pressure calibrant. A near-infrared laser beam was used to heat the sample from both sides of the DAC. A monochromatic x-ray beam with energy of 14 kiloelectronvolts was used to probe the samples. The x-ray emission spectra (XES) of the K_{β} fluorescence of iron were collected as a function of pressure and temperature up to 95 GPa and 2,000 kelvins, respectively. X-ray diffraction patterns were collected from some of the samples before, during, and after laser heating at high pressures.

The researchers performed an integrated absolute difference analysis of the x-ray emission spectra to determine the ratio of the high-spin and low-spin states in the sample. The derived fractions of the high-spin state were used to construct the spin-crossover phase diagram of iron in ferropericlase. Whereas the XES results revealed an electronic spin transition with a mixed population of high-spin and low-spin states

of iron at high pressures and temperatures, the x-ray diffraction patterns show that the (Mg_{0.75},Fe_{0.25})O sample is structurally stable before, during, and after the laser heating of the DAC, up to 95 GPa and 2,000 kelvins. High temperatures significantly affect the fraction of the high-spin state between 50 and 95 GPa where the spin crossover occurs. The researchers found that the observed spin transition is readily reversible with temperature. However, its width in ferroperricite is much narrower than that predicted by existing theoretical models.

This research, which was published in the September 21, 2007, issue of *Science*, has led to improved understanding of the properties of Earth's lower mantle at depths below 2000 kilometers.

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Unusual properties of dense liquid sodium

Livermore researchers have performed ab initio calculations that explain the unusual melting behavior in dense sodium that was observed in previous experiments. The results of the calculations show that molten sodium undergoes a series of pressure-induced structural and electronic transitions, analogous to those observed in solid sodium but commencing at much lower pressure in the presence of liquid disorder. The researchers found that as pressure increases, liquid sodium initially evolves by assuming a more compact local structure. However, a transition to a lower-coordinated liquid takes place at a pressure of around 65 gigapascals (GPa), accompanied by a surprisingly large, threefold drop in electrical conductivity.

To investigate the structural and electronic changes in compressed sodium, the researchers carried out a series of first-principles molecular dynamics (FPMD) simulations for pressures between 5 and 120 GPa, and temperatures up to 1,500 kelvins. To compute the melting curve over this pressure range, they used the 'heat-until-it-melts' approach. With this method, the

melting temperatures are deduced from a series of calculations, each done at progressively higher temperature, on the three solid structures of sodium known to be stable at room temperature up to a pressure of 130 GPa. The calculations confirmed the unprecedented pressure-induced drop in the melting temperature of sodium from 1,000 kelvins at 30 GPa down to room temperature (300 kelvins) at 120 GPa, which has been observed in previous experiments.

To understand the unusual melting curve of sodium, the researchers initially focused on a sequence of solid-phase transitions with increasing pressure corresponding to changes from less-compact to more-compact atomic structures. Generally, molten metals exhibit local orders similar to those of their crystalline solid-phases, thus liquid sodium may exhibit changes in the local order of atoms along the melting curve similar to that associated with the solid-phase transitions. To examine this possibility, the researchers determined from the calculations the distribution of atoms in the second coordination shell as a function of pressure and temperature. They found that the second coordination shell of the heated face-centered cubic (fcc) solid is contracted compared to that of the heated body-centered cubic (bcc) phase, in exactly the same way as the calculations predicted for the liquid between 0 and 60 GPa. This result showed that the changes in the liquid structure, which are noticeable in the second coordination shell, correlate with the unusual shape of the melting curve, and that these changes are characteristic of a transition from bcc to fcc local order at a finite temperature. At pressures above 60 GPa, the researchers observed another change in the atomic structure of liquid sodium corresponding to a local order that bears similarity to a distorted bcc-like structure (cI16 in the crystalline phase).

The researchers also used the FPMD simulations to investigate changes in the electronic properties of dense sodium that correlate with the changes in atomic structure observed with increasing pressure and temperature. For example, they found a dramatic drop, by a factor of three, in the electrical conductivity between 40 and 80 GPa,

the pressure range where the liquid structure becomes distorted bcc-like.

These results, which were published in the September 27, 2007, issue of *Nature*, will stimulate future experiments to verify the predictions of the simulations for molten sodium and to search for similar behavior in other dense liquid metals.

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Shedding light on dark matter

Livermore researchers, working with colleagues from Columbia University, have developed a novel general antiparticle spectrometer (GAPS) to shed light on weakly interacting massive particles (WIMPs), one of the possible constituents of dark matter in the universe. The researchers plan to use GAPS to indirectly measure WIMPs in cosmic rays by looking for the antiparticles the WIMPs produce when they interact with each other.

