Lawrence Livermore National Laboratory

Science & Technology REVIEW

March 2011

Lung Enzyme to Capture Carbon

Also in this issue:

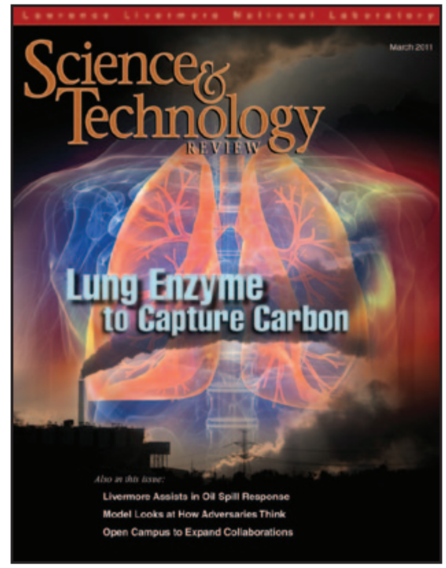
Livermore Assists in Oil Spill Response

Model Looks at How Adversaries Think

Open Campus to Expand Collaborations

About the Cover

Lawrence Livermore is collaborating with Babcock & Wilcox Company and the University of Illinois to create a molecule that mimics the behavior of carbonic anhydrase—a natural lung enzyme that transports carbon dioxide (CO_2) out of our blood. The article beginning on p. 4 describes the team's research, which is focused on making the synthesized molecule rugged enough to function under high pressures and temperatures. The project's goal is to use such catalysts in removing CO_2 from the flue gas of a coal-fired power plant. Replacing current scrubbing technologies with such an application could greatly increase the efficiency of the carbon-capture process. The artist's concept on the cover shows a human lung cavity above a typical power plant that emits greenhouse gases.



Cover design: George A. Kitrinos

About *S&TR*

At Lawrence Livermore National Laboratory, we focus on science and technology research to ensure 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 eight 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.

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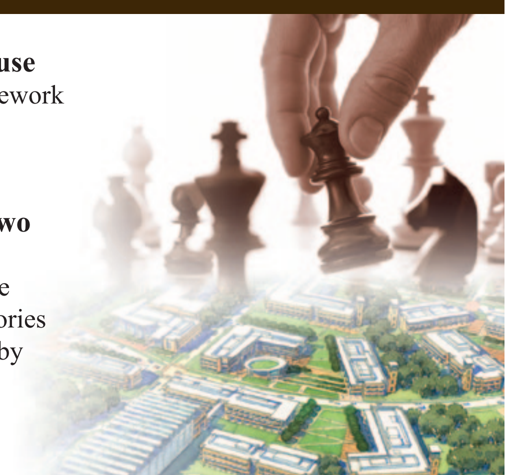

Departments

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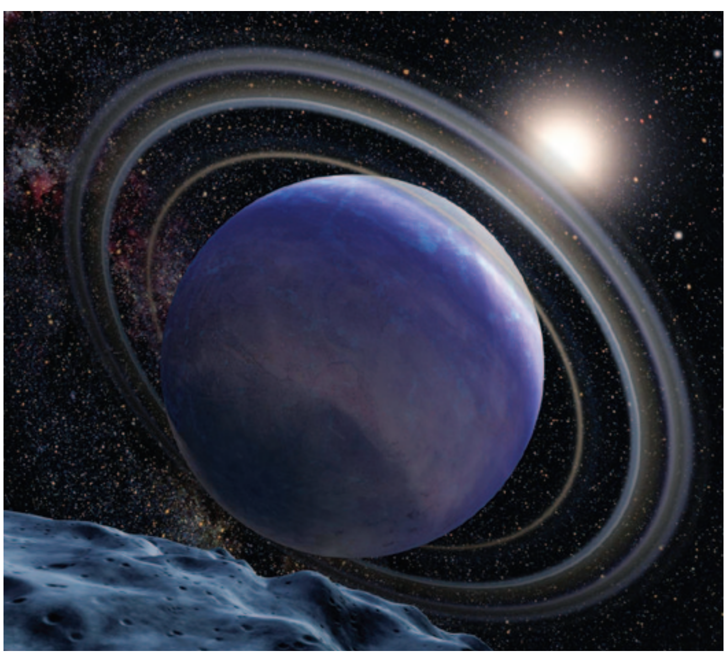
Fourth Planet Found in HR8799 Solar System

A research collaboration involving Livermore scientists has discovered a fourth giant planet in the HR8799 solar system—the first planetary system found to orbit another star other than our Sun. The new planet, dubbed HR8799e, is about seven times the mass of Jupiter. If it were orbiting the Sun, it would lie between Saturn and Uranus.

The research team, which also includes scientists from the National Research Council of Canada Herzberg Institute of Astrophysics, the University of California at Los Angeles, and Lowell Observatory, imaged the planet using high-contrast, near-infrared adaptive optics on the Keck II telescope in Hawaii. The team's results appeared in the December 23, 2010, issue of *Nature.*

Discovered in 2008, the HR8799 system is about 30 million years old, much younger than our 4.6-billion-year-old system. Although the giant system is much like ours, the combined mass of its four planets may be 20 times greater than that of the eight planets orbiting the Sun. In addition, the asteroid and comet belts in the HR8799 system are dense and turbulent. In fact, the massive planets pull on each other gravitationally, and the system may be on the verge of falling apart.

Livermore simulations of the system's evolution indicate that the three inner planets must travel on a clockwork schedule for the system to have survived this long. That is, the new planet must complete four orbits of the system's star in the exact time needed for the second planet to finish two orbits and the third planet to complete one. This behavior, first seen in the moons of Jupiter, had not previously been observed in such a large system.



According to Livermore astrophysicist Bruce Macintosh, the system's origin remains a puzzle. It follows neither the core-accretion model, in which planets form gradually close to stars where the dust and gas are thick, nor the disk fragmentation model, in which a turbulent planet-forming disk rapidly cools and collapses at its edges. "No simple model can predict all four planets at their current location," says Macintosh, the principal investigator for the Keck Observatory program. "It's a challenge for our theoretical colleagues to resolve."

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Arsenic Proves to Be a Building Block

A research team led by the National Aeronautics and Space Administration (NASA) and involving scientists from Livermore and the U.S. Geological Survey has found the first known living organism that appears to use arsenic in place of phosphorus in its major macromolecules. The findings, published in the December 2, 2010, issue of *Science,* could redefine origins-of-life research and alter the way scientists describe life on Earth.

Oxygen, carbon, hydrogen, nitrogen, sulfur, and phosphorus are the basic building blocks of life. These six elements make up nucleic acids, proteins, and lipids—the bulk of living matter. Results from the NASA collaboration indicate that a strain of Gamaproteobacteria isolated from California's Mono Lake may sustain its growth by substituting arsenic for phosphorus.

Mono Lake is an alkaline and hypersaline lake with high concentrations of dissolved arsenic. Researchers estimate the lake formed more than 760,000 years ago from neighboring volcanic eruptions. In the NASA study, researchers mixed lake sediment samples with a culture medium that had reduced phosphorus levels. The Livermore team then analyzed the samples using NanoSIMS, the Laboratory's nanometer-scale secondary-ion mass spectrometer. When the cultures were fed a steady supply of phosphorus along with other necessities, they produced flourishing colonies of the bacterium cells, as expected. However, when researchers removed the phosphorus and replaced it with arsenic, the microbes continued to grow. Subsequent analyses suggested that the arsenic was being used to produce the building blocks of new cells.

"The organism tolerated the heavy metal concentrations found in Mono Lake," says team member Jennifer Pett-Ridge, a scientist in Livermore's Physical and Life Sciences Directorate. "Arsenic is right below phosphorous on the periodic table, so this bacterium may have found a way to substitute arsenic for phosphorous in its biological makeup."

Pett-Ridge cautions that the team has yet to establish how the organism uses arsenic as a building block when it is a poison to most other life forms. The next step is to conduct protein biochemistry to determine if specific enzymes help transport arsenic into the cells.

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(*continued on p. 28*)

Serving the Nation as a Broad National Security Laboratory

OUR Laboratory was established in 1952 with a core mission: to advance nuclear weapons science and technology. But that was not our only focus. Fusion energy research was also part of our charter. Over time, our mission focus has continued to broaden. We've anticipated and developed innovative solutions to changing national needs by applying advanced capabilities that stem from the Laboratory's nuclear weapons mission. In the 1970s, for example, we grew energy and environmental programs and launched a biological research program that evolved into the Department of Energy's pioneering efforts to sequence the human genome.

Today, while our foremost responsibility remains ensuring the safety, security, and effectiveness of the nation's nuclear deterrent, we serve as a broad national security laboratory. Livermore's multidisciplinary approach to problem solving is well suited to tackling the complex issues that affect national security and global stability in the 21st century. Our portfolio of work includes nuclear security, international and domestic security, and energy and environmental security. The projects we engage in—often in collaboration with research partners—take full advantage of the Laboratory's expertise in wide-ranging scientific and engineering disciplines and our unique research capabilities.

The article beginning on p. 4 features a high-performance computing project to explore improved methods for reducing the carbon dioxide emitted by coal-fired power plants. In a collaboration with industry and academia using the Laboratory's supercomputers, researchers are simulating the performance of various molecules to find candidates that emulate the properties of the enzyme carbonic anhydrase—a natural catalyst found in our lungs. The most promising candidate molecules are synthesized for more extensive laboratory testing to determine if they can be adapted to capture carbon dioxide from flue gases before it reaches the atmosphere.

