Science & Technology REVIEW

October 2007

National Nuclear
Security Administration's
Lawrence Livermore
National Laboratory

*Livermore
Wins*

R&D
100

Awards

Also in this issue:

- Introducing a New Partnership
- Teller's Legacy in Basic Atomic Physics

About the Cover

Livermore researchers won five R&D 100 awards in *R&D Magazine*'s annual competition for the top 100 industrial innovations worldwide. This issue of *Science & Technology Review* highlights the award-winning technologies: noninvasive pneumothorax detector, microelectromechanical system-based adaptive optics scanning laser ophthalmoscope, large-area imager, *hypr* library of linear solvers, and continuous-phase-plate optics system manufactured using magnetorheological finishing. Since 1978, Laboratory researchers have received 118 R&D 100 awards. The R&D 100 logo (on the cover and p. 1) is reprinted courtesy of *R&D Magazine*.

Cover design: Daniel Moore

About the Review

Lawrence Livermore National Laboratory is operated by Lawrence Livermore National Security, LLC (LLNS), for the Department of Energy's National Nuclear Security Administration. LLNS is a partnership involving Bechtel National, Inc.; University of California; BWX Technologies, Inc.; Washington Group International, Inc.; and Battelle in affiliation with Texas A&M University. More information about LLNS is available at www.llnslc.com.

At Livermore, we focus science and technology on ensuring our nation's security. We also apply that expertise to solve other important national problems in energy, bioscience, and the environment. *Science & Technology Review* is published 10 times a year to communicate, to a broad audience, the Laboratory's scientific and technological accomplishments in fulfilling its primary missions. The publication's goal is to help readers understand these accomplishments and appreciate their value to the individual citizen, the nation, and the world.

Please address any correspondence (including name and address changes) to *S&TR*, Mail Stop L-664, Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, California 94551, or telephone (925) 423-3432. Our e-mail address is str-mail@llnl.gov. *S&TR* is available on the Web at www.llnl.gov/str.

© 2007. Lawrence Livermore National Security, LLC. All rights reserved. This document has been authored by Lawrence Livermore National Security, LLC, under contract DE-AC52-07NA27344 with the U.S. Government. To request permission to use any material contained in this document, please submit your request in writing to Library Report Orders, Lawrence Livermore National Laboratory, Mail Stop L-610, P.O. Box 808, Livermore, California 94551, or to our e-mail address report-orders@llnl.gov.

This document was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor Lawrence Livermore National Security, LLC, nor any of their employees makes any warranty, expressed or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or Lawrence Livermore National Security, LLC. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or Lawrence Livermore National Security, LLC, and shall not be used for advertising or product endorsement purposes.

Prepared by LLNL under contract
DE-AC52-07NA27344

Contents

S&TR Staff

SCIENTIFIC EDITOR

Diane J. Chinn

MANAGING EDITOR

Ray Marazzi

PUBLICATION EDITOR

Carolin Middleton

WRITERS

Rose Hansen, Arnie Heller, Kristen Light, Caryn Meissner, Ann Parker, Maurina S. Sherman, and Katie Walter

ART DIRECTOR

Daniel Moore

PROOFREADER

Pamela MacGregor

PRINT COORDINATOR

Charlie M. Arteago, Jr.

S&TR, a Director's Office publication, is produced by the Technical Information Department under the direction of the Office of Policy, Planning, and Special Studies.

S&TR is available on the Web at www.llnl.gov/str.

Printed in the United States of America

Available from
National Technical Information Service
U.S. Department of Commerce
5285 Port Royal Road
Springfield, Virginia 22161

UCRL-TR-52000-07-10
Distribution Category UC-99
October 2007

Features

2 A New Partnership for a Strong Future

The Laboratory introduces its new management contactor, Lawrence Livermore National Security, LLC.

4 Fast Detection of a Punctured Lung

A portable detector can reveal a life-threatening condition in seconds.

6 Retinal Camera Captures Early Stages of Eye Disease

Livermore's adaptive optics ophthalmoscope detects early-stage retinal disease.

8 Mobile Mapping for Radioactive Materials

A compact imager can quickly scan a large area and pinpoint radiation sources.

10 Linear Solutions at *Hypr* Speed

The Laboratory's *hypr* software offers fast solutions to linear equations.

12 Bringing Fusion Research into Focus

Continuous-phase-plate optics control the shape and size of laser beams.

Teller Centennial Highlight

14 Back to Basics

Throughout his career, Edward Teller maintained a passion for understanding the basics of atomic physics.

Departments

16 The Laboratory in the News

18 Patents and Awards

21 Abstracts

A New Partnership for a Strong Future

The limited-liability corporation now managing Lawrence Livermore is dedicated to delivering innovative science and technology to meet enduring national needs.

ON October 1, 2007, Lawrence Livermore National Laboratory started a new chapter in our remarkable history. A newly formed public-private partnership, Lawrence Livermore National Security, LLC (LLNS), began its contract with the Department of Energy to manage and operate the Laboratory. LLNS is honored to take on this responsibility. As president of LLNS and the

Laboratory's director, I foresee a bright future for Livermore in applying exceptional science and technology to solve important national problems.

LLNS is a limited-liability corporation made up of Bechtel National, Inc.; the University of California; BWX Technologies, Inc.; the Washington Group International, Inc.; and Battelle. Four small business subcontractors and Texas A&M University are also members of the team. The Department of Energy awarded the contract to LLNS in May 2007 in the first open competition for managing Lawrence Livermore. The University of California—one of the LLNS partners—had operated the Laboratory since its inception in 1952 as part of Ernest O. Lawrence's Radiation Laboratory.

The LLNS public-private partnership brings together enormous experience in science and technology, business and operations, and nuclear weapons complex-critical infrastructure capabilities. Drawing expertise from the parent organizations through the LLNS Board of Governors, we will build on the Laboratory's proud tradition of outstanding science and technology and fully integrate world-class business systems and safety and security practices.

Our senior management team at the Laboratory is a mixture of new and familiar faces. Deputy director Steven Liedle and Frank Russo, principal associate director for Operations and Business, both come to Livermore from Bechtel. John Doesburg,

In 1952, Livermore's senior management team included (from left) Ernest O. Lawrence, Edward Teller, and Herbert York, the Laboratory's first director.

George H. Miller

Steven D. Liedle

John C. Doesburg

Bruce T. Goodwin

Edward I. Moses

Cherry A. Murray

Frank M. Russo

who joins us from Batelle's Oak Ridge National Laboratory, is the principal associate director for Global Security. Readers of *Science & Technology Review* will recognize Cherry Murray, Bruce Goodwin, and Edward Moses from their commentaries in past issues. They are, respectively, the principal associate directors for Science and Technology, Weapons and Complex Integration, and National Ignition Facility (NIF) and Photon Science.

With the five principal associate directors (PADs), we are organized to sustain Livermore's deeply rooted heritage of mission-focused science and technology. National security is the Laboratory's defining mission, and a primary responsibility is ensuring that the nation's nuclear weapons stockpile is reliable, safe, and secure. The PAD for Weapons and Complex Integration leads this effort. He also directs our work in support of the National Nuclear Security Administration's 2030 goal to transform the nuclear weapons complex to be more responsive, cost-efficient, and highly secure.

Livermore also strives to anticipate future national needs, and we use innovative science and technology to deliver solutions to complex global, national, and energy security challenges. The Global Security PAD heads efforts to apply the Laboratory's science and technology to emerging 21st-century threats through expanded work-for-others programs, ranging from nonproliferation, intelligence, and homeland security to environmental quality. The PAD for NIF and Photon Science leads Livermore's third major program element. Experiments on NIF, the world's most energetic laser, will make a major impact on stockpile stewardship, global security, fusion energy, and basic science.