Matter that scientists can see or detect, such as the planets, stars, and interstellar dust, comprises only four percent of the total mass of the universe. The rest, most scientists believe, consists of dark matter—matter of unknown composition that does not emit or reflect electromagnetic radiation and is therefore difficult to observe directly. Determining the nature of this dark matter is one of the most important problems in modern cosmology and particle physics. Several kinds of particles have been proposed as dark-matter candidates, including WIMPs. Because WIMPs do not interact with electromagnetism or interact strongly with matter, they are nearly impossible to detect directly. A leading candidate for dark matter is a hypothetical particle called the neutralino—a stable, heavy WIMP predicted by some models in particle physics—which has properties similar to those of neutrinos.

The Livermore team's approach to searching for the neutralino involves identifying the unique "fingerprint" of elementary particles produced when one neutralino hits another. During the annihilation of the neutralinos, a bevy of particles and

antiparticles is produced, including antiprotons and antineutrons, which combine to form antideuterons. The researchers are planning to look for these antideuterons in the cosmic rays originating from the galactic center of the Milky Way.

The GAPS system is designed to reliably identify antiparticles amid enormous quantities of other particles. For instance, only one antideuteron might be observed for every 10^9 protons and 10^5 deuterons. To distinguish the types and energies of the antiparticles, GAPS combines a time-of-flight system, an energy degrader, and a chamber filled with a target gas or solid that is surrounded by x-ray spectrometers.

The time-of-flight system measures the velocity of an incoming particle. The particle then enters an energy-degrading block made of a material, such as lead, that slows the particle. The degrader's thickness is chosen so that it will slow down antiparticles of a specific type and energy by a specific amount of time. The slowed antiparticle enters the chamber, where it collides with an atom of the target material, knocking out and replacing an electron in the atom's outer electron shell. The resulting "exotic" atom is unstable, and it emits x-ray photons with discrete energies of 25 to 250 kiloelectronvolts as the antiparticles cascade to lower and lower energy levels. Finally, the antiparticle decays directly into the target atom's nucleus, annihilating itself and emitting a shower of pions. The segmented x-ray spectrometers, which surround the target chamber on all but one side, measure the energies of the emitted x rays and the pion shower. The energies of x rays and pions differ for each type of antiparticle, providing a fingerprint for particle identification.

The Livermore team completed a proof-of-concept prototype and tested it at the KEK Accelerator Test Facility in Japan. They looked for antiprotons resulting from the interaction of KEK's antiproton beam with the GAPS target material. High-quality antiparticle events were detected from four different targets. The experiment proved that GAPS could detect a specific antiparticle with a given energy amid a high flux of other particles. The next step is to fly GAPS on a high-altitude balloon in Antarctica, as part of a multinational collaboration

that includes groups from several institutions in the U.S. and Japan. The flight instrument, which will have 20,000 detectors versus the 128 on the prototype, will gather antiparticle data during the 20-day experiment. Because most galactic cosmic rays have energies too low to penetrate Earth's atmosphere, this balloon test will be the first opportunity for GAPS to detect a sizable number of antideuterons originating from space.

The progress with GAPS was highlighted in the September 2007 issue of **Science & Technology Review** (<https://www.llnl.gov/str/Sep07/Craig.html>) and published in the November 2007 issue of **Nuclear Physics B - Proceedings Supplements**.

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New camera captures early stages of eye disease

Livermore researchers, in collaboration with universities, medical centers, and industry, have developed an ophthalmoscope that uses adaptive optics and microelectromechanical systems (MEMS) technology to improve imaging of the retina in the eye. With the MEMS-based adaptive optics scanning laser ophthalmoscope (MAOSLO), clinicians can visualize microscopic cellular structures in the eye—a major advance over current ophthalmoscopes and retinal cameras. MAOSLO uses an adaptive optics system similar to that pioneered by the Laboratory for use in large astronomical telescopes. Instead of viewing astronomical objects, the MAOSLO system sharpens images of the retinal cell layers in a patient's eye to provide enhanced details. The Livermore collaboration received an R&D 100 Award for this new technology (see p. 22).

The new ophthalmoscope's optical system has tiny telescopes that relay light to two deformable mirrors and into the patient's eye. Horizontal and vertical scan mirrors focus a light beam onto the patient's retina in a raster, or uniform, pattern at the standard video rate of 24 frames per second. Light scattered by the retina follows the path of the

incoming light but in the reverse direction. A wave-front sensor measures optical aberrations in both the incoming and outgoing paths, and a MEMS-based deformable mirror corrects the distortions. The light then passes through a confocal pinhole and into a photomultiplier tube, which produces a high-resolution, digital video of the retina. MAOSLO is the first clinical instrument that automatically measures aberrations, makes the necessary corrections, and allows both clinician and patient to view the compensated image immediately.

The device also performs other useful functions. For example, having a second deformable mirror enables the system to correct for large refractive errors and quickly shift the focal depth in the retina. This feature produces clear views of distinct retinal cell layers, allowing clinicians to examine specific areas such as photoreceptors, blood vessels, or nerve fibers. The MEMS-based deformable mirrors also reduce the size and cost of the system without sacrificing speed or accuracy.