Livermore's wide-ranging expertise also draws us into a broad range of activities of national importance. A recent example, described in the article beginning on p. 10, is the technical support provided by the Laboratory following the explosion of the Macondo oil well in the Gulf of Mexico on April 20, 2010. Secretary of Energy Steven Chu offered the expertise of Lawrence Livermore, Los Alamos, and Sandia national laboratories to help in the effort to contain the spill and cap the leaking well. All three laboratories provided technical staff for 24-hour coverage at the BP crisis center in Houston, Texas, as well as significant "home team" scientific efforts. At Livermore, up to 60 scientists and engineers engaged in the assistance efforts.

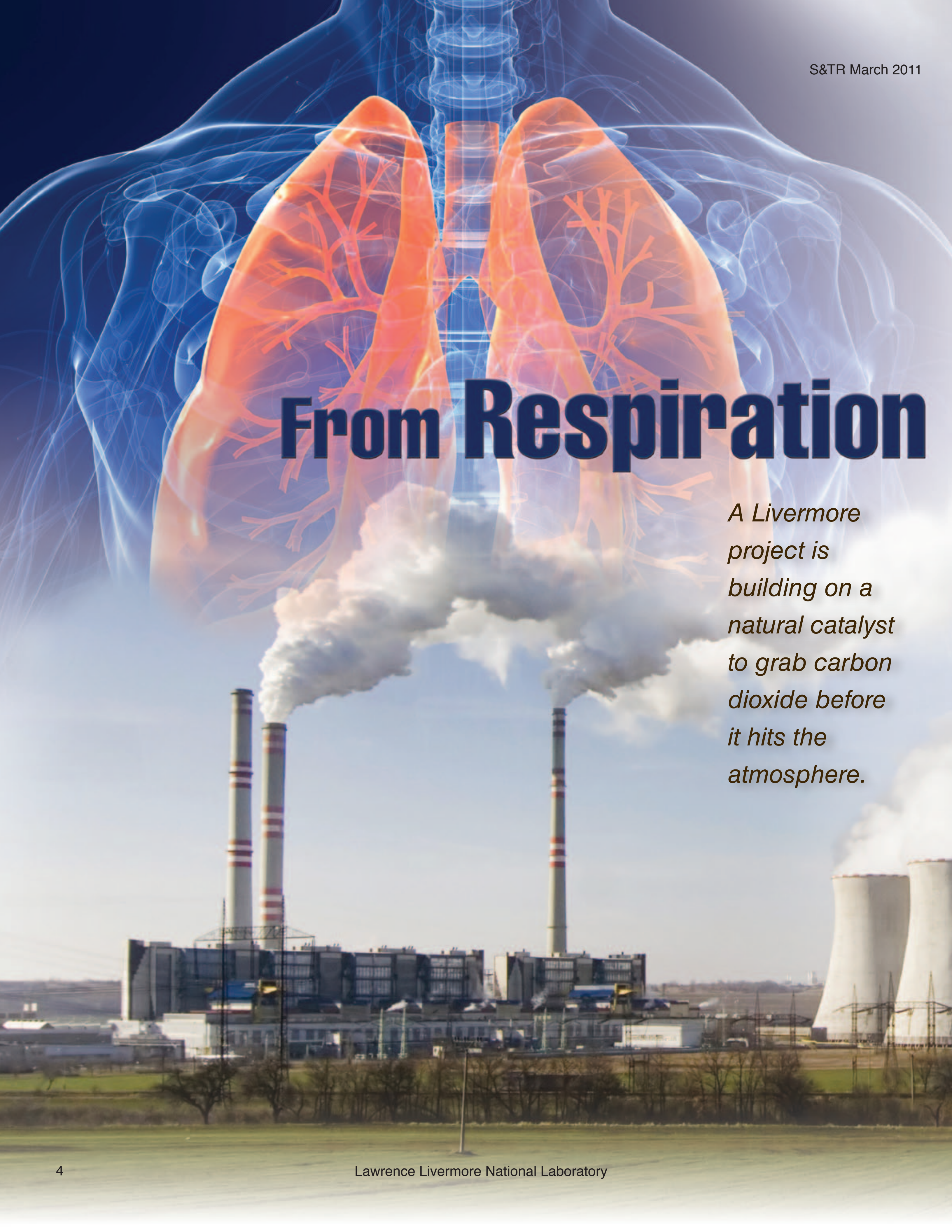
The Laboratory's expertise in areas such as computer simulations, engineering, and diagnostics proved vital for addressing flow, capture, and containment issues. BP came to value the technical competence, problem-solving abilities, and alternative viewpoints offered by the national laboratory teams. In the process, we developed effective working relationships with BP engineers, experts from other oil companies, and government agencies such as the U.S. Geological Survey and the National Oceanic and Atmospheric Administration.

Livermore scientists are also developing innovative computer modeling systems that process decisions as we humans do, by recognizing and adapting to changes in our environment. In this project, which is discussed in the highlight beginning on p. 18, the team's goal is to use these systems to analyze adversarial relationships that threaten security.

As these articles show, the Laboratory's outstanding technical staff offers the nation a wide range of resources and technology whether they are needed to assist in disaster response or are directed toward solving important national security problems. To expand such activities, we are strengthening our many current partnerships and developing new ones with other work sponsors and collaborators in academia and industry. As part of this effort, Lawrence Livermore and Sandia are developing the Livermore Valley Open Campus (LVOC) on 110 acres of contiguous land adjoining the southeast corner of Livermore's main site and the northeast corner of Sandia's California site. The highlight beginning on p. 22 details the plans for LVOC, which will build on the two laboratories' existing programs and strengths.

We are excited about our future as a broad national security laboratory and the opportunities LVOC will create. By increasing collaborations with the talented minds in industry and academia, we can continue to develop innovative technologies that strengthen national security, help to improve international relationships, and ensure that the U.S. maintains its economic competitiveness.

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



From Respiration

A Livermore project is building on a natural catalyst to grab carbon dioxide before it hits the atmosphere.

to Carbon Capture

OUR lungs separate, capture, and transport carbon dioxide (CO_2) out of blood and other tissues as part of the normal respiration process. The catalyst that initiates this natural response in the lungs is carbonic anhydrase, the fastest operating natural enzyme known.

Other enzymes play an "energy" role in our bodies as well. For example, ribulose-1,5-bisphosphate carboxylase oxygenase, more commonly known as RuBisCO, catalyzes the first major step of carbon fixation. In that process, molecules of atmospheric CO_2 are made available to organisms in the form of energy-rich molecules such as glucose. Methane monooxygenase, or MMO, oxidizes the carbon–hydrogen bond in methane.

Medical researchers have used these enzymes as guides for designing synthetic catalysts that speed up chemical reactions. Now, a collaboration led by Lawrence Livermore is examining carbonic anhydrase as the basis for a new molecule that does for coal-fired power plants what the enzyme does for our bodies: quickly separate CO_2. But instead of transporting it out of blood or tissue, the catalyst will remove the greenhouse gas before a power plant emits it to the atmosphere. (See box on p. 7.)

"Developing a synthetic molecule to replace CO_2 scrubbing processes that use amines could greatly speed up carbon capture," says geochemist Roger Aines, the principal investigator for the catalyst project. "Current analysis indicates that efficient catalysts might increase the capture rate for CO_2 separation by as much as 1,000 times."

It Takes a Team

In 2010, the collaboration, which involves researchers from Lawrence Livermore, Babcock & Wilcox Company, and the University of Illinois, received funding from the Department of Energy's Advanced Research Projects Agency–Energy (ARPA-E). The team's goal is to develop robust, small-molecule catalysts that mimic the behavior of carbonic anhydrase and can be adapted to capture CO_2 from power-plant emissions.

Each institution brings different expertise to the three-year project.

Computational biologists and synthetic chemists in Livermore's Physical and Life Sciences Directorate are working with the Laboratory's powerful supercomputers to computationally design hundreds of molecular compounds and synthesize the most-promising candidates for laboratory testing. Babcock & Wilcox's Power Generation Group, a leading supplier of steam-generation and environmental equipment for the electric utility market, will provide benchtop and full-scale testing and process modeling to determine which molecules can be implemented in existing and new processes. The University of Illinois will design and fabricate specific applications for the catalysts selected.

Before the ARPA-E project began, Livermore was already working on methods to design and synthesize such a catalyst through Laboratory Directed Research and Development funding. Results from this early effort showed that key technologies must be improved for global air-capture systems to be feasible. In particular, researchers must speed up the chemistry of the CO_2 removal process to keep the capture device to a manageable size. If a new molecule is tough enough, it might also enable the direct capture of CO_2 from such emission sources as airplanes and home heating systems.

Supercomputers Aid the First Steps

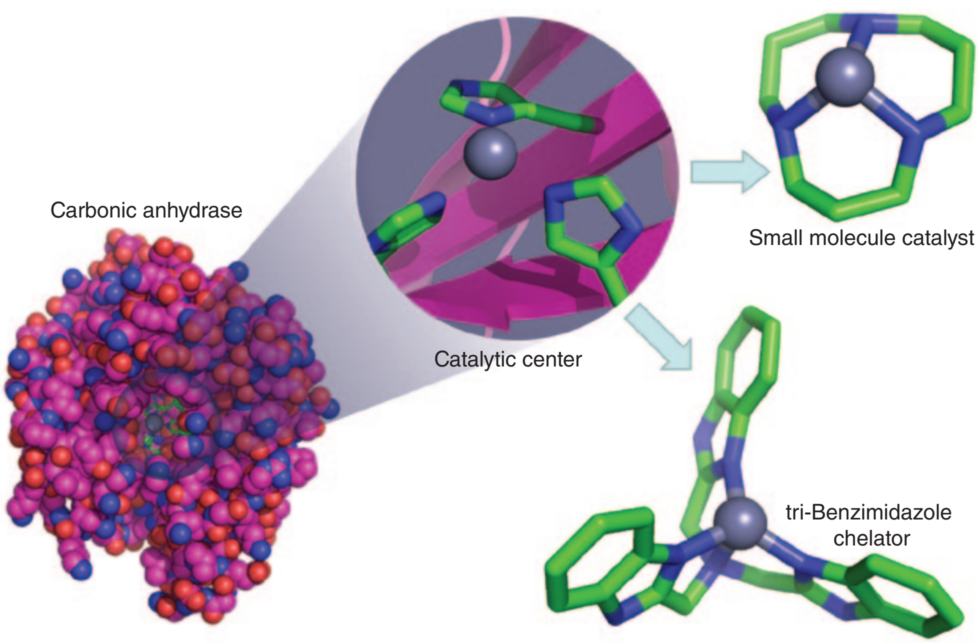
Experiments by others show that adding a carbonic anhydrase enzyme to CO_2 interactions dramatically enhances the kinetics of carbon capture. In the ARPA-E project, researchers want to modify the enzyme, making it less chemically complex than the native protein and better able to withstand the high pressures and temperatures of the flue gas from a coal-fired power plant.