Program success in our mission areas is made possible by outstanding science and technology using safe, secure, and efficient operations and business functions. A hallmark of the Laboratory is its application of multidisciplinary teams that combine innovative science and engineering, challenging program goals, and operational considerations to tackle complex

problems—from basic science research to prototype development. Scientists and engineers from Science and Technology directorates and professional staff from Operations and Business organizations work in integrated teams with program personnel to make advances in support of our missions.

Some of our recent breakthroughs are highlighted in the features beginning on p. 4. Each year, *R&D Magazine* selects the top 100 technological advances that contribute to meeting an important national or societal need. This year, the Laboratory and its partners earned five R&D 100 awards. Livermore has captured a total of 118 of these "Oscars of Invention" since the competition began in 1978. The winning technologies demonstrate the wide range of expertise at the Laboratory: an advanced radiation detection system for interdicting illicit nuclear materials; a novel optics technology to improve NIF experimental capabilities; software to speed supercomputer simulations; a new ophthalmoscope that could revolutionize retinal imaging; and a diagnostic device to promptly detect pneumothorax, a medical condition that can cause death in minutes.

The R&D 100 Award winners also highlight a few of the Laboratory's many partnerships. Livermore is an active participant in the broad scientific and technical community, and our continuing success depends on strong ties with research universities and U.S. industry. The award-winning work described in this issue involved collaborators from five universities, four industrial partners, and another national laboratory.

In addition, these feature articles introduce readers to some of the outstanding scientists and engineers at the Laboratory. Our staff is key to our success. Livermore is an exceptional national laboratory because of its exceptional people. We have an important mission full of science and technology frontiers to explore.

■ George H. Miller is director of Lawrence Livermore National Laboratory.

Fast Detection of a Punctured

The noninvasive pneumothorax detector connects to a standard personal digital assistant. A graphical user interface guides diagnosis.

PNEUMOTHORAX is a respiratory condition in which air is trapped in the pleural space—the space between the wall of the chest cavity and the lung. The condition is usually attributed to a fractured rib puncturing the lung. If not treated quickly, it can become life-threatening in minutes. Prompt diagnosis is difficult, especially in remote or combat environments where x-ray and computed tomography (CT) systems are not available. The noninvasive pneumothorax detector, developed by Livermore scientists in collaboration with ElectroSonics Medical, Inc., can diagnose this serious condition in seconds.

The project team, led by Livermore engineer John Chang, won a 2007 R&D Award for the handheld detector. Detroit Receiving Hospital and Sinai-Grace Hospital, both of the Detroit Medical Center, collaborated on the project. The device uses the ultrawideband (UWB) technology pioneered by Lawrence Livermore, and the development effort received early support from Livermore's Laboratory Directed Research and Development Program.

The battery-operated detector is ideal for trauma situations where low weight, low power consumption, and insensitivity to acoustic and electromagnetic noise are critical. "The concept came about in 1999 from my experience and interest as an emergency medical technician for search and rescue operations," says Chang.

Faster, Lighter, Cheaper

The traditional process for diagnosing pneumothorax is time-consuming. Emergency response personnel first examine the patient, looking for signs

of respiratory distress, feeling for broken ribs, and listening for sounds of diminished breathing capacity. A definitive diagnosis requires a chest x ray or CT scan. If a diagnostician cannot interpret the images immediately, results may not be available for hours. In addition, x-ray and CT systems are so large and require so much electrical power that emergency squads and battlefield medics cannot use them in the field.

The noninvasive pneumothorax detector has a graphical user interface that guides the user in collecting data and displays the diagnosis on a readout screen. The procedure takes only 15 seconds, and results are processed immediately. The device is so simple to use that patients at risk of developing pneumothorax from a congenital defect or following a surgical procedure can carry a detector and continuously monitor their condition.

Livermore's UWB technology is compact and insensitive to acoustic and electromagnetic background noise. On an emergency rescue mission or in a chaotic trauma situation such as a moving ambulance, technicians using a stethoscope cannot always hear a person's breathing sounds. Detecting pneumothorax is especially important if a patient is to be airlifted to a treatment facility because the drop in air pressure could exacerbate symptoms.

To test the effectiveness of the UWB technology in a noisy environment, the Livermore team placed the cardiovascular monitor on the flight jacket worn by a helicopter pilot during takeoff. Even with the background noise from the helicopter, the monitor gave an accurate (negative) test result.

Lung

The portable detector measures 1 centimeter by 2 centimeters and weighs less than 0.45 kilogram. Because the UWB technology uses commercial components, the projected cost is \$1,000 per unit. For comparison, x-ray equipment can cost more than \$15,000, and CT scanners run up to \$250,000.

One Breath at a Time

Now licensed by ElectroSonics Medical, Inc. (previously called BIOMECH, Inc.), the noninvasive pneumothorax detector underwent final commercial development and clinical trials in 2000. In 2001, the Livermore team collaborated with BIOMECH and the MetroHealth Medical Center in Cleveland, Ohio, to assess the detector's accuracy.

Experiments using a pig established the technical feasibility of the device. The goal in these tests was to detect a pneumothorax with a volume as small as 60 milliliters, or about 4 tablespoons. Experimental results were remarkable, showing that the UWB signal clearly detected a pneumothorax as small as 30 milliliters.

In 2003, the National Institutes of Health funded a project to investigate the detector's capabilities in humans. For this research, the team tested a prototype device on 53 patients who had been examined for pneumothorax and were waiting to receive results from a chest x ray or CT scan. All patients in the study pool gave informed consent to participate in the research. In these tests, a clinician placed the detector's UWB antenna at eight defined locations on the patient and took readings at each location.

The overall accuracy of the prototype was 91 percent, with four false positives

Project team for the noninvasive pneumothorax detector (from left): Mark Vigars, Gregory Dallum, John Chang, Christine Paulson, Patrick Welsh, and Garth Pratt.

and one false negative. Accuracy decreased to 85 percent in tests to determine on which side of a patient's chest the pneumothorax was located. Researchers attributed the errors in part to the UWB antenna used in the prototype device. The antenna's wide beam spread caused its signal to cross over from one side of the chest to the other. For example, a measurement taken on the left side received echoes from a pneumothorax on the right side. According to Chang, reducing the beam spread and optimizing antenna placement on the body will improve the results. The team is looking at different antenna designs to control the beam spread.

In High Demand

Rapid diagnosis and treatment of pneumothorax can save lives and reduce morbidity. The noninvasive pneumothorax detector is in high demand in medical air transports, ambulances, hospital

emergency rooms, and intensive care units. Veterinarians are also interested in the device because x-ray procedures on animals are expensive and can be difficult to perform. The project team expects civilian and animal services to create a demand of about 20,000 units in the U.S. alone—an attractive market for the device.

"We're making progress in moving the technology from bench-top prototype to clinical validation," says Chang. "We hope the detector will be implemented by emergency response teams and health-care providers to improve the outcome for critically injured individuals."

—Kristen Light

Key Words: chest trauma, chest x ray, collapsed lung, noninvasive pneumothorax detector, R&D 100 Award, ultrawideband (UWB) technology.

For further information contact John Chang (925) 424-4624 (chang16@llnl.gov).

Retinal Camera Captures Early Stages of

LAURENCE 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 retinal imaging. With the MEMS-based adaptive optics scanning laser ophthalmoscope (MAOSLO), clinicians can visualize microscopic cellular structures in the eye—a major advancement over current ophthalmoscopes and retinal cameras. The Livermore collaboration received an R&D 100 Award for this new technology.