Researchers at the University of Southern California's Doheny Eye Institute conducted clinical trials of the device. Results from these studies demonstrated that MAOSLO identifies abnormalities in patients who show no symptoms of disease. The results highlighted the device's potential for early disease detection and intervention and for helping researchers better understand how a disease originates and progresses. MAOSLO is available for licensing and has been in clinical operation at the Doheny Eye Institute for over a year.

The technology was highlighted in the October 2007 issue of **Science & Technology Review** (<https://www.llnl.gov/str/Oct07/Olivier.html>).

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New detector for mobile mapping of radioactive materials

Livermore researchers, in collaboration with colleagues at Oak Ridge National Laboratory and the University of California at Berkeley's Space Sciences Laboratory, have developed a large-area

gamma-ray imager for detecting stolen nuclear materials. This device combines gamma-ray detection and imaging into a compact instrument for mobile operation to pinpoint the source of radioactivity. It quickly scans a sizable area and maps the radiation field with a range and accuracy unmatched by other available technologies. In tests with a prototype mounted on a truck traveling 40 kilometers per hour, the imager detected a 1-millicurie sample of a cesium isotope located 50 meters away. The research team received an R&D 100 Award for this new technology (see p.23).

A key challenge for detecting gamma rays from nuclear materials is background radiation, the intensity of which varies from place to place. Search instruments generally can detect radiation sources only at close ranges (within a few meters) or when a source is much stronger than the area's background radiation levels. Sources of modest strength cannot be detected with confidence beyond a few meters because the signal they induce in a detector may appear the same as the normal variation in background radioactivity.

To solve the background clutter problem, the researchers adapted an imaging method developed for astrophysics. In this technique, a coded aperture—a lead mask with openings arranged in a special pattern—is placed in front of a detector array. The radiation incident on the mask casts shadows on the detector elements, and the imager records these patterns. The pattern in the mask is designed so that each possible source location in the field of view produces a unique shadow pattern on the detector array. Processing software uses these patterns to determine the signal count and the source's location. To eliminate signals from gamma-ray sources outside an instrument's viewing field, which can cause blurring of the image, the team added a second imager. The mask for this imager has open and closed elements arranged in a pattern, which is the exact reverse of the pattern used on the first imager's mask.

The instrument can measure gamma-ray energies from 60 to 3,000 kiloelectronvolts—the range of interest for most homeland security applications. The current design fits on the back of a small truck or trailer and can be used to search

neighborhoods with low-rise commercial buildings and houses. The aperture mask pairs on each side of a detector array are coded with different patterns so the imager can sample both sides of the road as the vehicle travels through an area. This design combines speed, sensitivity, and detail. The imager can sweep an area about 25 times faster than other detection technologies, dramatically reducing the time necessary to conduct a search. The device can also pinpoint a radiation source within a 5-by-5-meter area.

This technology was highlighted in the October 2007 issue of ***Science & Technology Review*** (<http://www.llnl.gov/str/Oct07/Fabris.html>), and published earlier in the June 2006 issue of ***IEEE Transactions on Nuclear Science***.

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Unraveling the ionization balance in gold plasmas

In a paper published in the November 9, 2007, issue of ***Physical Review Letters***, Livermore researchers reported the results of benchmark measurements of well-characterized gold plasmas that were not in local thermodynamic equilibrium. The plasmas had electron densities near 10^{21} cm⁻³ and electron temperatures spanning the range 0.8 to 2.4 kiloelectronvolts (keV). The researchers analyzed the measured time- and space-resolved emission spectra of M-shell gold ions using a sophisticated collisional-radiative model to deduce the ion charge state distribution (CSD) as a function of plasma conditions. They also investigated the effects of external radiation fields on the CSD. The measured spectra and inferred average charge states provide a stringent test for non-local-thermodynamic-equilibrium (NLTE) models of complex high-Z ions.

The experiments were conducted at the OMEGA laser at the Laboratory for Laser Energetics, University of Rochester. The targets were thin disks composed of a 200-micrometer-diameter, 0.5-micrometer-thick gold layer (gold co-mixed with potassium chloride) embedded within a 400

micrometer-diameter, 10.8-micrometer-thick beryllium disk, which acted as a hydrodynamic tamper. The tamper ensured that heating of the target produced gold plasmas with nearly uniform, within 5-10 percent, electron density and temperature. The targets were illuminated directly on two sides by four nanosecond-long laser pulses from OMEGA. Some of the targets were placed inside cylindrical radiation cans (hohlraums) coated with tungsten, which heated the gold plasma indirectly with soft x-rays.

The researchers used a set of four independent measurements to diagnose the plasma conditions and to measure the M-shell emission spectra of gold: Thomson scattering of probe beams to determine the electron temperature; pinhole images of the plasma expansion to infer the electron density; an absolutely calibrated diode array (Dante) to determine the radiation temperature of the hohlraum; and a time-gated, spatially-resolving x-ray spectrometer to measure the M-shell spectra of gold, and the K-shell spectra of potassium and chlorine (co-mixed in the gold disks). The K-shell spectra were used to deduce the electron temperature independent of the measured gold spectra.