Felice Lightstone, a computational biologist at Livermore, is leading the initial effort to evaluate potential candidates. "We are developing a computational library of molecules, all of which are designed to protect the zinc ion that activates the catalyst," says Lightstone. "Using quantum molecular calculations, we can experiment with different configurations, placing nitrogen atoms at various angles and distances from the zinc. The idea is to build scaffold structures that protect the metallic ion in a power plant's harsh operating environment and optimize the molecule for capturing CO_2." The computational team, which includes Sergio Wong, Lawrence Fellow Yosuke Kanai, and Donghwa Lee, also examined cobalt as a replacement for zinc but found it to be less effective in many configurations.

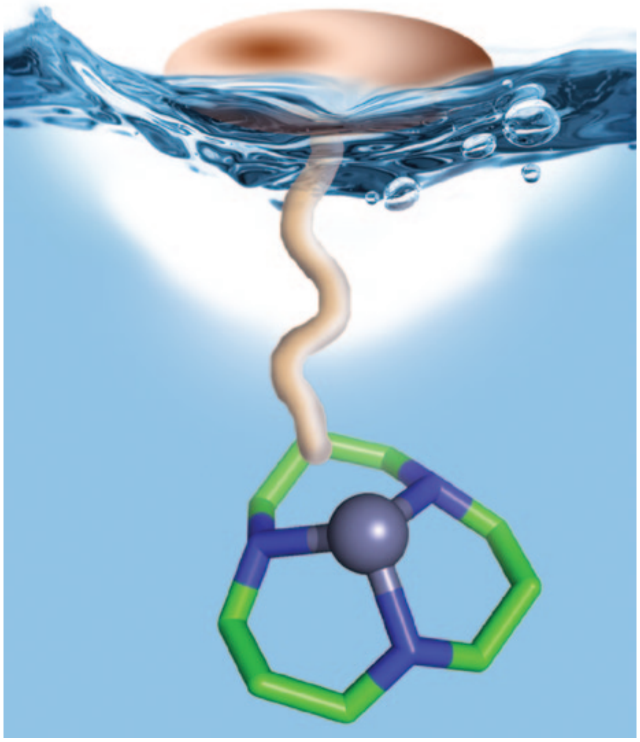
Quantum molecular calculations can predict activity at the electronic scale—a dimension comparable to about 1/50,000 of a slice of human hair—allowing scientists to examine processes occurring at dimensions that experiments often cannot create. Kanai and Lee are applying density functional theory (DFT) to model the atomic motion and complex dynamics of each candidate's material interactions. DFT starts from first principles. That is, it uses the laws of quantum mechanics without any ad hoc assumptions to describe the electronic density of a molecular or condensed system.

Kanai notes, however, that at the scale of molecular vibrations, chemical reactions are rare events. A simple application of first-principles molecular-dynamics simulations does not allow researchers to investigate reaction kinetics, which largely determine catalytic reactivity. "To address this challenge, we interface DFT with other computational tools such as the 'nudged elastic band' and 'string' methods to locate the reaction coordinates and obtain the reaction barrier."

The ARPA-E team is examining two possible molecular designs. One is a relatively simple dissolved catalyst system that could be applied immediately in industrial practice. This technology, known as regenerable solvent absorption technology, or RAST, is being developed largely by Babcock & Wilcox. The second, a Livermore design, is a "tethered" molecule that holds the catalyst at the air–liquid interface where the CO_2



Chemical scaffolds are designed to protect the zinc ion in carbonic anhydrase, which is critical for capturing carbon dioxide (CO_2).



"Tethered" molecules, such as the model shown at left, will cling to the gas–water interface much as mosquito larvae (above) hang from the surface of still water. (Photo courtesy of James Gathany, Centers for Disease Control and Prevention.)

transfer typically takes place. The tethered molecule looks much like mosquito larvae floating just below the surface of water. This approach promises very high efficiency, but using it in power plants may require changes in industrial practices.

Challenges to Overcome

Several challenges remain to make the synthetic catalysts suitable for a commercial CO_2 capture process. First, the molecular scaffolding must be structurally stable to preserve the metal ion in the catalytic pocket under high temperatures and pressures.

Addressing structural robustness and fast catalytic rates would normally be a slow, expensive process. Because of Livermore's computational and synthetic chemistry capabilities, the ARPA-E team can quickly evaluate hundreds of candidate compounds computationally, synthesize dozens, and test the most promising ones in the laboratory. Aines estimates that in just two years, the team will be ready to conduct long-term stability experiments

Keeping Carbon Dioxide Out of the Atmosphere

About 50 percent of electricity consumed in the U.S. comes from coal-fired power plants. In 2006, these plants accounted for 83 percent of the carbon dioxide (CO_2) emitted during the process of electricity generation. Capturing CO_2 before it enters the atmosphere could have enormous environmental benefits, yet to date, no CO_2-capture technology has advanced to the demonstration phase. The costs for the postcombustion process are still very high at about $60 per ton of CO_2, and precombustion capture technology has stalled because of increasing capital costs to retrofit or redesign power plants.

The current method for CO_2 removal involves scrubbing the flue gas with amines, or nitrogen compounds, but this process uses copious quantities of water to heat and cool the gas. The energy required to strip CO_2 from the amine solvent is as much as 2.1 billion British thermal units per hour (or more than 0.6 gigawatts). "Considering additional equipment such as pumps, fans, and heat, we estimate that an optimal scrubbing system consumes 15 percent of the energy produced by the power plant," says Livermore geochemist Roger Aines.

And coal-fired power plants are just one of many facilities that emit CO_2 to the atmosphere. Natural gas plants, refineries, steel mills, cement plants, even home heating appliances produce this greenhouse gas. Substantially increasing the rate of CO_2 separation would reduce the size and cost of industrial processes designed to reduce CO_2 emissions.

For years, researchers have considered adapting the natural CO_2 lung catalyst carbonic anhydrase to capture carbon emitted in industrial operations. "An effective catalyst would make the separation process much more efficient," says Aines, "although at this point we can't project how much energy could be saved." The limiting factor with carbonic anhydrase is the difficulty of maintaining a viable enzyme in the intense conditions of industrial processes. Because hot, high-pH flue gas quickly degrades the molecule, modifying the catalyst to make it more robust is essential.

Livermore chemist Carlos Valdez synthesizes molecules based on the elemental structures proposed by the computational team. Thus far, only a few have offered the structural stability and ease of construction that would make them candidates for CO_2 capture.

on candidate molecules in large-scale testing facilities.

In addition, catalysts for the tethered molecule design must remain within about 100 micrometers of the gas–water interface, where they are most effective. If the catalyst is distributed throughout the solvent, more of it must be produced overall. The team is investigating an approach that adds a hydrophobic molecule to tether the molecule at the gas–water interface. Livermore's preliminary calculations show that such tethers do not deform the catalyst and should preserve full functionality. Another design possibility uses very small particles containing the catalyst on their surface. These particles move with the solvent and can be easily extracted before thermal desorption.

As candidate molecules move closer to commercialization, team members at Livermore and Babcock & Wilcox will work together to balance the cost of catalyst production with the molecule's expected lifetime. "For now, we are estimating that a catalyst will live at least a few days, possibly longer," says Aines. "Surviving the high temperature is the greatest challenge in designing an effective catalyst and will be the limiting factor with this technology."

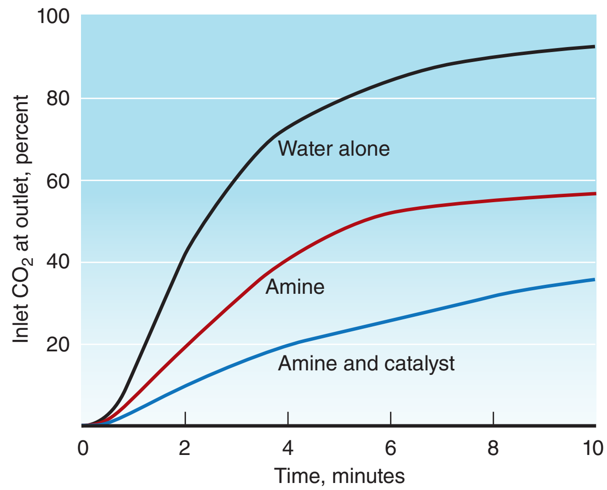
Molecules Made to Order

Synthetic chemist Carlos Valdez notes that the desired catalyst must be easily assembled in a concise operation. A reaction scheme should involve two to five steps to keep costs down and facilitate commercialization. The catalyst's structure must also be amenable to further chemical enhancement so that properties such as solubility, thermal stability, surface attachment, and efficiency can be improved when necessary.