The research team, led by Livermore physicist Scot Olivier, used an adaptive optics system similar to that pioneered by the Laboratory for use in large telescopes, such as those at the W. M. Keck Observatory in Mauna Kea, Hawaii. Instead of viewing astronomical objects, the MAOSLO system sharpens images of the retinal cell layers in a patient's eye to provide enhanced details. Livermore's Laboratory Directed Research and Development Program funded early research efforts for the ophthalmoscope.

Clinical trials showed that clinicians using the system can diagnose the early stages of retinal diseases such as macular degeneration (an age-related disease in which the center of the eye's lining thins and atrophies), diabetic retinopathy (damage to the retina resulting from diabetes), and retinitis pigmentosa (a group of inherited diseases that cause the retina to degenerate). The MAOSLO system can also be used to monitor a patient's treatment.

The microelectromechanical systems— (MEMS-) based adaptive optics scanning laser ophthalmoscope captures images of the individual cellular layers of the retina. The ringlike pattern in the inset indicates photoreceptor cell loss, which causes visual disturbances in a patient's line of sight.

The Science behind the Image

The Livermore ophthalmoscope 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. MAOSLO'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 wavefront 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.

As with other retinal imagers, MAOSLO provides digitized, permanent records that can be used to track changes in a patient's eyesight over time. The device also performs functions that other instruments do not. 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.

Eye Disease

Imaging the Unexpected

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. One study examined several members of a family affected by Stargardt's disease, an inherited genetic retinal disorder.

As expected, MAOSLO revealed varying degrees of missing photoreceptors. The high-resolution images also exposed an unexpected defect in the photoreceptor layer of a family member who had no obvious symptoms and an otherwise normal clinical exam. This observation highlighted the device's potential for early disease detection and intervention and for helping researchers better understand how a disease originates and progresses.

Another clinical study involved a patient who complained of a visual disturbance in his central vision. A ringlike pattern of photoreceptor cell loss found in the MAOSLO images correlated with the patient's complaints. Researchers believe the patient has a rare retinal disorder known as coffee and doughnut maculopathy. The MAOSLO study may be the first to demonstrate the anatomic basis for this poorly understood disorder.

Positive Prognosis

MAOSLO gives eye doctors an affordable system to diagnose retinal disease in its early stages and effectively monitor treatment. It can also be used for vision research in animals, and it

Development team for the MEMS-based adaptive optics scanning laser ophthalmoscope (from left): Dennis Silva, Steven Jones, Scot Olivier, and Diana Chen.

can be enhanced with additional light sources and detection channels to image fluorescent signals from the retina. In addition, the system can be designed to test pharmaceutical and molecular therapies developed for blinding diseases.

MAOSLO is available for licensing and has been in clinical operation at the Doheny Eye Institute for approximately one year. As the baby boomer population continues to age, their risk of age-related retinal diseases will increase. MAOSLO will be an important tool for ophthalmologists, optometrists, and

scientists who are combating vision loss and blindness in their patients. It has the potential to improve the quality of life for millions of people.

—Caryn Meissner

Key Words: deformable mirror, microelectromechanical systems— (MEMS-) based adaptive optics scanning laser ophthalmoscope (MAOSLO), optical aberrations, R&D 100 Award, retinal imaging, wavefront corrector.

For further information contact Scot Olivier (925) 423-6483 (olivier1@llnl.gov).

Mobile Mapping for Radioactive Materials

AS part of Livermore's national security mission, Laboratory researchers are applying their expertise in radiation sensing to develop technologies that can detect and intercept stolen nuclear materials. One recent success is the large-area imager (LAI), which uses gamma-ray imaging to pinpoint the source of radioactivity. (See *S&TR*, May 2006, pp. 4–10.) Developed in collaboration with Oak Ridge National Laboratory and the University of California at Berkeley's Space Sciences Laboratory, 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.

The research team, led by Laboratory engineer Lorenzo Fabris and physicist Klaus Ziöck (both now at Oak Ridge), received an R&D 100 Award for the innovative technology. Other team members include Livermore engineers Jeff Collins, Dennis Carr, and Chris Cork; engineering technician Marianne Ammendolia, also from Livermore; and computer programmers Thomas Karnowski from Oak Ridge and Will Marchant from the Space Sciences Laboratory. The team received funding from Livermore's Laboratory Directed Research and Development Program and the Department of Homeland Security. 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 team completed the prototype design in July 2006, and the instrument is being commercially licensed.

The large-area imager (LAI) fits on the back of a small truck or trailer. Team members at Oak Ridge National Laboratory (from left): Lorenzo Fabris, Thomas Karnowski, and Klaus Ziöck.

Locating a Radiation Source

LAI uses gamma rays to pinpoint various radiation sources—from chunks of uranium to a truck filled with bananas. Gamma rays, produced through radioactive decay, have the highest energy in the electromagnetic spectrum and thus can penetrate most materials. Because of this extreme penetrability, researchers can use gamma rays to detect radioactivity even if the radiation source is shielded by concrete, dirt, or a few centimeters of lead.

However, gamma rays can only be viewed indirectly by observing their interactions with detector materials. The intensity and energy of gamma rays emitted by a source provides clues to the type of material producing the radiation. Because

gamma radiation is a high-energy type of light, it travels in straight lines from the source to the detector. Imaging gamma rays thus shows the material's location.

Background radiation levels vary from place to place. Search instruments generally 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 beyond a few meters because the signal they induce in a detector may appear the same as the normal variation in radioactivity. If an instrument's sensitivity were adjusted to account for these fluctuations, naturally occurring radioisotopes emitted by harmless materials would falsely appear

as a dangerous radiation source. The similarity between hazardous and benign sources makes the detection of weak but significant signals impossible unless variations in background radiation are known in advance, which is unlikely.

Seeing through the Background

To conquer the clutter problem, the research team 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. As the array picks up gamma-ray signals, the radiation incident on the mask casts shadows on the detector elements, and the imager records these patterns. 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.

One disadvantage of coded-aperture imagers is that gamma-ray sources outside an instrument's viewing field can contribute to the signal count and generate artifacts in the image. To correct for this blurring effect, the team added a second imager. The mask for this imager has open and closed elements arranged in the reverse pattern of that used on the first imager's mask.

As the instrument travels through an area, it takes snapshots of the radiation field and uses them to produce a two-dimensional map showing where each source is generated. LAI's navigation system tracks the imager's location and orientation so that gamma-ray data can be superimposed on satellite images of an area.

The LAI development team at Livermore (from left): Dennis Carr, Marianne Ammendolia, and Jeff Collins. Not pictured: Chris Cork.

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

Homeland Security Applications

“Gamma-ray imaging is highly effective at distinguishing illicit sources from harmless background radiation,” says Fabris. “We foresee this technology

being adapted for various scenarios, such as scanning buildings or monitoring port and harbor entries.” For example, Ziock is extending the technology to track radioactive materials in vehicles. Other applications include routine surveillance of key targets, facility inspections prior to special events, and searches based on intelligence information.

LAI is an important contribution to improving the nation's security. Accurately mapping radioactive sources will help border agents, customs inspectors, law-enforcement officers, and incident response personnel to locate illicit nuclear material.

—Rose Hansen

Key Words: coded aperture, gamma rays, large-area imager (LAI), radiation detection, R&D 100 Award.

For further information contact Lorenzo Fabris (865) 576-2474 (fabrisl@ornl.gov).