For electron temperatures between 0.8 and 2.4 keV, gold ions with charge states between 41 and 53 contribute to the M-shell x-ray spectra of the plasma. The researchers determined the CSD in the plasma by fitting the measured x-ray spectra of the plasma to the spectra of each gold ion with a given charge state, as calculated using the collisional radiative model. Because of the complexity and spectral overlap of the x-ray emission from each charge state, the fitting procedure is not trivial. The researchers employed a genetic algorithm to search a wide range of possible CSDs, seeking the best fit to 27 intensity points in the 2.9–3.6 keV spectral range. They found that for plasmas with electron density near $6 \times 10^{20} \text{ cm}^{-3}$, the average charge state varied from 42.2 ± 1.2 at 0.8 keV electron temperature to 49.5 ± 0.5 at 2.4 keV. They also found that at the lower temperatures, the spectra exhibited significant sensitivity to the external radiation field produced by the hohlraum.

The results of this research will lead to improved understanding of the internal energy,

radiative properties, and interaction with external radiation fields of NLTE plasmas relevant to inertial confinement fusion.

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Lab-on-chip analyzes picoliter droplets

Livermore researchers have demonstrated the first lab-on-chip system that generates picoliter droplets and performs biochemical reaction and analysis on its content. The system performed polymerase chain reaction (PCR), with real-time fluorescence detection, in isolated droplets with volumes a million times smaller than commercial PCR instruments. The use of advanced digital microfluidics is the key to this dramatic reduction in reaction volume for such biochemical reactions. The technology promises high-throughput, massively parallel analyses by partitioning the bulk sample into millions of discrete reaction vessels on-chip. In this way, each constituent can be isolated and assayed at the single cell, virus, protein, or nucleic acid level.

The Livermore system utilizes a shearing T-junction in a silicon device to generate a stream of monodisperse, picoliter droplets that are isolated from the microfluidic channel walls and from each other by an oil-phase carrier. An off-chip valving system stops the droplets on-chip, allowing them to be thermally cycled through the PCR protocol without droplet motion. With this system, the researchers found that a 10-picoliter droplet, encapsulating less than one copy of viral genomic DNA through Poisson statistics, exhibited real time PCR amplification curves with a threshold of 18 cycles, some 20 cycles earlier than commercial instruments. The combination of the established real-time PCR assay with digital microfluidics is ideal for isolating single-copy nucleic acids in a complex environment.

The primary advantage of digital PCR is its ability to detect a single copy of the target nucleic acid in a complex background. Reducing digital PCR reactor volumes by several orders of magnitude allows earlier detection due to decreased diffusion

distances, a wider range of sample concentrations, and reduced reagent consumption. While techniques have already been demonstrated for performing PCR on picoliter samples using bulk emulsion methods, they could only include end-point amplification detection. To perform real-time detection, the droplets must be focused into a channel so that background fluorescence from droplets above or below the focal depth does not affect the fluorescence intensity measurement. Otherwise, the optical interrogation of individual reactors, which is key to the digital PCR concept, cannot be achieved.

In the Livermore-developed lab-on-chip, monodisperse droplets with tunable volumes are generated using microfluidic chips with a T-junction shearing zone. Droplet size is adjusted by varying channel geometry, flow rate, and dispersed-phase viscosity. Two infusion syringe pumps independently drive the aqueous and mineral oil streams at predetermined flow rates through two off-chip valve systems, which are connected to the chip's fluid ports.

This research was published in an article that was featured on the cover of the November 15, 2007, issue of *Analytical Chemistry*.

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Measuring the relaxation of fast electrons in solids

Livermore researchers, in collaborations with colleagues from other institutions, have measured the relaxation time for fast electrons generated by short-pulse laser-solid interactions at very high laser intensities. The experiments, performed at the Compact Multi-pulse Terawatt Laser (COMET) at the Jupiter Laser facility in Livermore, showed that the conversion of laser energy to fast electrons increased as the laser intensity became relativistic. Using time-resolved x-ray spectroscopy, the researchers found that the thermalization of the fast electrons in the solid occurs over time scales on the order of

10 picoseconds, which is much longer than the duration of the laser pulse.

In the experiments, a laser pulse containing 6-7 joules of energy with duration of 500 femtoseconds was focused on the solid target at a 45-degree angle of incidence. In best focus (8-9 micrometer-diameter focal spot) the laser intensity was 10^{19} Watts per square centimeter (W/cm^2). By systematically changing the spot size on the target, the team was able to vary the laser intensity between 10^{19} and 10^{17} W/cm^2 while keeping the laser energy constant. The target consisted of a 12.5-micrometer-thick titanium (Ti) foil coated with a layer of aluminum (Al) 0.1 micrometer thick. The latter prevented direct illumination of the titanium foil, thus eliminating any direct laser heating. The fast electrons, which were generated in the aluminum plasma, penetrated into the cold titanium foil where they ionized and excited the titanium atoms, leading to the emission of K_{α} x-rays.