For this project, Valdez is applying what he learned during his postdoctoral research at the Scripps Research Institute under K. Barry Sharpless, who in 2001 won the Nobel Prize in Chemistry. Sharpless is the father of "click chemistry," a process designed to speed up drug discoveries by building chemical libraries and rapidly screening them for molecules with a desired activity. Click chemistry changed the search for effective drug formulas from a needle-in-a-haystack operation, in which numerous attempts led to only a few successes, into a winnowing process that more quickly identifies a successful candidate.

The ARPA-E researchers want to achieve a similar advance with their combinatorial approach. Their goal is to ensure that each reaction in the multistep synthesis process is fast, efficient, and highly predictable. "The computational aspect of the project involves arbitrarily shuffling and arranging atoms around the metal center," says Valdez. "For the

Chemists Roger Krueger (left) and Sarah Baker operate the wetted wall apparatus. This Livermore-designed test device measures the combined rates of all chemical and mass-transfer processes, including the concentration of CO_2 being vented.



Initial experiments indicate that adding the carbonic anhydrase enzyme would dramatically reduce the amount of CO_2 emitted during the combustion process compared with the amount captured with scrubbing processes that use only amine or water.

synthetic chemistry phase, I use an array of scaffolds that have been developed without regard for their linkage stability or synthetic tractability."

Combinations that are not stable or would require an extensive construction process are eliminated from the list of candidates for synthesis. Only about 2 percent of the computationally derived scaffolds have made it to the synthesis stage, which is currently under way.

Synthesized molecules go through two tests, run by Livermore chemist Sarah Baker, to evaluate how well the candidates actually work. In the first test, a stopped-flow spectrophotometer determines a candidate's absolute hydration kinetics and stability. The spectrophotometer heats the dissolved catalyst to 80°C and mixes it with CO_2 gas in less than 500 microseconds. The color of the resulting solution indicates the rate of CO_2 capture. In the second test, a wetted wall apparatus built at Livermore measures the combined rates of all chemical and mass-transfer processes, including the concentration of CO_2 emitted by the operation.

The Process Continues

The feedback loop is constant. If a candidate cannot be synthesized, the computational team will take another look at its molecular structure. If laboratory tests are unsuccessful, similar analysis may reveal the problem. "We currently have a 'map' showing the expected performance of hundreds of structures based on each one's bond length and angle around the zinc atom," says Aines. "We've also synthesized 16 candidates, including 6 molecules previously identified."

Even when combinations of bond length and angles cannot be synthesized, computational methods such as click chemistry allow the team to consider options more quickly. "We originally thought we could synthesize five new molecules a year," says Aines. "By combining advanced computation and experimental tools, we now expect to test up to 20 specific examples a year. The synergy exhibited in our team's multidisciplinary approach is critical to our success."

Aines notes that one day, the technology could be fast enough to remove CO_2 directly from the atmosphere. Until then, researchers will focus on capturing this greenhouse gas at the source—removing it from the numerous industrial processes we rely on every day.

—Katie Walter

Key Words: carbon capture, carbon dioxide (CO_2), carbonic anhydrase, density functional theory (DFT), greenhouse gas.

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Lending a Hand to an

Livermore experts joined the international effort to end the

ON April 20, 2010, oil, gas, and cement exploded from the borehole of BP's Macondo oil well on the seafloor of the Gulf of Mexico, igniting the floating drilling rig Deepwater Horizon. The tragedy cost 11 crew members their lives, and the raging fire was quenched only when the rig eventually collapsed and sank. The well was, by then, leaking oil into the deep waters of the Gulf. Within days, Livermore scientists and engineers joined what became an international effort to plug the well and address the environmental damages caused by the massive spill, applying their expertise in engineering, modeling, and diagnostics to the largely unfamiliar arena of undersea oil-well technology.

The Laboratory's contributions to the response involved a short-term atmospheric modeling effort and a longer

Oily Problem

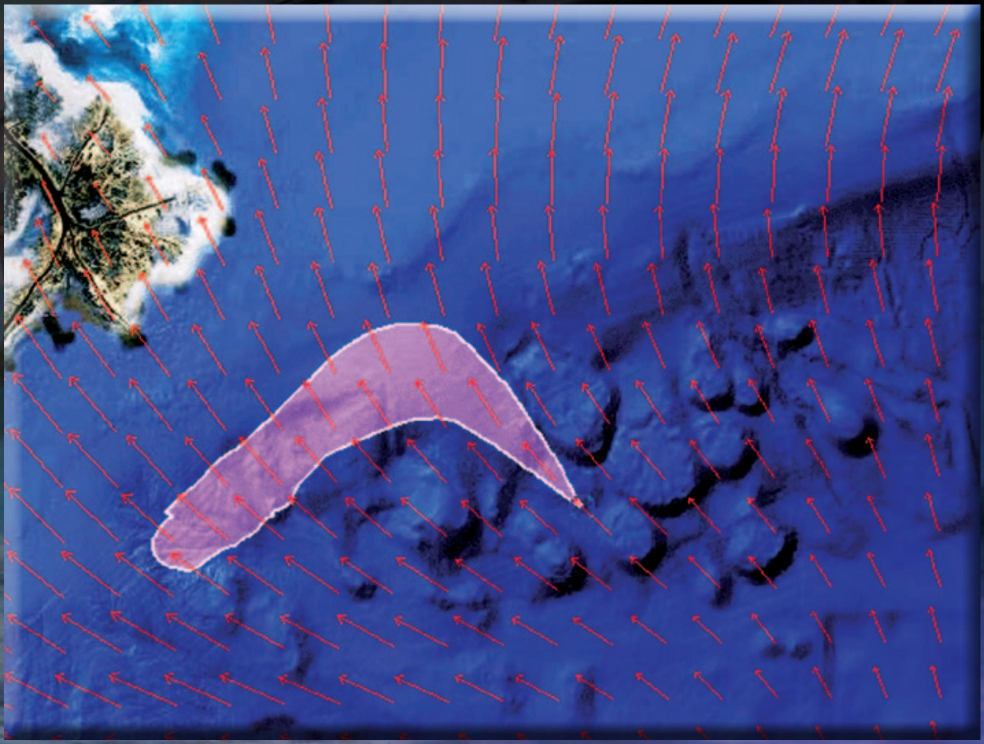
largest-ever undersea oil spill.

effort to provide technical capabilities and peer review to the U.S. Coast Guard–led endeavor to plug the leak. The Department of Homeland Security's Interagency Modeling and Atmospheric Assessment Center (IMAAC) provided plume predictions of the April 23 fire on the Deepwater Horizon oil platform. The National Atmospheric Release Advisory Center at Livermore, which serves as the IMAAC operations hub, forecast the particulates that might be released from planned surface-oil test burns—one of several methods used to remove spilled oil from the Gulf. The center predicted the extent of particulate dispersal and the areas in which air-quality standards might be exceeded.

A week after the explosion, Secretary of Energy Steven Chu, at the direction of President Barack Obama, asked the national laboratories to quickly come up with ideas for spill mitigation and environmental remediation. He also requested that Sandia, Los Alamos, and Lawrence Livermore national laboratories send personnel to BP's crisis center in Houston, Texas, to assist with response efforts. (See the box on p. 13.)

Thus began a sustained advisory and technical support role for the three laboratories, both at the crisis center and back at their home sites. Working with BP, other oil companies, and government agencies such as the U.S. Geological Survey and the National Oceanic and Atmospheric Administration, the three laboratories drew on their expertise and experience in areas such as diagnostics and fluid dynamics to support work to stop the oil leak.

The leak was securely capped on July 15, 2010, and on September 19, operations at the well site were successfully completed. Retired Coast Guard Admiral Thad Allen, who had overseen spill containment and mitigation,



Results from a computer model run by the National Atmospheric Release Advisory Center show the projected dispersal of smoke plumes from a surface-oil burn in the Gulf of Mexico. (Background map courtesy of Google.)

declared the well "effectively dead." From late April until September, up to 60 Livermore engineers and scientists provided oil-spill analysis and assistance under the coordination of Rob Sharpe, the deputy associate director for Science and Technology in Livermore's Engineering Directorate. Los Alamos and Sandia provided comparable technical expertise.

"Support from the three labs focused on flow, capture, and containment," says Sharpe. "We soon demonstrated that the labs could offer expertise and technology that were not in general commercially available to the drilling industry." Bruce Warner, who led the Livermore task force assigned to assemble technical resources to aid the oil-spill effort, says, "Very quickly, it became clear that the national labs had the technology necessary to help. It was basically a self-selection process."

Into the Deep

Two major challenges throughout the crisis were the undersea location of the well and the dearth of information about the leak site and flow rate. Julio Friedmann, a geoscientist who serves as deputy program director for Energy and Environmental Security in Livermore's Global Security Principal Directorate, says, "The Macondo well environment was inhomogeneous, and characterizing the geology near the surface of the seafloor was complicated." Without understanding characteristics such as the effects of stress on rocks in the upper 200 meters of the oil well, scientists had to eliminate the more daring proposals, such as using

Fireboat crews battle the blazing remnants of the offshore oil rig Deepwater Horizon on April 21, 2010. An explosion in the Macondo well led to the catastrophic rig fire and oil leak. (Courtesy of U.S. Coast Guard.)

explosives to collapse the well casing. Detailed geologic information about the oil reservoir and seafloor topography was also often unavailable. Compounding the problem was that the blowout likely changed the conditions of the drilling structures and rocks around the well bore.

Even with thorough documentation and complete information, performing repairs on an oil well located under 1,500 meters of water posed enormous challenges. At this depth, water temperature is nearly freezing, and its pressure is about 17 megapascals—enough to compress a basketball to the size of an orange. BP used remotely operated vehicles (ROVs), which Sharpe describes as "relatively crude robots," to acquire videos of the leaking well and perform most undersea operations.