Linear Solutions at *Hypre* Speed

TODAY'S supercomputers allow researchers to simulate large-scale physical phenomena with a level of detail previously impossible to achieve. These simulations are increasingly important in exploring fundamental scientific issues, particularly when experiments are prohibitively expensive or simply not feasible, as in studying global climate change or stellar evolution.

Livermore's *hypre* library of linear solvers makes possible larger, more detailed simulations by solving problems faster than ever before. The *hypre* development team, which received initial funding from Livermore's Laboratory Directed Research and Development Program, won an R&D 100 Award for their innovative software.

A solver is an algorithm for calculating the solution to a set of mathematical equations. A linear solver works on a system of linear equations, such as those found in a high school algebra textbook. Unlike the equations in high school algebra, however, the linear systems that arise in scientific simulations often have millions or billions of equations. Computer scientist Rob Falgout, who leads the *hypre* team, says, "When it comes to efficiently processing huge sets of linear equations, not all systems are created equal. Some are fairly easy to solve, while others require specialized algorithms."

The physical world can be described by complicated sets of mathematical equations. To translate these equations into something suitable for a computer, scientists restrict a problem to a grid and assign one or more physical characteristics to each grid point, a process called discretizing. In a groundwater-flow

The *hypre* library of linear solvers helps speed up calculations for a range of simulations. (a) A simulation predicting the results of a maxillofacial surgery compares well with the patient's postoperative computed-tomography scan. (Image courtesy of C&C Research Laboratories, NEC Europe, Ltd.) (b) Results from a Livermore calculation of the hydrodynamic stress caused by large currents in pulsed-power experiments show the transient magnetic field and eddy currents occurring in a helical coil with two side-by-side wires.

simulation, for example, the grid points represent discrete locations underground. The characteristics describing these locations might include the concentration of chemical contaminants and the direction and speed of contaminant travel.

The main goal of a simulation is to assign meaningful values to the physical properties at each point. In a large-scale simulation, the most time-consuming component in determining these values is often processing the solution for a huge system of linear equations. *Hypre*'s linear solvers make quick work of the equations and are effective on systems that define a variety of physical phenomena. For example, Livermore researchers applied *hypre*'s structured solvers in simulations of inertial confinement fusion experiments, reducing the calculation time by as much as 30 times that required

by other linear solvers. They are also using the *hypre* library to improve the detail and reduce computational time of simulations such as elastic deformation in explosive materials, explosively driven magnetic flux compression generators, and molecular dynamics.

The Challenge of Scalability

Although many software packages include parallel linear solvers, not all of them are scalable. Scalability—the ability to use additional computational resources effectively—is both a challenge and a necessity in designing parallel algorithms. Falgout's team developed the algorithms in *hypre* with scalability in mind.

Hypre's solvers are based on an iterative multilevel approach. An iterative solver begins with a "guess" of the solution and then uses an algorithm to generate an

improved guess. This procedure repeats until the iterations converge with the solution. The multilevel solvers in *hypre* accelerate the iterative process by using a sequence of smaller linear systems, each associated with a smaller, or coarser, grid. The coarse-grid system enables *hypre* to significantly improve each successive guess with little added computational expense because the calculations primarily involve small problems.

Most importantly, the computational cost with a multilevel approach is proportional to the number of equations. Thus, a large problem can be solved in the same time as a smaller one by proportionally increasing the number of processors working on the calculation. *Hypre*'s algorithms facilitate scalability on current supercomputers, with tens of thousands of processors, and are expected to operate just as effectively on future systems with hundreds of thousands or even millions of processors. The library's flexibility also allows researchers to use *hypre* on a laptop computer or individual workstation.

Hypre's specialized algorithms take advantage of easy-to-use interfaces for scientific software. Most parallel linear solver packages access information only from the equations to be processed. Many *hypre* solvers, in contrast, work faster by using information from the interface, such as the grid, the type of discretization, or known error components that are slow to converge.

Algorithms range from structured multigrid solvers for simple problems to a fast, adaptive composite solver for problems requiring adaptively refined grids. *Hypre*'s algebraic multigrid solver can process complex problems requiring arbitrary

The *hypre* development team (from left): Van Emden Henson, Rob Falgout, Ulrike Meier Yang, Tzanio Kolev, Charles Tong, Allison Baker, Barry Lee, Jeffrey Painter, and Panayot Vassilevski.

unstructured grids and has been scaled up to 125,000 processors. In addition, the library's unstructured Maxwell solver, AMS, is the first provably scalable solver for semi-definite electromagnetic problems involving general unstructured meshes.

Free and Flexible

Hypre is open-source software and is available for free from the project's Web site (www.llnl.gov/CASC/hypre/). In 2006, scientists in more than 35 countries downloaded it nearly 1,000 times. Research institutions and private companies have used *hypre* to simulate maxillofacial surgeries, magnetic fusion energy plasmas in tokamaks and stellarators, blood flow through the heart, fluid flow in steam generators for nuclear power plants, and pumping activity in oil reservoirs.

The *hypre* library offers the most comprehensive suite of scalable parallel linear solvers available for large-scale scientific simulation, with some algorithms appearing for the first time in a linear solver library. "The *hypre* library is the result of nearly nine years of mathematical research and software development," says Ulrike Meier Yang, a computer scientist on the *hypre* team. "It was a significant undertaking, but one that is benefiting scientists all over the world."

—Katie Walter

Key Words: *hypre* linear solver, open-source software, parallel computing, R&D 100 Award, supercomputing.

For further information contact Rob Falgout (925) 422-4377 (falgout2@llnl.gov).

Bringing Fusion Research into Focus

The no mystery that high-powered laser systems such as the National Ignition Facility (NIF) are at the forefront of scientific discovery—especially in the field of high-energy-density physics. What has puzzled researchers, however, is developing a method to accurately manipulate certain properties of the megajoule-level laser beams to better enhance inertial confinement fusion (ICF) research.

The continuous-phase-plate (CPP) optics system developed by a Livermore research team offers an elegant solution to this challenge. The team, led by chemist Joe Menapace of the Laboratory's Chemistry, Materials, and Life Sciences Directorate, received an R&D 100 Award for the novel technology. Livermore has partnered with Zygo Corporation of Middlefield, Connecticut, and QED Technologies of

Rochester, New York, to make the new technology commercially available.

To create the best environment for achieving nuclear fusion with a high-powered laser such as NIF, researchers must precisely characterize and control each beam's illumination at the target plane. With Livermore's CPP optics system, they can manipulate a beam's shape, energy distribution, and wavefront profile. This level of control will allow scientists to design rigorous fusion experiments that examine details of phenomena such as how the universe began and how nuclear weapons age.

Behind the Plate

Continuous phase plates are large-aperture diffractive optics that can adjust and fine-tune a laser beam to a prescribed size and shape while maintaining the

coherent properties of the laser light. CPPs work with a focusing element, such as a lens, to define a beam's characteristics.

For example, using only a lens, researchers can focus a 360-millimeter-square laser beam to a spot about 15 micrometers in diameter on the target. The focused beam has a high intensity, but because of its small diameter, it cannot illuminate a large area (up to 1 millimeter in size) with coherent light. In addition, the lens-only configuration results in nonuniform illumination of the target. The spot size can be increased to about 100 micrometers by defocusing the lens. However, this process does not produce the optimal beam shape for ICF experiments, and the beam's intensity diminishes away from the center.