The researchers used an absolutely calibrated electron spectrometer to measure the number and energy distribution of fast electrons passing through the target. They used an x-ray streak camera with a time resolution of 1 picosecond to measure the time evolution of the K_{α} emission from both Ti and Al. A time-integrated, spatially resolving x-ray spectrometer viewed the back of the target providing information about the heating of the Ti foil and the size of the x-ray emitting region.

The researchers found that the number of fast electrons produced increased by a factor of five as the laser intensity increased from 10^{17} and 10^{19} W/cm^2 , while their characteristic energy also increased from 100 to 520 kiloelectronvolts (keV). The measured time duration of the Ti K_{α} emission varied from about 12 to 16 picoseconds, which was much longer than the laser pulse (0.5 picosecond). This result is in contrast to earlier experiments at lower laser intensities where the measured K_{α} emission time and laser pulse duration were the same order of magnitude. To explain the unexpectedly long duration of the Ti K_{α} emission, the researchers proposed that some of the emission is induced by energetic secondary electrons, which are produced during M-shell ionization of Ti atoms by the primary fast

electrons. Using a combination of models that included K_{α} generation, collisional coupling, and plasma expansion, the researchers verified that the observed rise-time of the Ti K_{α} emission is consistent with the proposed mechanism.

These results, which were published in the November 2007 issue of *Physical Review E*, will help scientists better understand the physics underlying the fast ignition concept for inertial confinement fusion.

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Using supercomputers to elucidate the behavior of quarks

Livermore researchers, working with theoretical physicists from around the world, are using the world's fastest supercomputer at Livermore to improve scientists' understanding of the behavior of quarks, the building blocks of all nuclear matter. Their calculations, based on the theory of quantum chromodynamics (QCD), are exploring how quarks coalesce to form larger subatomic particles like the proton, neutron, and their more exotic brethren.

QCD explains how a vast array of particles could arise from only a few types of quarks. It describes the "strong force," whimsically termed color (chroma in Greek), which prevents quarks from running free except under extreme conditions. It postulates the mass-less gluons that bind the quarks together in the proton and the neutron. Experiments done during the past few years at the Relativistic Heavy Ion Collider (RHIC) at Brookhaven National Laboratory have succeeded in freeing the constituent quarks for a very short time. In the experiments, gold ions collided at very high velocities compressing matter in their nuclei to high densities and temperatures. A major goal of the Livermore calculations is to help explain some of the unexpected results of these experiments.

In their calculations, the researchers use lattice QCD, a computational methodology ideally suited for massively parallel computers. In this method, space and time are represented on a four-dimensional grid of points. The quarks live on the lattice points, and the interactions among them occur along the links connecting the grid points. A version of lattice QCD, which has been

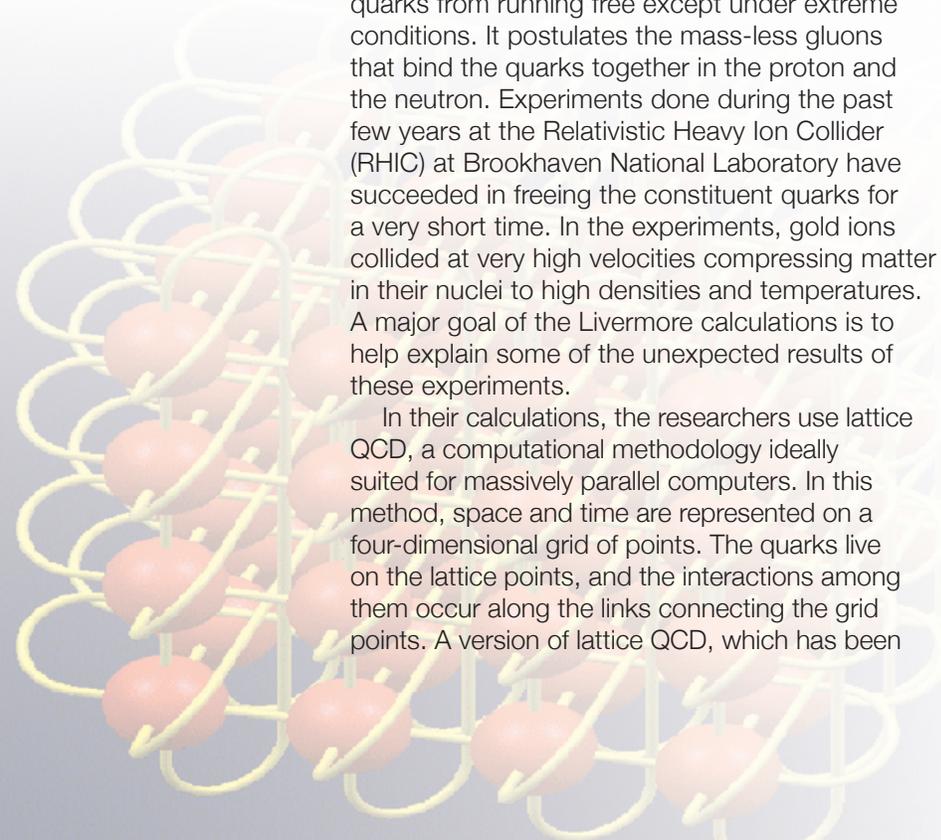
implemented on BlueGene/L, the world's fastest computer, has achieved almost perfect scaling with the number of processors up to 130,000. The code, optimized for BlueGene/L's architecture, demonstrated a sustained operating speed of 70.4 trillion floating-point operations per second (teraflops). The researchers received the 2006 Gordon Bell Prize for Special Achievement for their work.