Attached to ships by umbilical cables and controlled by operators onboard, the robots moved extremely slowly and, with their large claws, could perform only basic grasping and twisting maneuvers. Underwater activities were further limited by the robots' 8-hour power supply and 140-kilogram lifting limit. "Operators might spend 15 minutes making the robot pick up a socket wrench, put it on a nut, and turn it," says Livermore engineer Bob Ferencz. "They called it 'undersea time.' BP had to have a lot of contingency plans for each action in case something went wrong, for example, if a nut was distorted."

Expertise in extracting information indirectly was crucial to understanding the state and stability of the well and its associated structures, how much oil was escaping the well, and where it was flowing. An early opportunity for the national laboratories was in helping BP diagnose the condition of the blowout preventer, a 20-meter-high mass of interconnected valves and piping that topped the oil well.

Blowout preventers are designed to close off a well should oil or gas uncontrollably rush to the top—precisely the sort of event that precipitated the explosion and leak. Because the preventer on the Macondo well did not activate, the Deepwater Horizon crew had to abandon the rig. Extending from the top of what Sharpe called "a giant spigot for oil" was more than a kilometer of collapsed piping that originally linked the well to the Deepwater Horizon at the surface. Now crumpled on the ocean floor, the piping was still connected at one end to the blowout preventer and had oil leaking from several spots.

Looking and Listening for Clues

Engineers needed to "see" inside the blowout preventer to determine why its five redundant valves did not sever the pipes and seal off the well. They also

At the Heart of Spill Operations

In addition to the "home team" scientific efforts at Lawrence Livermore, Los Alamos, and Sandia national laboratories, a small pool of scientists and engineers from the three laboratories worked shifts at the BP crisis command center in Houston, Texas. Twelve technical staff members traveled to Houston from Livermore, ensuring that at least one Laboratory representative was available daily, including weekends and holidays, from May to September. During a few key operations, the national laboratories' team maintained round-the-clock coverage at the crisis center.

Livermore engineer Scott Perfect became known as the Laboratory's Iron Man for volunteering the most time at the center. He saw his role and that of other personnel from the national laboratories as an intermediary. "We were in Houston conducting an orchestra at Livermore," says Perfect. "We were reaching back to our home organizations, supplying them with information so they could do their work and communicate the results back to us in Houston." Daily conference calls involving staff from the BP crisis center, national laboratories, and government agencies as well as Secretary of Energy Steven Chu ensured that all participants were well informed. Perfect notes that especially in the early stages, an essential part of his role was knowing the capabilities available at Livermore and the other national laboratories and recognizing opportunities where he could offer their resources. Livermore engineer Bob Ferencz, who also spent time in Houston, says, "It was an ongoing triage effort. We determined which issues had the highest priority and what lab could offer help on each one."

This role evolved significantly as BP came to appreciate the depth of knowledge and experience available from the national laboratories and as Secretary Chu extended their involvement. Laboratory personnel in Houston spent much of the summer assessing designs and ideas presented by BP scientists. They asked questions, drafted procedures, looked for reactions, previewed concepts, and facilitated reviews to evaluate designs and suggest the best next steps. Representatives from the three laboratories also provided updates on containment efforts to the Department of Energy and at times the White House. Diane Chinn, a division leader in Livermore's Engineering Directorate, notes that although the laboratories were rarely in a design role, they were vital in helping BP determine whether proposals for capping the well or collecting the oil would work.

Shifts at the crisis center were long, occasionally lasting more than 24 hours, and the stress level was high because of the disaster's scope and urgency. But Livermore team members were glad they had participated. According to Perfect, the atmosphere of cooperation held its own appeal. "I enjoyed working with the people from the other labs," he says. "We all shared the same sense of mission and duty."

wanted to assess the structure's baseline state before proceeding with plans to cap the well. Sharpe notes that despite the unwieldy size and thickness of the preventer, x-ray imaging would have been relatively easy aboveground. Underwater imaging was more challenging.

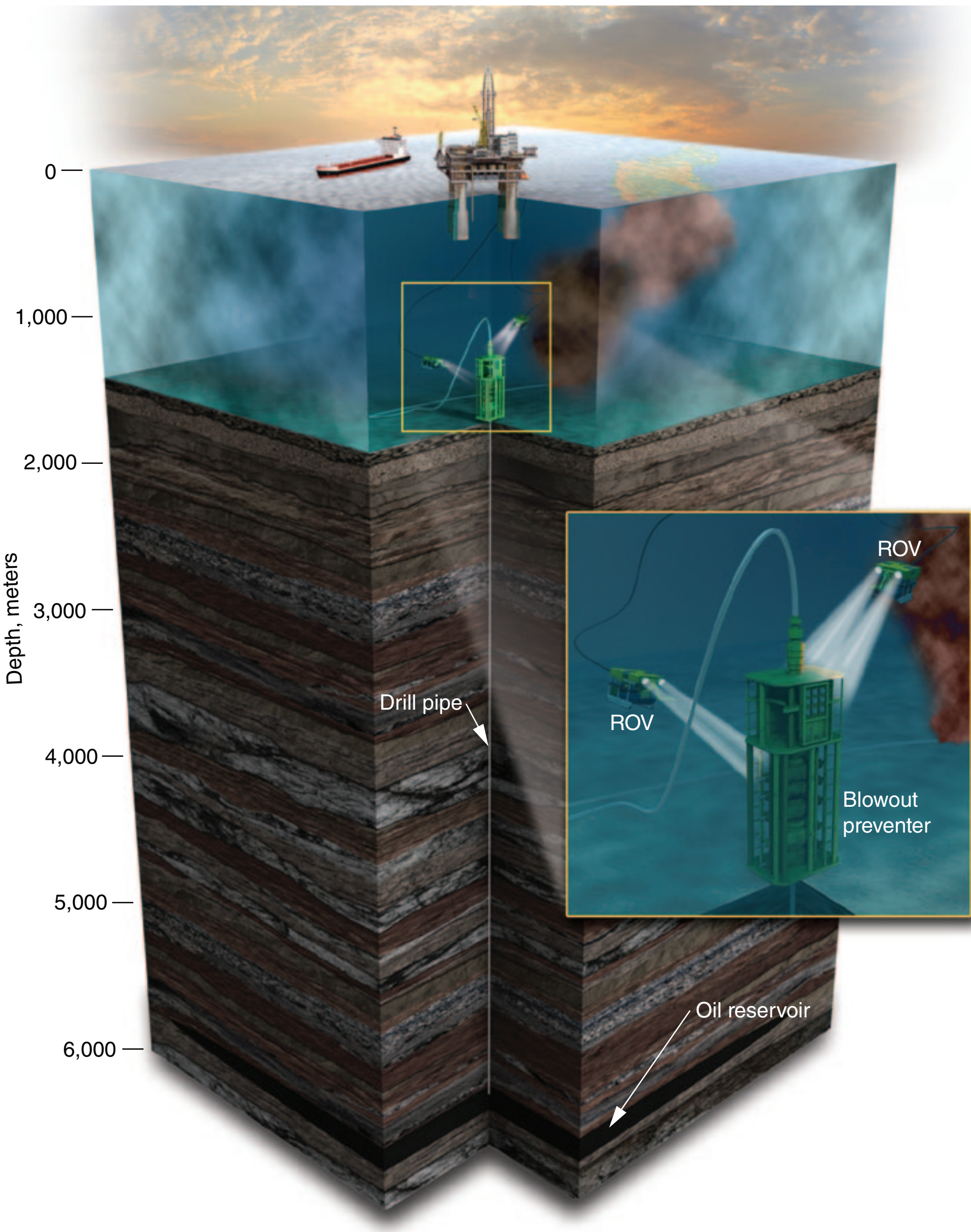
A Los Alamos team led by Scott Watson used gamma radiography to examine the blowout preventer. The operation involved placing a 1- × 10^9-becquerel source of cobalt-60 and a phosphor detector in water- and pressure-proof tubes. ROVs moved the detector and source into position underwater to image the valves in the device—the first time gamma-ray imaging had been successfully used at such a depth.

A Livermore team led by Maurice Aufderheide, a radiography expert in the Weapons and Complex Integration Principal Directorate, analyzed the resulting data. The team found that the preventer's internal valves were partially closed and somewhat restricting the flow of oil. Information from the imaging contributed to the decision to try sealing the leak with heavy drilling mud, an operation known as a "top kill."

When the top-kill operation failed, efforts turned to plugging the piping above the blowout preventer. This option, which proved successful, involved cutting the pipe and capping it. However, oil wells of this type are generally built with a number of nested pipes. Before the main pipe, or dogbone, could be cut, operators needed to know what was inside it.

The Los Alamos imaging team obtained radiographs of the bent, kinked dogbone, and analysis teams at Los Alamos and Livermore located interior drill pipes within it. As part of this effort, Ed Kokko, who works in Livermore's Engineering Directorate, converted a Sandia model of nested pipes into a model that used the Livermore hydrodynamics code ALE-3D. The conversion allowed Aufderheide to examine the images with HADES, a radiographic simulation code developed at Livermore. Aufderheide further analyzed the nested pipe geometries using models constructed with BRL-CAD, an open-source, computer-aided design system developed by the Army Research Laboratory.