Introducing a CPP into the optics chain solves this problem. CPPs take advantage of the apparent bend in a light wave when it encounters a topographic change on an optical surface. To design CPPs for NIF, Menapace's team uses a computer program to generate a continually varying phase profile that will achieve the required energy profile. The topographic changes are then imprinted onto the surface of defect-free fused-silica optics. The variations in surface topography perturb the wavefront of the incoming laser beam either before or after the beam passes through the final focusing element. This process yields a beam footprint at the target with the desired characteristics.

A CPP can be designed to convert a square or circular laser beam to an elliptical or circular spot with the required dimensions. Other spot shapes are possible, including triangles, squares, and closed polygons.

A laser beam can be controlled with a lens (a) focused to its diffraction limit, (b) moved out of focus, or (c) combined with Livermore's continuous-phase-plate (CPP) optics system. CPP optics allow researchers to control a laser beam's size and shape and maintain its uniformity across the target area.

With Energy to Burn

Researchers must tailor CPP optics for a particular experiment. For example, in ICF experiments, NIF laser beams will focus on a tiny gold hohlraum that surrounds a sphere filled with gaseous and liquid or solid deuterium and tritium. The laser shot creates very high-energy-density matter, and the generated x rays blow off from the capsule surface, compressing the fuel sphere. Under these extreme conditions, the fusion fuel core implodes, ignites, and generates thermonuclear burn, yielding many times the input energy. In such a scenario, CPPs would be designed to spread the laser energy uniformly over the hohlraum interior, producing a symmetric implosion. The optics also shape the initially square laser beams into elliptical spots, which, because of their angle of entry, project as circles on the hohlraum walls.

In ICF applications, CPPs control each beam's spot size so light does not impinge on critical components in the target area. In addition, they help maintain a beam's projection angle and keep its energy uniform as it illuminates the target. CPPs also eliminate high-intensity areas, which can cause hydrodynamic performance to deteriorate.

Magnetic Attraction

Menapace's team designed the highly precise optics so they will survive extremely powerful laser pulses without being damaged. CPPs also do not add unwanted distortion to the focused laser beam.

To manufacture optics to the extreme tolerances required, the team developed a magnetorheological finishing (MRF) technology for polishing surface topography onto optical surfaces. This method pairs an

The project team for Livermore's continuous-phase-plate optics system (from left): Christopher Haynam, Gregory Rogowski, Jeff Atherton, Joe Menapace, Pete Davis, Jack Campbell, and Sham Dixit.

electromagnet with a magnetic fluid that contains microscopic abrasive particles. A computer program determines how the electromagnet and fluid interact to imprint the desired topographic structure on the optics. The MRF system, which combines interferometry, precision equipment, and computer control, is a key technology for CPP optics. "Traditional methods for polishing optics are more of an art than a science," says Menapace. "Imprinting varying topographies is simply not possible with those techniques. The MRF approach is pushing the technological limits of optical polishing, allowing us to make not only more precise parts but also more complicated optics."

And these more complex optics are enabling systems that could never have

been imagined with current technology. "NIF is just one example," says Menapace. "Using traditional techniques to develop optics for this powerful laser was an impossibility. We had to create a new technology to make the system work."

—Maurina S. Sherman

Key Words: continuous-phase-plate (CPP) optics system, inertial confinement fusion (ICF), laser optics, magnetorheological finishing (MRF), National Ignition Facility (NIF), R&D 100 Award.

For further information contact
Joe Menapace (925) 423-0829
(menapace1@llnl.gov).

Back to Basics

Teller's Contributions to Atomic and Molecular Physics

January 15, 2008, marks the 100th anniversary of Edward Teller's birth. This highlight is the seventh in a series of 10 honoring his life and contributions to science.

EDWARD Teller kept a small statue in his Livermore office of the Greek philosopher Democritus. Born about 460 B.C., Democritus advanced an early concept of atomic theory when, at one of Plato's seminars, he proposed that the universe was composed of two indivisible elements: the atom and the void.

At the dawn of the 20th century, scientists continued to question the existence of atoms. Atomic theory worked well in chemistry, but it conflicted with the well-established classical laws of physics. The birth of quantum mechanics in the 1920s provided the theoretical framework needed to study atomistic behavior. The powerful physical picture and mathematical tools of quantum mechanics allowed physicists, including Teller, to describe the behavior of atoms and molecules and explain, often for the first time, phenomena that previously puzzled them.

Teller studied quantum mechanics at the University of Leipzig under Werner Heisenberg, a major contributor to the theory. At this time, scientists did not completely understand even the simplest molecule—the hydrogen ion, which has two protons and one electron in a bound state. The theories being proposed to explain the molecule's behavior often contradicted each other.

For example, two physicists, Carl Jensen Burrau of Denmark and A. H. Wilson from the U.S., derived different results in their separate calculations

of the lowest energy state for the hydrogen ion. In 1929, Heisenberg asked the 20-year-old Teller to determine which result was correct. A few days later, Teller reported that Burrau's calculation was accurate. Heisenberg then had Teller analyze the higher energy levels of an excited hydrogen ion, a topic that became Teller's doctoral thesis. In *Memoirs*, Teller recalled that the project involved

"lots of busy work, a little diligence, and no originality." It also required him to use a noisy calculating machine in a room below Heisenberg's living quarters. According to Teller, Heisenberg declared the thesis work completed when he tired of the machine's racket. The resulting paper, "Hydrogen Molecular Ion," appeared in 1930 in *Zeitschrift für Physik*. It was the first of many in which Teller applied quantum mechanics to molecular physics.

Teller worked with László Tisza, a friend from Hungary, on another molecular physics problem. In this project, the two physicists examined the spectral consequences of coupling the nuclear vibration and molecular rotation of a methyl halide molecule. Methyl halide has one carbon atom, three hydrogen atoms, and one atom of a halogen, either iodine, bromine, chlorine, or fluorine. Teller and Tisza extended the Franck–Condon principle, which explains the electronic transitions occurring in a polyatomic molecule as it vibrates and rotates. Their 1932 paper, also published in *Zeitschrift für Physik*, was the first of a series examining how polyatomic molecules behave when, under varying circumstances, the electronic levels cross.

Teller's work on molecular physics culminated in a collaboration with Hermann Jahn. Their 1937 paper, "Stability

The Teller family enjoyed playing chess: (from left) Teller's son, Paul; wife, Mici; daughter, Wendy; and Teller.

Edward Teller graduated from the Minta Model School in Budapest, Hungary, in 1925.

of Polyatomic Molecules in Degenerate Electronic States,” presented the Jahn–Teller theorem. Published in the *Proceedings of the Royal Society*, this paper described how electrons force nominally symmetric molecules with more than two atoms to readjust and break the symmetry in specific ways. At the time, scientists considered this effect to be rare, but Jahn and Teller showed that it, in fact, is ubiquitous.

The Jahn–Teller theorem remains an important contribution to molecular physics research. Its significance extends through the modern physics of materials and their chemistry—from measuring spectral interactions to calculating chemical reactivity and determining molecular and condensed-matter crystal structures. For example, in 1986, the Jahn–Teller theorem was instrumental in the discovery of high-temperature superconductivity. The discoverers, Georg Bednorz and Alex Müller, chose to examine perovskites because the materials exhibited strong Jahn–Teller distortions and thus offered the promise of strong electron couplings.

Teller also explored basic atomic physics issues, most notably the two-photon decays of the metastable states of excited hydrogen and helium atoms. The resulting paper with his colleague Gregory

Edward Teller demonstrates a physics principle in the classroom.

Nothing exists except atoms and empty space; everything else is opinion.