A multi-institutional collaboration, called HotQCD, is using the simulations to study the conditions of nuclear matter reached in the RHIC experiments. The researchers are calculating the equation of state (the pressure and energy density as a function of temperature) of the hot quark-gluon plasma that was formed momentarily from the protons and neutrons in the colliding gold nuclei. This equation of state is required for a full hydrodynamic simulation of the collisions at RHIC, including the time when quarks begin to coalesce to form protons and neutrons. Previous research suggests that this transition occurs when the temperature drops below 170 megaelectronvolts (MeV), give or take 20 MeV. The Hot QCD collaboration is aiming to reduce the uncertainty to a few MeV.

Another collaboration, Nuclear Physics with Lattice QCD, has been studying the interaction of quarks at much lower temperatures. The researchers used the results of QCD calculations to predict the scattering length for several pairs of nuclear particles, including pion-pion and pion-kaon, which have a very short half-life. The scattering length is directly related to the interaction between the two particles at low collision energies. This research will lead to the very first calculations of the interactions of three nucleons for which no direct experimental data exist.

Parts of this work were published in the proceedings of the *Twenty-fifth International Symposium on Lattice Field Theory* (<http://arxiv.org/pdf/0710.1655>). The research was also featured in the winning essay entitled "Simulating the Birth of the Universe" that appeared in the November/December 2007 issue of *Computing in Science and Engineering*, and highlighted in the January/February 2008 issue of *Science & Technology Review* (<https://www.llnl.gov/str/JanFeb08/soltz.html>).

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2

People in the News

*Valuing scientific excellence,
leadership, and visibility*



The scientific and technological accomplishments of the staff in the Physical Sciences Directorate are recognized inside and outside the Laboratory through prizes, awards, and front-page publicity. Highlights in 2007 include:



John Lindl received the 2007 **James Clerk Maxwell Prize for Plasma Physics** from the **American Physical Society**. Lindl, who is currently the Chief Scientist for the National Ignition Facility, was the Fusion Energy Program Leader in the Physics and

Advanced Technologies Directorate from 2000 to 2004. He was recognized “For 30 years of continuous plasma physics contributions in high energy density physics and inertial confinement fusion research and scientific management.” Lindl’s work in inertial confinement fusion (ICF) has spanned a wide range of topics including high-gain target designs for lasers and particle beams, hydrodynamic instabilities in ICF, implosion symmetry and hohlraum design, high-energy electron production and plasma evolution in hohlraums, and the physics of compression and ignition. He is the previous recipient of the Edward Teller Medal (1993), the E. O. Lawrence Award (1994) and the Fusion Power Associate Leadership Award (2000).



Retired physicist **Ken Kulander**, now a Laboratory Associate in V Division, received the 2008 **Will Allis Prize for the Study of Ionized Gases** from the **American Physical Society**. He was recognized

“For the development of time-dependent methods and models that have advanced our understanding of strong field ionization processes in rapidly ionizing gases.” Kulander’s research has focused on developing

and exploiting computational methods to study the time-dependent quantum dynamics of atoms and molecules either during collision processes or when subjected to ultra-short, intense laser pulses. His research encompassed electron-atom and ion-atom collisions, molecular photodissociation, collision induced dissociation, dissociative electron-ion recombination, and a variety of strong field, multiphoton processes in atoms and molecules.



Peter Celliers, an experimental physicist in V Division, was elected **Fellow of the American Physical Society** (APS) in 2007. He was recognized by the APS Topical Group in Shock Compression of Condensed Matter “For developing a new generation

of high-precision ultra-fast diagnostics, which have enabled accurate laboratory measurements of shock compressed condensed matter in the ~1 to 100 Mbar regime.” The APS Fellowship recognizes those members who have made significant advances in knowledge through original research or who have made significant, innovative contributions in the application of physics to science and technology. Each year, no more than one-half of one percent of the current APS membership is elected to the status of Fellow. Currently there are 48 APS Fellows in Physical Sciences (PhySci).