BP also used acoustic scanning with commercial sensors to examine pipes and valves. Just as a doctor places a stethoscope on a patient, an ROV positioned a sensor against the piping at



This conceptual drawing shows the Macondo well, blowout preventer, and broken piping after the BP well exploded and the Deepwater Horizon drilling rig sank. BP's remotely operated vehicles (ROVs) were the sole source of real-time images from the underwater leak site and the primary devices for performing repair and containment work. (Rendering by Sabrina Fletcher.)

four points to "hear" what was going on inside the pipe just below the blowout preventer. "The three labs brought in experts to analyze those signals," says Sharpe. "We were looking for loose or moving pieces of metal and seeking to understand the conditions at the blowout preventer." Sean Lehman, Dave Chambers, and Karl Fisher, signal-processing experts in Livermore's Engineering Directorate, analyzed the data to diagnose the condition inside that area of the well.

In an ideal situation, ROVs would place sensors on multiple spots around a pipe and produce measurements simultaneously. However, because of constraints on time and ROV availability, BP could acquire only a snapshot of acoustic data. Even with the limited data, the engineers confirmed that a loose piece of metal was floating inside the pipe. Lehman credits the Laboratory's experience in processing raw signal and image data from various types of experiments with facilitating the imaging work at many stages of the oil-spill response.

BP's crisis command center in Houston, Texas, was called the HIVE because it offered a highly immersive visualization environment. From these consoles, command center staff controlled 40 to 60 ships and 12 to 16 ROVs during containment and oil-recovery operations. (Courtesy of BP PLC.)

For the modeling and analysis efforts, Livermore engineers and scientists worked in parallel with teams from Los Alamos and Sandia. Teams performed independently but sometimes discussed approaches during the process. Their results were then compared with those from BP's analyses. "BP didn't want us to just replicate their work," says Livermore engineer Scott Perfect. "They wanted fresh eyes and independent calculations from the labs."

Modeling a Giant Garden Hose

Another contribution by the three laboratories was to estimate the size of the Macondo well leak, using complementary techniques such as measurement, observation, particle velocimetry, fluid mechanics modeling, and imaging. Livermore engineer Diane Chinn led a team of image-processing and fluid mechanics experts who reviewed ROV-supplied images of the leak frame by frame and estimated the velocity of particles escaping the well.

Two other Livermore groups, one led by Roger Aines and Todd Weisgraber in conjunction with the National Energy Technology Laboratory and the other by Wayne Miller and Mark Havstad, performed independent fluids modeling and analysis to calculate the flow. Crisis response activities such as designing a cap for the well, predicting the extent to which oil would befoul Gulf wetlands, and determining how many ships were needed to collect oil depended on an accurate flow estimate from the leak. The measurement task, which would be quite straightforward on land, became an enormous challenge deep underwater.

According to Miller, a thermal fluids analyst in the Engineering Directorate, his group approached the flow-rate problem as if they were trying to determine the amount of water flowing from a garden hose that had a spigot at one end and a pressurized reservoir at the other. For this calculation, the team needed to know the size of the "hose" (in this case, the well), the pressure inside it, and the physical properties (viscosity and resistance) of the medium flowing through it, whether water or oil.

Unfortunately, the oil well was not simply one pipe stretching deep into the subsurface. As with the piping above the blowout preventer, the well contained a series of concentric pipes and casings that provided support and enabled drilling operations. To calculate the oil pressure and flow rate, engineers needed to determine whether oil was flowing only through the central oil string, a pipe less than 25 centimeters in diameter, or between the various piping and casing components, a condition known as annular flow.

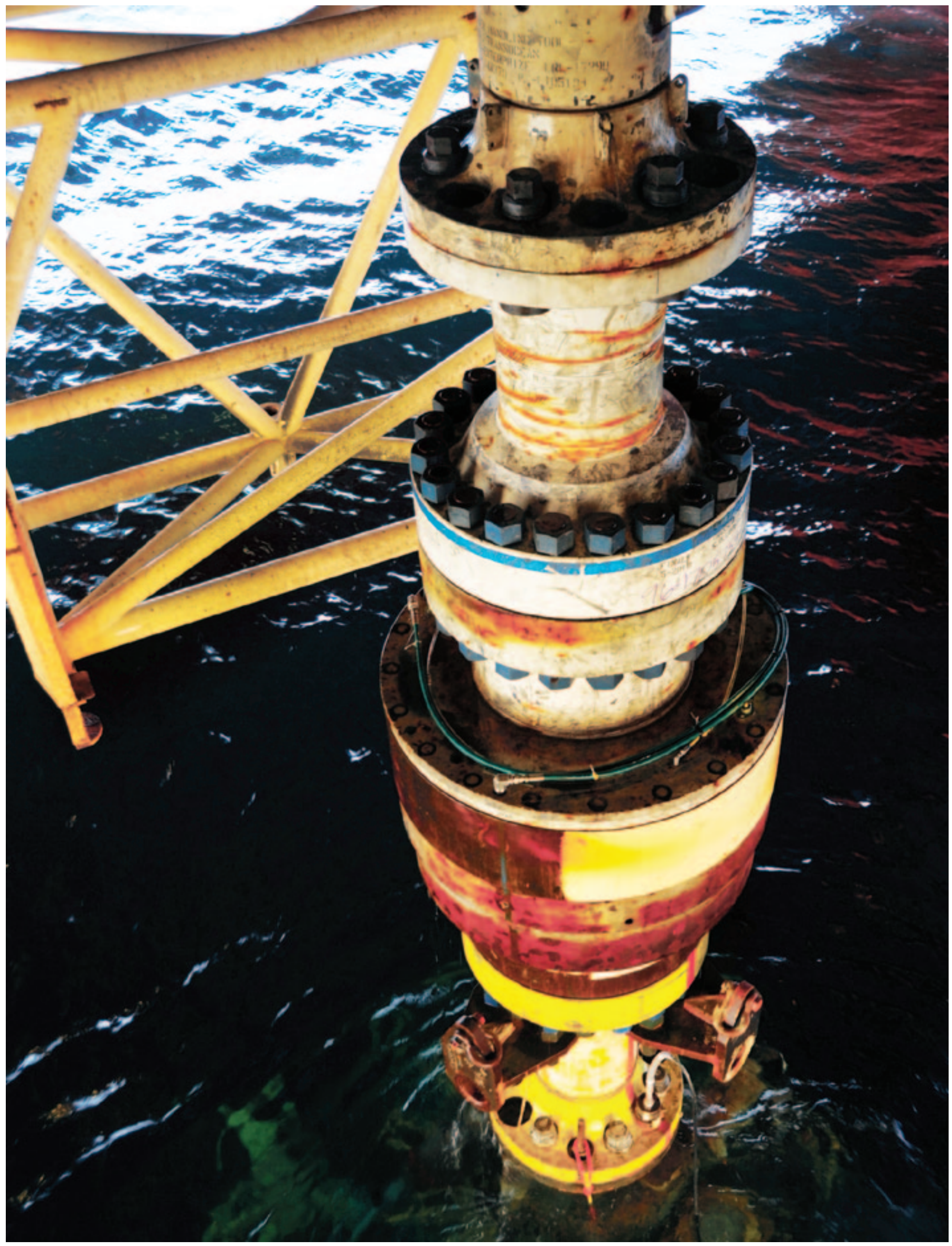
Several weeks before the explosion, BP engineers had measured the pressure in the oil reservoir, some 4,000 meters below the seafloor. At that time, it was about 83 megapascals, but the engineers knew it had dropped as oil continued to leak. Pressure at the entrance to the well pipe—a key area for creating an accurate flow model—depended on the quantity of reservoir sediments that the oil was flowing through to reach the pipe. During the early calculations, the pressure at the top of the well was also uncertain. Readings from the original gauge on the blowout preventer were suspect and eventually found to be inaccurate.

Complicating the calculations were the oil's physical properties. Deep underground, oil is hot and full of emulsified gas, a viscous mixture that Miller compares to carbonated water under pressure. As hot oil rises through the well and contacts the nearly freezing seawater, it cools, and its pressure gradually drops. In addition, the gas begins to bubble and separate from the liquid. Accounting for these two changing phases of material complicates calculations of oil density and flow rate.

In June, ROVs sliced off the bent pipe and installed piping to transport the escaping oil to the surface for collection. During this procedure, BP attached several pressure gauges to the new structure, to more accurately measure the pressure at the blowout preventer and the surface. Although engineers could now better understand the current pressure and flow rate, they still had to determine the past rate and the total overall because flow had not been constant. In fact, installing new structures, such as the oil-collection piping, increased the total pressure in the system.

At the same time, the reservoir was gradually being depleted, which reduced the pressure of oil entering the well piping. The U.S. Geological Survey estimated that pressure dropped from 83 to 34 megapascals during the three-month leak. Researchers now project that the flow rate decreased from 10,000 to 8,400 cubic meters (63,000 to 53,000 barrels) of oil a day over the duration of the spill, as the well was depleted and new structures were attached to the blowout preventer.

Engineers from the three laboratories developed estimates independently, refining calculations over time and adding new information as it became available. Ultimately, their results agreed within 10 percent. "We didn't have the luxury of writing journal articles," says Miller. "We needed quick, practical solutions, so we had to make flow calculations with incomplete information."