—Democritus,
Greek philosopher

Breit, “Metastability of Hydrogen and Helium Levels,” appeared in 1940 in *Astrophysical Journal*. Their work had particular relevance to astrophysics, including cosmology, and the physics of magnetic fusion. In the corona of a star or in the early universe, when the density of atoms is low, they can exist in metastable states whose lifetimes are controlled by the two-photon rates.

In 1962, Teller returned to the behavior and properties of molecules in his paper, “On the Stability of Molecules in the Thomas–Fermi Theory,” which appeared in *Reviews of Modern Physics*. Written for a Festschrift, or tribute publication, to honor his friend Eugene Wigner, this concise paper addressed whether the Thomas–Fermi approximation can provide an adequate simplification to the full Schrödinger equation of quantum mechanics when applied to molecules. Teller showed that the approximation did not sufficiently capture the physics described by the more complex Schrödinger equation and thus would not predict stable, bound molecules. His result was significant in later basic analyses of the stability of matter. (See *S&TR*, April 2007, pp. 25–26.)

These discoveries, combining insights of basic atomic, molecular, and mathematical physics, continue to be important in research at Lawrence Livermore and elsewhere. From the creation of first-principles molecular dynamics simulations to the spectra of atoms and ions in gases and plasmas, Teller’s legacy lives on.

—Ann Parker

Key Words: atomic physics, Edward Teller, hydrogen molecular ion, Jahn–Teller theorem, molecular physics, polymolecules, Thomas–Fermi approximation, quantum mechanics.

For further information contact Stephen B. Libby (925) 422-9785 (libby1@llnl.gov).

An improved measure of DNA damage

A team of Livermore researchers led by Paul Henderson of the Chemistry, Materials, and Life Sciences Directorate reported a new understanding of how damaged nucleic acid is incorporated in DNA and subsequently repaired. The findings—which resulted from a study using accelerator mass spectrometry (AMS)—were featured on the cover of the July 3, 2007, issue of the *Proceedings of the National Academy of Sciences*.

AMS allows patients or cells to be dosed with tiny amounts of radioactive compounds that can be traced in vivo or in vitro without disturbing normal metabolic processes. In this study, which was funded by the National Institutes of Health and the California Breast Cancer Research Program, researchers tagged human breast cancer cells with carbon-14 to track how living cells process oxidized guanosine (8-oxodG), a precursor to one of the most prevalent forms of DNA damage. If not repaired, the damaged DNA can cause cell mutations.

The sensitivity of AMS allowed the researchers to measure the 8-oxodG incorporated into DNA even though the amount in some cells was less than one atom of carbon-14. This minute quantity is too small to be characterized using standard non-AMS methods. Nevertheless, it was orders of magnitude higher than the researchers expected.

In this study, the Livermore team established the mechanism by which 8-oxodG is metabolized. The team hopes that scientists can use this new understanding of mutagenesis to develop treatments aimed at reducing cancer mutation rates.

Contact: Paul Henderson (925) 423-2822 (henderson48@llnl.gov).

Climate models reflect observed ocean temperatures

A study by Laboratory scientists in the Program for Climate Model Diagnosis and Intercomparison in collaboration with colleagues at Scripps Institution of Oceanography shows that climate models are reliable tools for helping researchers better understand the observed record of ocean warming and variability. Results from this collaboration appeared in the June 26, 2007, issue of the *Proceedings of the National Academy of Sciences*.

The observational record shows substantial variability in ocean heat content over time scales ranging from several years to decades. The Livermore–Scripps team demonstrated that climate models represent this variability much more realistically than previously believed. Using 13 numerical climate models, the researchers found that the apparent discrepancies between modeled and observed variability can be explained by accounting for changes in observational coverage and instrumentation and by including the effects of volcanic eruptions.

The research also casts doubt on recent findings that the 0- to 700-meter layer of the global ocean cooled markedly from 2003 to 2005. Results indicate that the perceived cooling is largely an artifact of a systematic change in the observing system. Previous studies combined ocean temperature observations from several types of instruments, and the averaged measurements indicated an apparent cooling trend. When the Livermore–Scripps researchers looked at readings from individual instruments, they found no cooling. When the climate models included the cooling effects of intermittent volcanic eruptions, modeling results agreed even more closely with observations.

Contact: Benjamin Santer (925) 422-2486 (santer1@llnl.gov).

Laboratory signs technical agreement with BP

Lawrence Livermore has partnered with BP (formerly British Petroleum) to provide technical expertise in developing underground coal gasification (UCG) technology to convert in situ coal deposits into fuels and other products. In a technical cooperation agreement signed in July, Livermore agreed to work with BP to address three areas of UCG technology: determining the feasibility of storing carbon dioxide underground; assessing the environmental risks associated with UCG and developing methods to mitigate those factors; and modeling UCG processes to evaluate test results over time.

Underground coal gasification offers the potential to produce fuels and hydrocarbon feedstock from coal deposits that otherwise cannot be recovered. Introducing a controlled supply of air or oxygen into a coal seam produces syngas, which can be pumped to the surface. The recovered syngas can be used as fuel to generate power or as feedstock to produce chemicals and other hydrocarbon products. Additionally, the carbon dioxide produced in the UCG process can be captured and pumped into the excavated coal seam or into a nearby formation. This capability could dramatically reduce carbon dioxide emissions, which have been linked to global climate change.

Livermore has worked on developing UCG technology for more than 30 years. In the partnership with BP, Laboratory researchers will provide their expertise in advanced computation and modeling, engineering, environmental management, and carbon management, including carbon sequestration.

Contact: Julio Friedmann (925) 423-0585 (friedmann2@llnl.gov).

Detailing algae's role in nutrient cycle

Scientists from Lawrence Livermore, Portland State University, and the University of Southern California used nanometer-scale secondary-ion mass spectrometry (NanoSIMS) to image

and track nutrient uptake in blue-green algae. Blue-green algae are key players in global nutrient cycling. They take in, or fix, nitrogen gas from the atmosphere and convert it into a usable nutrient, enabling photosynthesis in nutrient-poor waters. The bacteria fix both nitrogen and carbon, an intriguing capability. Fixing carbon dioxide during photosynthesis produces oxygen, which inhibits nitrogen fixation. Each blue-green algae species solves this problem in its own way, and many of the methods are poorly understood. The collaboration, which includes Livermore researchers Peter Weber, Jennifer Pett-Ridge, Stewart Fallon, and Ian Hutcheon, focused on the freshwater algae *Anabaena oscillarioides*, a species that separates the two processes into adjacent cells.

NanoSIMS allows researchers to map distributions of elements and isotopes to a resolution of 50 to 100 nanometers. The research results, published in the August 2007 issue of the *International Society for Microbial Ecology Journal*, demonstrate that the technique could effectively track the uptake and movement of carbon and nitrogen in two cell types in the algae: carbon-fixing vegetative cells and nitrogen-fixing heterocysts. “We can see cell by cell how newly fixed nitrogen is rapidly exported from the heterocysts to vegetative cells, keeping pace with the nitrogen demands of the growing and dividing vegetative cells,” says Weber. “Now, we can take these results and apply them to poorly understood species.”

Contact: Peter Weber (925) 422-3018 (weber21@llnl.gov).

Dusty mirror experiment inspires new research

A group of researchers at Lawrence Livermore and several American and European institutions have developed 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. An x-ray laser pulse directed at the target blows up the plastic sphere and then bounces off the mirror, allowing the researchers to look at the sphere after it explodes. The resolution for this experiment is greater than 3 femtoseconds. Light passing through the sphere combines with light bouncing from the mirror back through the object and causes interference, which forms a hologram, or three-dimensional image, of the object. With this setup, the team can study material dynamics under the extreme conditions created by an intense laser pulse, both during the pulse and as it turns into plasma.