Five teams of Livermore researchers won 2007 **R&D 100 Awards**, known as the “Oscars of Invention.” Each year, R&D Magazine selects the 100 most technologically significant new products and processes, ones that are likely to produce the most benefits for the world at large. Two of the awards involved R&D led by current or former staff members of the PhySci Directorate:

- *MEMS-based adaptive optics scanning laser ophthalmoscope* (MAOSLO) is a clinical instrument that uses adaptive optics and microelectromechanical systems (MEMS) technology to improve retinal imaging. With MAOSLO, doctors

can visualize microscopic cellular structures in the eye—a major advancement over current ophthalmoscopes and retinal cameras. Clinical trials showed that the instrument could diagnose the early stages of retinal diseases such as macular degeneration (age-related thinning and atrophy of the



eye's lining), diabetic retinopathy (damage to the retina resulting from diabetes), and retinitis pigmentosa (genetically induced retinal degeneration). **Scott Olivier** in AP Division led the multi-institutional research and development team that included

researchers at the University of Southern California's Doheny Eye Institute, where the clinical trials of the device took place.

- **Large Area Imager (LAI)** is a novel radiation detector, which uses gamma-ray imaging to pinpoint the source of radioactivity. LAI combines radiation detection and imaging into a compact instrument for mobile operation. The device quickly scans a sizable area and maps the radiation field



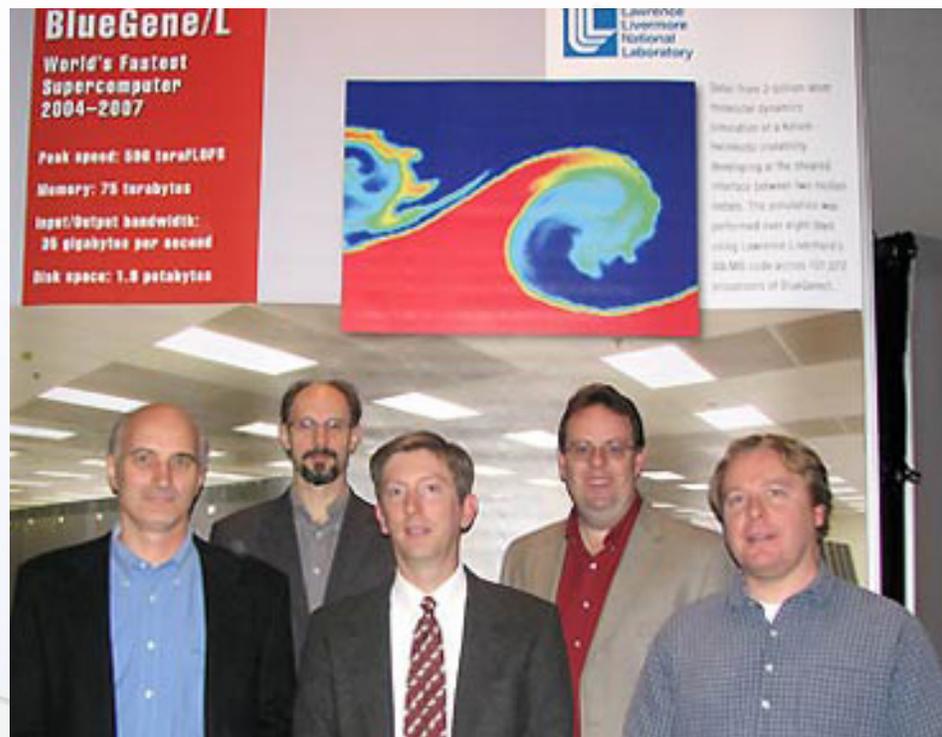
with a range and accuracy unmatched by available technologies. In tests with a prototype mounted on a truck traveling 40 kilometers per hour, the imager detected a 1-millicurie sample of a cesium isotope located 50 meters away.



Lorenzo Fabris and **Klaus Ziock** from AP Division (both now at Oak Ridge National Laboratory) led the multidisciplinary team, which also included researchers from Oak Ridge and the Space Science Laboratory in Berkeley.

A team of scientists from Livermore and IBM received the 2007 **Gordon Bell Prize** for their first-of-a-kind simulation of Kelvin-Helmholtz instability in molten metals on BlueGene/L, the world's fastest supercomputer. By performing

extremely large-scale molecular dynamics simulations enabled by groundbreaking computational techniques, the team was able to study, for the first time, how a Kelvin-Helmholtz instability develops from atomic scale fluctuations into micron-scale vortices. Named for one of the founding fathers of supercomputing, the prestigious Gordon Bell Prize is awarded to innovators who advance high-performance computing. Members of the award-winning team were **Jim Glosli**, principal investigator, **Fred Streitz**, project leader, **Kyle Caspersen**, **David Richards**, **Robert Rudd**, all from H Division, and John Gunnels of IBM. The researchers were recognized for "Extending Stability Beyond CPU Millennium: A Micron-Scale Simulation of Kelvin-Helmholtz Instability."



From left to right, Jim Glosli, Fred Streitz, Robert Rudd, David Richards and Kyle Caspersen won the Gordon Bell Award at the 2007 Supercomputing Conference (SC07) in Reno, Nevada.