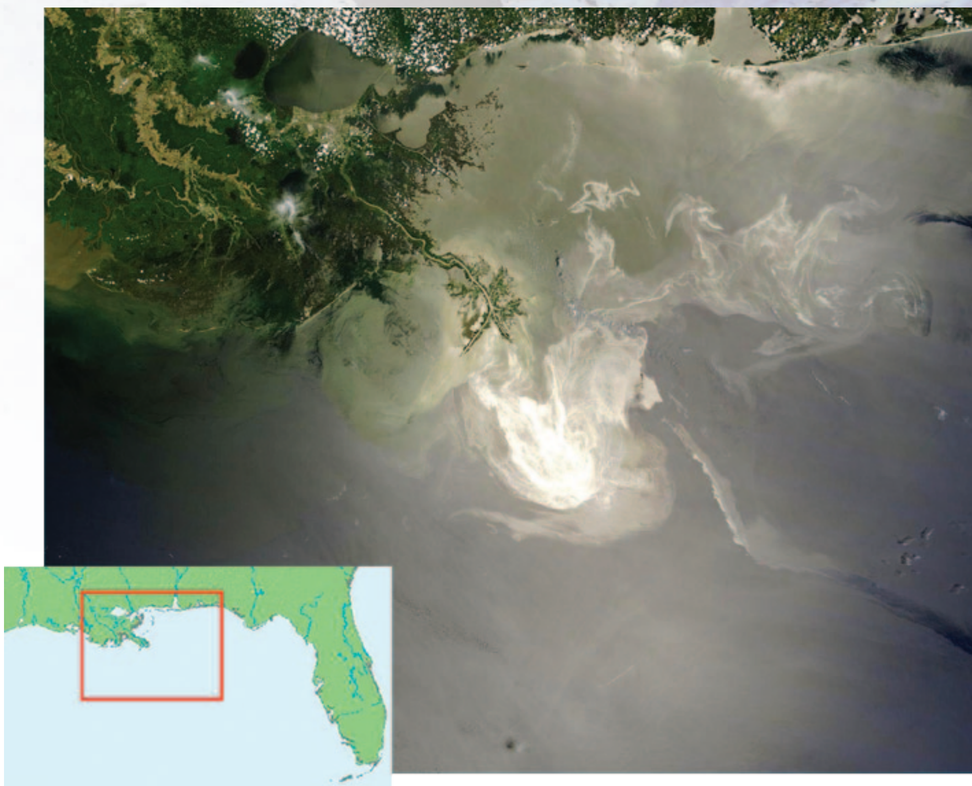


The damaged blowout preventer was eventually removed from the well and replaced. The 20-meter-high device, shown here as it is lifted aboard a ship, will be examined to better understand the events leading up to the oil leak. (Courtesy of U.S. Coast Guard.)

Preparing for the Next Crisis

The largest accidental spill in the history of the petroleum industry has been stopped, although environmental assessment and remediation continue in much of the Gulf. Many scientists and policy makers are now focused on preventing future disasters of this magnitude. Having received a crash course in oil-drilling technology, Laboratory engineers have had an opportunity to consider methods that might improve the safety of fossil-fuel exploration and drilling operations. Suggestions include deploying more in situ diagnostic techniques, adding layers of safety with standardized and certified hardware, and modifying equipment and technologies to operate in harsh environments, for example, building faster, more dexterous ROVs.

Several participants noted that the national laboratories would be an excellent resource in developing relevant technology. For example, Lehman's group has expertise in building "smart parts," integrating acoustic, electromagnetic, and other sensors into equipment or a structure (say, an engine or bridge), to monitor its "health"—usage, wear, and deterioration that might affect its safety or reliability. Perhaps in the future, the Laboratory could be engaged to design "smart" blowout preventers.



On May 24, 2010, the Terra satellite captured sunlight illuminating the growing oil slick off the Mississippi Delta. (Courtesy of National Aeronautics and Space Administration.)

Supporting BP during the crisis also led Livermore engineers and scientists to consider their broader role in preparing for and responding to national emergencies. "The next crisis won't be an oil spill," says Perfect. "The question is how do we, as national labs, set up for a quick response, whatever the emergency might be. If we are called on, we need to be ready." To that end, groups within the Engineering Directorate are doing best-practice exercises to assess the effectiveness of their procedures and ensure that they can promptly provide the technical expertise to address an unknown scenario.

In responding to the disaster, scientists and engineers from Livermore, Sandia, and Los Alamos also had a chance to build relationships with technical experts and government agencies outside their research communities and professional networks. Sharpe notes that, despite initial skepticism, BP came to value the technical competence and alternative viewpoints offered by the staff from the national laboratories. "Part of what made us effective is that although most of us knew little about the oil industry," says Perfect, "we're good problem solvers." The broad interdisciplinary experience of national laboratory researchers allowed them to respond quickly and provide measurable support to a large, complex effort.

For participants, the experience was unique. "Many aspects of the crisis response were quite different from our normal operating environment," says Aufderheide. "Working in this unusual setting has given us a chance to improve our craft for future efforts." Adds Warner, "It's not often that we get to see our work on television every day. We played a supporting role, but an important one."

—*Rose Hansen*

Key Words: acoustic imaging, blowout preventer, Deepwater Horizon, fluid dynamics, gamma-ray imaging, Interagency Modeling and Atmospheric Assessment Center (IMAAC), Macondo well, oil reservoir, remotely operated vehicle (ROV).

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A Complex Game of Cat and Mouse

IN chess, whether one is playing against a human or a computer, each move typically builds on the opponent's previous maneuvers. Humans have one significant advantage, however: their innate ability to analyze many factors before taking a turn. For example, human players may consider what they know about an opponent's behaviors or past strategies. They then use this knowledge to devise a game plan that gives them the advantage.

Traditional artificial intelligence systems, even those that model real-world adversarial scenarios, are less adaptive. In these systems, players, or "agents," are programmed to process a far less nuanced, narrow set of conditions before making a decision, and they often select moves with little or no regard for the behavior of others in the game environment.

As part of a two-year project funded by the Laboratory Directed Research and Development Program, a research team in Livermore's Engineering Directorate is attempting to develop computer modeling systems that process decisions more like humans do, adapting to the changing environment. The team, which includes computer scientists Brenda Ng and Kofi Boakye, operations researcher Carol Meyers, and former summer intern Andrew Wang from the Massachusetts Institute of Technology, wants to devise a system that can analyze adversarial relationships for a wide range of national security and law-enforcement applications. "The idea is to create a framework that takes into account an agent's intent rather than simply its static behavior," says Ng, who leads the project. This type of system will improve the effectiveness of computer simulations designed to analyze response scenarios against real-world adversaries.

Outwitting the Enemy

In single-agent decision models, the agent can choose from a given set of actions to advance from one state to another within the simulation environment. The agent selects an action based on the rewards or penalties it will incur for that turn. Most of the time, the information available for evaluating these options is imperfect. That is, the agent cannot be certain about its current state before deciding which optimal action to take. In these situations, the agent must infer its state through the noisy observations it receives from the environment. To do this, the agent maintains beliefs, in the form of probability distributions, over all of its possible states.

"This process is analogous to attempting to optimize a retirement portfolio," says Ng. "One can only surmise through day-to-day reports (observations) the general health of his or her investment (the agent state). Possible actions are to buy, sell, or cash out, but each action has an associated cost—a reward or a penalty."

As the number of agents increases, the models become more complex. The interactive, partially observable Markov decision process (I-POMDP) model is well suited for adversarial scenarios between multiple agents because it allows agents to consider the capabilities and beliefs of their adversaries before making the next move. Within such an environment, agents repeatedly interact with one another, and each agent's actions affect the joint state of all agents, which in turn affects every agent's observations.

One drawback with the I-POMDP model is with the built-in assumption that agents know all of the model parameters. In the real world, many conditions remain unknown until people interact with each other, whether they are allies or adversaries. To make the agents' simulated behavior more realistic, the Livermore team incorporated reinforcement learning into the I-POMDP model.

With the new framework, agents learn as they make choices within the established environment. Each interaction provides information that helps them select the optimal action for a given situation, allowing the agents to maximize their rewards. Model parameters are not fully known beforehand, but agents learn them through trial and error as the players interact.

"Our goal is to bridge the gap between theory and practice in what an I-POMDP can model in an adversarial scenario," says Meyers. A framework that simulates how agents "learn" from their opponents and change strategies based on observed behavior has major potential for law-enforcement and national security applications.

Show Me the Money

During the project's first year, the team applied the conventional I-POMDP to a simplified money-laundering scenario to evaluate its potential for accurately modeling dynamic adversaries. Considered a high-stakes game of cat and mouse, money laundering typically involves a complex series of financial transactions intentionally designed to be difficult to trace. Adversaries who think their actions are being monitored are likely to change their behavior, taking steps to evade detection or deceive the other agent.

Interactive, partially observable Markov decision process (I-POMDP) models incorporate the idea of nested belief to emulate adversarial relationships between multiple agents. In I-POMDP models, each agent tries to anticipate an opponent's behavior and makes choices to counter those actions.

"The money-laundering scenario is appealing because both agents have nested beliefs," says Ng. "Each one acts on what it 'believes' the other is thinking." The nested-belief framework attempts to model each player's thought processes and actions in a manner that better simulates human behavior—what Ng calls an I-think-that-you-think-that-I-think pattern.

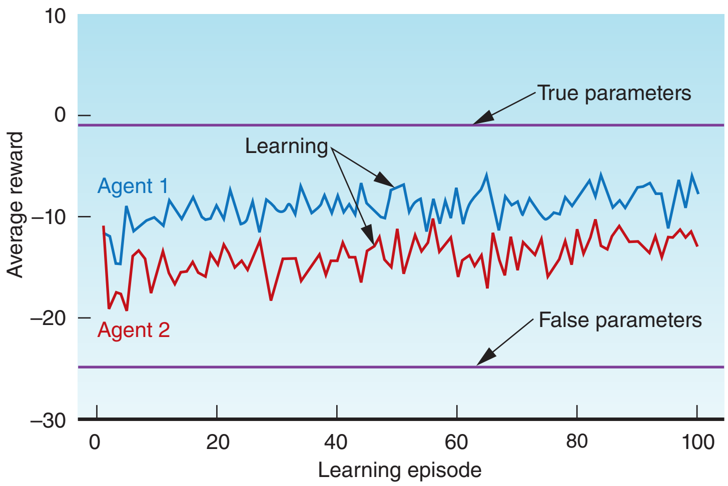
The team's initial model consisted of two agents. The first agent, a money launderer, is trying to diffuse and integrate its assets, "dirty" money, into the mainstream economy without being detected. The second agent, a law-enforcement officer, wants to confiscate this money before the money launderer can "cash out" via transactions with legitimate businesses.