“From previous work at FLASH, we know the target does not explode during the initial 25-femtosecond pulse, which forms the known reference wave of the hologram,” says Livermore physicist

Henry Chapman. “We can thus use the reference wave to determine the unknown object wave, which is actually the same object but a few femtoseconds later.”

The experiment design was inspired by Chapman’s visit to the Chabot Space and Science Center in Oakland, California. An optics exhibit at the science museum demonstrated Sir Isaac Newton’s dusty mirror experiment, in which Newton made one of the earliest observations of interference. Chapman realized that his group could create the same effect using laser pulses and x-ray mirrors. The research, which appeared in the August 9, 2007, edition of *Nature*, is part of a Laboratory Directed Research and Development project to develop the technique and determine the feasibility of single-molecule imaging experiments to be performed at Stanford’s Linac Coherent Light Source.

Contact: Henry Chapman (925) 423-1580 (chapman9@llnl.gov).

Each month in this space, we report on the patents issued to and/or the awards received by Laboratory employees. Our goal is to showcase the distinguished scientific and technical achievements of our employees as well as to indicate the scale and scope of the work done at the Laboratory.

Patents

Super-Hydrophobic Fluorine Containing Aerogels

Paul R. Coronado, John F. Poco, Lawrence W. Hrubesh

U.S. Patent 7,211,605 B2

May 1, 2007

An aerogel material with surfaces that contain fluorine atoms exhibits exceptional hydrophobicity, the ability to repel liquid water. Hydrophobic aerogels efficiently absorb solvents from water. Solvents miscible with water can be separated from the aerogel because they are more volatile than water. Thus, they enter the porous aerogel as a vapor across the liquid water–solid interface. Solvents that are immiscible with water are separated from it by selectively wetting the aerogel. The hydrophobic property is achieved by formulating the aerogel with fluorine-containing molecules. These molecules can be added directly during the solgel process or indirectly by treating a standard dried aerogel with the vapor of fluorine-containing molecules.

Method for Producing High Surface Area Chromia Materials for Catalysis

Alexander E. Gash, Joe Satcher, Thomas Tillotson, Lawrence Hrubesh, Randall Simpson

U.S. Patent 7,211,607 B2

May 1, 2007

This method includes nanostructured chromium(III) oxide–based materials using solgel processing and a synthetic process for producing such materials. Monolithic aerogels and xerogels with surface areas between 150 and 520 square meters per gram have been produced. The synthetic method uses stable and inexpensive hydrated chromium(III) inorganic salts and common solvents such as water, ethanol, methanol, 1-propanol, t-butanol, 2-ethoxy ethanol, ethylene glycol, dimethyl sulfoxide, and dimethyl formamide. A metal salt is dissolved in a solvent, and a proton scavenger, such as an epoxide, is added to induce timely gel formation. Both critical-point (supercritical extraction) and atmospheric (low-temperature evaporation) drying may be used to produce monolithic aerogels and xerogels, respectively.

Method for Characterizing Mask Defects Using Image Reconstruction from X-Ray Diffraction Patterns

Stefan Peter Hau-Riege

U.S. Patent 7,212,282 B2

May 1, 2007

This invention applies techniques for image reconstruction from x-ray diffraction patterns on the three-dimensional imaging of defects in extreme ultraviolet lithography (EUVL) multilayer films. The reconstructed image gives information about the out-of-plane position and the diffraction strength of the defect. The positional information can be used to select the correct defect repair technique. This invention enables the fabrication of defect-free (since repaired) x-ray molybdenum silicon (Mo–Si) multilayer mirrors. Repairing Mo–Si multilayer-film defects on mask blanks is a key for the commercial success of EUVL. During the fabrication process, particles are added to the Mo–Si multilayer film, and this contamination limits mask yields. All suggested repair strategies must account for the out-of-plane position of the defects in the multilayer.

Liquid Heat Capacity Lasers

Brian J. Comaskey, Karl F. Scheibner, Earl R. Ault

U.S. Patent 7,212,558 B2

May 1, 2007

The heat-capacity laser concept is extended to systems in which the heat-capacity lasing media is a liquid. The laser active liquid is circulated from a reservoir, where the bulk of the media and waste heat resides, through a channel configured for both optical pumping of the media for gain and for light amplification from the resulting gain.

Portable Convertible Blast Effects Shield

John W. Pastrnak, Rocky Hollaway, Carl D. Henning, Steve DeTeresa, Walter Grundler, Lisle B. Hagler, Edwin Kokko, Vernon A. Switzer

U.S. Patent 7,219,588 B2

May 22, 2007

A rapidly deployable portable convertible blast-effects and ballistic shield includes a set of two or more telescoping cylindrical rings to convert between a collapsed configuration for storage and transport and an extended upright configuration forming an expanded inner volume. One upright configuration provides shielding against such effects as blast pressures, shrapnel, and fireballs. A second upright configuration shields against ballistics such as incoming weapons fire and shrapnel. Each ring has a high-strength material construction such as composite fiber and matrix material that can substantially inhibit blast effects and projectiles from passing through the shield. The rings are connected with click locks.

Design and Fabrication of 6.1-Å Family Semiconductor Devices Using Semi-Insulating AlSb Substrate

John W. Sherohman, Arthur W. Coombs, III, Jick Hong Yee, Kuang Jen J. Wu

U.S. Patent 7,224,041 B1

May 29, 2007

An aluminum antimonide (AlSb) single-crystal substrate is used to lattice-match to overlying semiconductor layers. The AlSb substrate establishes a new design and fabrication approach to construct high-speed, low-power electronic devices with interdevice isolation. Such lattice matching between the substrate and overlying semiconductor layers minimizes the formation of defects such as threaded dislocations, which can decrease the production yield and operational lifetime of 6.1-angstrom (0.61-nanometer) heterostructure devices.

Remotely-Interrogated High Data Rate Free Space Laser Communications Link

Anthony J. Ruggiero

U.S. Patent 7,224,905 B2

May 29, 2007

This system remotely extracts information from a communications station by interrogating it with a low-power beam. Nonlinear phase conjugation of the low-power beam results in a high-power encoded return beam that automatically tracks the input beam and is corrected for atmospheric distortion. Intracavity, nondegenerate four-wave mixing used in the communication station of a broad-area semiconductor laser produces the return beam.

Microwave Hemorrhagic Stroke Detector**Waleed S. Haddad, James E. Trebes**

U.S. Patent 7,226,415 B2

June 5, 2007

The microwave hemorrhagic stroke detector is based on low-power pulsed microwave technology combined with specialized antennae and topographic methods. The detector includes a low-power pulsed microwave transmitter with a broadband antenna for producing a directional beam of microwaves, an index-of-refraction matching cap to place over the patient's head, and an array of broadband microwave receivers with collection antennae. The microwave transmitter and receiver system scans around a patient's head or up and down the axis of the head. The noninvasive device is designed to rapidly detect and localize pooling blood and clots, common indicators of hemorrhagic stroke, and to measure blood flow. The system can also be used to detect a hemorrhage within a patient's body.

Automated Macromolecular Crystal Detection System and Method**Allen T. Christian, Brent Segelke, Bernard Rupp, Dominique Toppini**

U.S. Patent 7,227,983 B1

June 5, 2007

This automated macromolecular system detects crystals in two-dimensional images, such as light microscopy images obtained from an array of crystallization screens. Edges are detected by identifying local maxima of a phase congruency-based function associated with each image. The detected edges are segmented into discrete lines, which are compared to identify crystallike qualities such as parallel lines, similarity in length, and relative proximity. This evaluation allows researchers to determine whether crystals are present in an image.