George Chapline, a theoretical physicist in N Division, received the 2007 **Computing Anticipatory Systems Award** at the CASYS'07 International Conference hosted by the Centre for Hyperincursion

and Anticipation in Ordered Systems at the University of Liege in Belgium. Chapline was recognized for seminal research that explained the relationship between quantum mechanics and the so-called Helmholtz machine approach to pattern recognition. His work also suggests that mathematical techniques developed for inverse scattering problems might provide an alternative to conventional pattern recognition algorithms.



Physicist **Hope Ishii** has been selected for the Alameda County Women's Hall of Fame as the **2007 Outstanding Woman in Science**. Ishii, who works in the Institute of Geophysics and Planetary Physics, was honored for research she performed as a member of Livermore's Stardust team. The NASA Stardust mission, which was launched seven years ago, brought back to Earth particulate materials captured from the comet Wild 2. These bits of dust offer a snapshot of the building materials available in the solar system around the time that planets were forming.

Two teams of Livermore researchers received awards from the **Federal Laboratory Consortium (FLC) for Technology Transfer**. FLC is a nationwide network of federal laboratories that assists the U.S. public and private sectors in utilizing technologies developed by federal government research laboratories. The awards recognize excellence in technology transfer.

Both of the Livermore awards involved research contributions by members of the PhySci Directorate:

- *Dielectric Wall Accelerator (DWA) For Proton Therapy* is the first compact proton therapy system for treating cancer patients. Proton therapy is considered the most advanced form of radiation therapy for cancer, but size and cost have limited the technology's use to only six cancer centers nationwide. The compact DWA-based system was developed at Livermore and then licensed to TomoTherapy Incorporated. The company will fund development of the first clinical prototype, which will be tested on patients at the University of California Davis Cancer Center. **George Caporaso**, who has led the development of the DWA, and **Yu-Jiuan Chen**, both in the Fusion Energy Program, were members of the award-winning R&D team.
- *ORTEC Fission Meter™* is the first portable neutron detector that can assist in detecting and interdicting illegal nuclear materials. Several years ago, Livermore researchers developed an advanced neutron source identification system to assist in the interdiction of fissionable materials, which are a critical ingredient for nuclear explosives. The technology was licensed in 2005 to AMETEK's Advanced Measurement Technology ORTEC Division. The ORTEC Fission Meter™ is the first portable neutron detector that can distinguish between a fissile and non-fissile neutron source in real time. **Neal Snyderman** in N Division was a member of the award-winning R&D team.

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Dmitri Ryutov in the Fusion Energy Program and **Henry Chapman** in AP Division were awarded **Teller Fellowships** by the Laboratory to pursue self-directed research. Ryutov, a theoretical physicist, will focus his efforts on the Z-pinch approach to inertial confinement fusion, while continuing his collaborations with experimentalists on simulating astrophysical phenomena using laser-produced plasmas. Chapman, an experimental physicist, will continue his research on using coherent x-ray imaging with free-electron lasers to reveal the three-dimensional structure of proteins and other large molecules. One of his goals is to develop experiments for the Linac Coherent Light Source at the Stanford Linear Accelerator, which is due to become operational in 2009.



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Ed Synakowski, who is the Fusion Energy Program leader, has been invited to be a member of the international committee tasked with developing the initial Research Plan for ITER, the International Tokamak Experimental Reactor. ITER is a joint international research and development project that aims to demonstrate the scientific and technical feasibility of magnetic fusion power. The facility is under construction in Cadarache, France. Synakowski is one of three fusion energy researchers from the U.S. to serve on the committee. One of the primary tasks of the committee is to analyze how advances in the physics understanding of tokamak plasmas over the last five years will affect experiments at ITER. The findings and recommendations will have an impact on how ITER operates and may have an impact on the design of ITER itself.

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Ed Hartouni, leader of N Division, was a member of the Long Range Plan Working Group of the Nuclear Science Advisory Committee (NSAC), which produced the 2007 Long Range Plan: "The Frontiers of Nuclear Science." This document describes the vision and direction for US research in nuclear science from 2007 to 2012. The 2007 Long Range Plan, the culmination of many separate workshops in which scores of Livermore researchers participated, crafts the vision and roadmap that will guide the national basic research program in nuclear science sponsored by the Department of Energy (DOE) Office of Science and the National Science Foundation (NSF) throughout the next five years. NSAC is chartered to provide official advice to DOE and NSF in the area of basic nuclear science research.

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Lisa Poyneer of the Engineering Technologies Division, who is a member of the Adaptive Optics program in Physical Sciences, received the **Jain Prize** from the University of California (UC) Davis for her dissertation, "Signal Processing for High-Precision Wavefront Control in Adaptive Optics," which she completed in June 2007. The annual award recognizes the best Ph.D. dissertation in the Electrical and Computer Engineering Department at UC Davis. Poyneer's research, which has focused on applying innovative signal processing techniques to adaptive optics, has helped Livermore to secure a \$24 million contract to build, in collaboration with other institutions, the Gemini Planet Imager. This instrument, which is a coronagraph utilizing extreme adaptive optics, will be installed at the Gemini telescope for the purpose of detecting planets about 30 to 150 light years from Earth.

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