Speaker Verification System Using Acoustic Data and Non-Acoustic Data**Todd J. Gable, Lawrence C. Ng, John F. Holzrichter, Greg C. Burnett**

U.S. Patent 7,231,350 B2

June 12, 2007

This system for characterizing speech collects acoustic and nonacoustic data from a speaker as a method for speaker verification. The data are used to generate a first set of "template" parameters. A second set of parameters is generated using acoustic and nonacoustic data from a claimant's real-time identity claim form. The two sets are then compared to determine whether the claimant is the speaker. Both sets have at least one purely nonacoustic parameter, including a nonacoustic glottal shape parameter derived from averaging multiple glottal cycle waveforms.

Tamper to Delay Motion and Decrease Ionization of a Sample during Short Pulse X-Ray Imaging**Richard A. London, Abraham Szoke, Stefan P. Hau-Riege, Henry N. Chapman**

U.S. Patent 7,236,565 B2

June 26, 2007

In this x-ray imaging system, a tamper is connected to a sample, and short, intense x-ray pulses are directed onto the tamper and the sample. Through this process, an image is detected from the sample. The tamper delays the explosive motion of the sample when it is irradiated with the short, intense x-ray pulses, thereby extending the time to obtain an image of the sample's structure.

Compact Imaging Spectrometer Utilizing Immersed Gratings**Michael P. Chrisp, Scott A. Lerner, Paul J. Kuzmenko, Charles L. Bennett**

U.S. Patent 7,239,386 B2

July 3, 2007

This compact imaging spectrometer with an immersive diffraction grating compensates for optical distortions. An entrance slit transmits light to a device for receiving the light, which directs the light to an immersion grating. The immersion grating receives the light and directs it back to the receiving device, which transmits light to the detector array.

Radiation Detection Method and System Using the Sequential Probability Ratio Test**Karl E. Nelson, John D. Valentine, Brock R. Beauchamp**

U.S. Patent 7,244,930 B2

July 17, 2007

This system uses the sequential probability ratio test (SPRT) to enhance the detection of elevated radiation levels. The system determines whether a set of observations is consistent with a specified model within the limits of statistical significance. In particular, SPRT's processing mechanisms maximize the detection range by estimating the dynamic background radiation and adjusting the models to reflect this amount. The system then analyzes the current sample to determine the sample's statistical significance and determine when it has returned to the expected background conditions.

Trigger Probe for Determining the Orientation of the Power Distribution of an Electron Beam**John W. Elmer, Todd A. Palmer, Alan T. Teruya**

U.S. Patent 7,244,950 B2

July 17, 2007

This probe determines the orientation of electron beams being profiled. The probe is designed to accurately time the location of an electron beam by accepting electrons from a narrowly defined area. The signal produced is then used as a timing or triggering fiducial for a data-acquisition system. Such an arrangement eliminates changes in slit geometry, an additional signal feedthrough in the wall of a welding chamber, and a second timing or triggering channel on a data-acquisition system. As a result, the probe minimizes the adverse effects of current slit triggering methods and thus accurately reconstructs electron- or ion-beam orientations.

Video Surveillance with Speckle Imaging**Carmen J. Carrano, James M. Brase**

U.S. Patent 7,245,742 B2

July 17, 2007

When a surveillance system looks through the atmosphere along a horizontal or slanted path, turbulence along the path can cause blurring. The blurring is corrected by speckle processing short-exposure images recorded with a camera. The exposures are short enough to effectively freeze the atmospheric turbulence and thus improve the quality of the recovered images.

Awards

In September, *Science Spectrum* recognized two Laboratory scientists as top performers in their respective fields.

Dean Williams of the Computation Directorate received a **Senior Investigator Emerald Award**, which recognizes consistent leadership in advancing basic science knowledge or discovering, developing, and implementing entirely new technologies. Williams is deputy division leader for Computation's Biology, Atmosphere, Chemistry, and Earth Division and group leader for Atmospheric Science Computer Applications. In 2006, *Science Spectrum* honored him with a Trailblazer Award.

Kimberly Budil, who leads the Science, Technology, and Experiments Program in the Defense and Nuclear Technologies Directorate's B Division, received a **2007 Top Minorities in Science Trailblazer Award**. The Trailblazer Award honors minority men and women who create new paths for others in science, engineering, or technology; show leadership in their workplaces and communities; are role models and mentors; and demonstrate commitment to recruiting and retaining minorities in the nation's science and technology enterprises.

Livermore researcher **Nelson Max** of the Computation Directorate received the **Steven A. Coons Award for Outstanding Creative Contributions to Computer Graphics** given by the **Association for Computing Machinery Special Interest Group on Graphics and Interactive Techniques**.

The association presents this award every other year to honor an individual's lifetime contribution to computer graphics and interactive techniques.

Max, who is jointly appointed to the Laboratory and the University of California at Davis, was recognized for his work in pioneering scientific visualization, his extensive technical contributions, and his role in stimulating ideas and intellectual exchange in computer graphics. His research focuses on realism in nature images, molecular graphics, computer animation, and three-dimensional scientific visualization.

The **U.S. Air Force** presented Livermore employee **Greg Simonson** with a **medal for Exemplary Civilian Service** for his efforts to help protect the nation's capital and surrounding region from terrorist attacks. Simonson is one of the few individuals outside the Department of Defense to receive this award. Simonson has worked on assignment in Washington, DC, since November 2006, serving as the senior scientist for the Counter-Chemical, Biological, Radiological, Nuclear, and High Yield Explosives Center for the Air Force District of Washington. In this role, he collaborates with various governmental agencies to advance science and technology in defending the region against terrorism. Prior to this assignment, Simonson served as a division leader in the Laboratory's Nonproliferation, Homeland and International Security Directorate.

Livermore's R&D 100 Award Winners

Laboratory researchers turned in another strong showing in the annual R&D 100 competition, winning five awards. Each year, *R&D Magazine* presents these awards to the top 100 industrial, high-technology inventions submitted to its competition. The noninvasive pneumothorax detector is a handheld device designed to detect a collapsed lung, which if not promptly diagnosed and treated, can cause death within minutes. The microelectromechanical system–based adaptive optics scanning laser ophthalmoscope will allow clinicians to image microscopic structures of the living eye and measure aberrations. The large-area imager provides mobile radiation detection and imaging, allowing investigators to locate and interdict illicit nuclear materials.

Livermore's *hypr* library of linear solvers is open-source software designed to process extremely large sets of linear equations, which often form the primary bottleneck to many large-scale computer simulations. Continuous-phase-plate optics is a precise system for fine-tuning the laser beam of kilojoule- and megajoule-class laser systems such as the National Ignition Facility.

Contact:

Roger Werne (925) 423-7302 (werne1@llnl.gov).

Simulating Electromagnetic Phenomena

A versatile code called EMSolve helps scientists understand and predict electromagnetic fields.

Also in November

- *Livermore researchers have developed multiplexed assays that simultaneously detect bacteria, viruses, and toxins.*
- *A powerful electron microscope provides resolution at the atomic level.*
- *Laboratory scientists lend their expertise on peaceful nuclear applications to their counterparts in other nations.*

Coming Next Month

Science & Technology Review
Lawrence Livermore National Laboratory
P.O. Box 808, L-664
Livermore, California 94551

PRSRT STD
U.S. POSTAGE
PAID
LIVERMORE, CA
PERMIT NO. 154

Printed on recycled paper.