The two agents operate within a defined number of states where the laundered money may be placed or found. For the money launderer, each state represents a location through which money can be diverted, such as bank accounts, trusts, or securities, as well as businesses that can integrate the large sums, for example, casinos and real-estate agencies. For law enforcement, each state represents a location where the officer can probe for suspicious activities. Both agents take actions not only to gather intelligence information on the opponent but also to transition from state to state. The "game" resets when the money is either successfully laundered or confiscated.

One challenge for the Livermore team was reducing the computational burden required to calculate the solution. "We had to substantially scale down our model to make it run efficiently," says Meyers. "Even in the simplified version, the number of actions, observations, and states was 20 times greater than that in any game previously solved by an I-POMDP." The researchers also modified algorithms designed to solve the I-POMDP models. They introduced additional approximations to a technique called reachability tree sampling, in which possible paths forward in the game are based on the likelihood of each path. These modifications are designed to focus the agents' attention only on the highly probable observations as determined by computing the optimal actions.

Throughout an I-POMDP simulation, both agents maintain beliefs about the physical states of their environment and are knowledgeable of model parameters, such as how the other's actions will contribute to the next state. After experimenting with the model, the Livermore team determined that under most conditions, the money launderer has the advantage. However, when both agents are set to focus on achieving immediate rewards, the law-enforcement officer wins more often and does so much faster.

The tiger problem is a standard benchmark used to evaluate agent modeling and decision-making frameworks. In the two-player version of this game, agents in identical scenarios on adjacent floors must decide which door to open. Behind one door is a jackpot, but behind the other is a tiger. The agents can take one of three actions: open the left door, open the right door, or listen in an attempt to learn from the other agent's choice. (Rendering by Sabrina Fletcher.)



This graph compares the rewards acquired by two agents using the Livermore Bayes-adaptive I-POMDP model, which allows agents to learn the model parameters, and the conventional I-POMDP model, which bases agent decisions on known parameters that are either true or false.

A Risky Proposition

In the second phase of the project, the team adapted the lessons learned from the money-laundering experiment to create a Bayes-adaptive I-POMDP framework. Standard I-POMDPs can model only the agents' attempts to reason. Bayes-adaptive I-POMDPs, however, can also model their attempts to learn. In this new framework, agents interact with their opponents to acquire information about their state and the dynamics governing states and observations. The Bayes-adaptive I-POMDP thus improves results produced when modeling human adversarial relationships.

"We assume that the state, action, and observation spaces are finite and known, but the model parameters—namely, the probabilities with which the agents change states and get specific information—are not fully known," says Ng. "This approach is more realistic because in the real world, agents would face a number of uncertainties as both parties try to deceive each other."

To demonstrate how adversaries continually adapt to an opponent, the team applied the model to the tiger problem, a standard benchmark used in academia. In the two-agent scenario, two adjacent rooms contain an object, either a ferocious tiger or a jackpot. The two agents have access to their own set of doors and can hear but not see the other agent. Each agent can take one of three actions: open the left door, open the right door, or listen.

An agent choosing to listen might hear a tiger growl, a door creak, or only silence. However, observations are obscured by background noise, so the agent cannot completely trust what it hears. After listening, the agent can update its belief state, learn about the truthfulness of the observations, and then choose the next optimal action. At the same time, both agents are trying to anticipate the action, observation, and evolving belief of the opponent.

The model now has more states to track because the state space includes parameters that enable learning. As a result, the team had to add further algorithmic approximations. "We transferred our approximations from the money-laundering model," says Boakye, "and then revised them to work for the larger state space." The tiger simulations revealed that when both agents are learning, the agents reap more rewards as the accuracy of their learned parameters increases. In essence, the learned behavior allows the agent to significantly improve its rewards compared with those attained from an incorrect model with no learning. In addition, when both agents are learning, rewards take longer to acquire, which is similar to a real scenario in which adversaries try to "game" each other.

I See You

Ng cautions that although the team's demonstration was successful, the framework does not yet provide a complete platform for modeling complicated human adversarial systems. "Even more algorithmic approximations would be required," she says. "Our work does however provide a major advance in fundamental adversarial modeling. It has great promise for a variety of national security applications, including counterterrorism efforts."

Ongoing research will focus on developing ways to enable more states, actions, and observations in the model while keeping the computation tractable. With more realistic adversarial models in the works, national security and law-enforcement officials may one day have a better tool for understanding their intelligent opponents. As a result, these systems may also help answer a fundamental question: how might adversaries act differently if they knew they were being watched?

—Caryn Meissner

Key Words: adversarial modeling; artificial intelligence; counterterrorism; interactive, partially observable Markov decision process (I-POMDP); law enforcement; money laundering; reinforcement learning.

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New Campus Set to Transform Two National Laboratories

FOR more than half a century, Lawrence Livermore and Sandia national laboratories have thrived as neighbors on the eastern edge of the Livermore Valley in California. Much of the research conducted by the two laboratories addresses national security issues. Although classified aspects of that work must be performed in strictly controlled environments, the underlying science and technology is not classified. In addition, both laboratories have a broad range of unclassified programs that focus on complex problems of national importance. Throughout the years, these programs have benefited from participation by colleagues in academia and industry.

To promote even greater collaboration between researchers at the two laboratories and their counterparts outside the Department of Energy (DOE) complex, Livermore and Sandia are planning to create an open research and development campus. The Livermore Valley Open Campus (LVOC), a partnership involving Livermore, Sandia, DOE, and the National Nuclear Security Administration (NNSA), creates a shared space between the two adjacent sites.

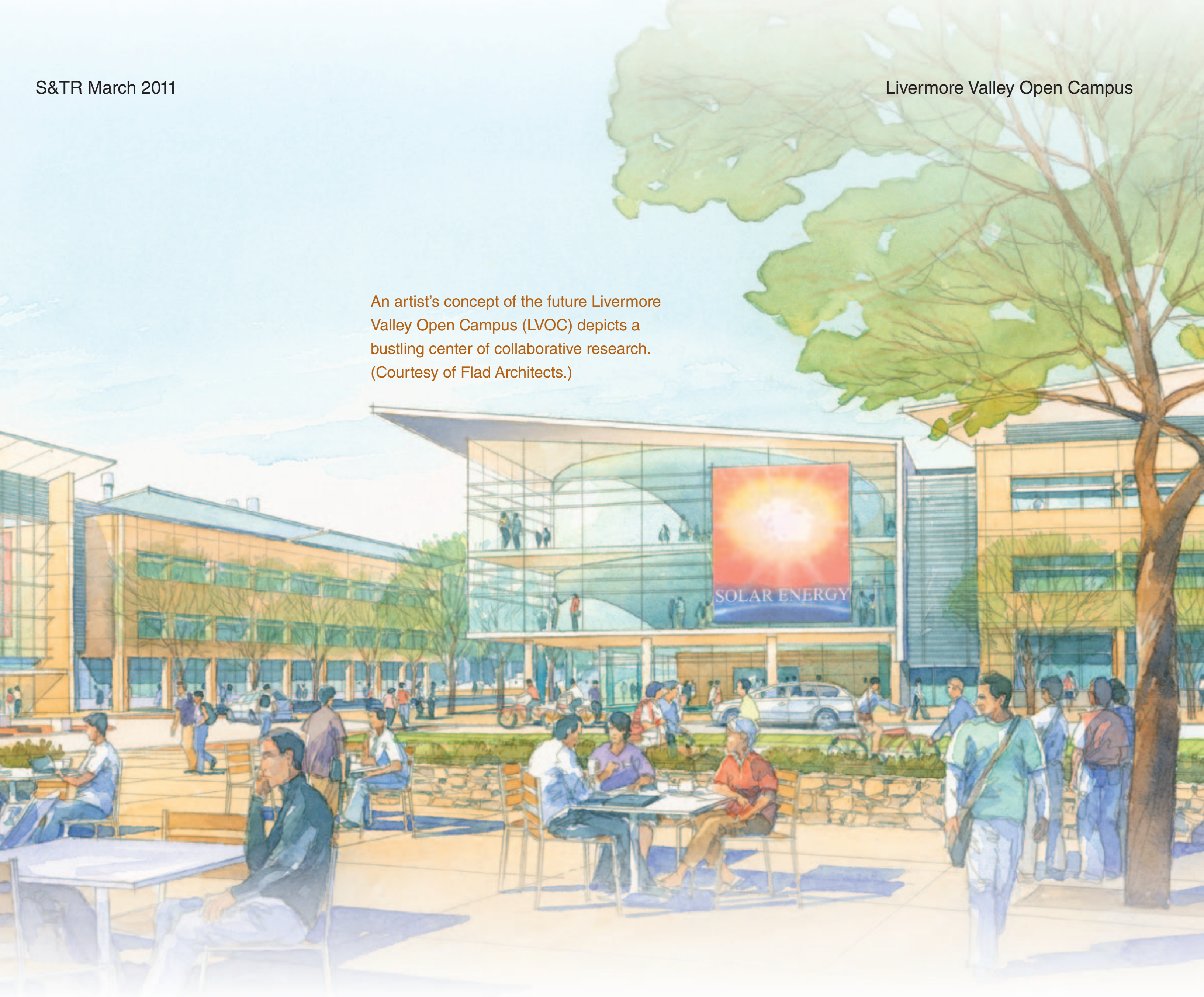
According to James "Buck" Koonce, senior adviser to Livermore Director George Miller, the new campus is in keeping with DOE's vision for increased scientific interaction and collaboration. "LVOC will position the two laboratories to more fully address their broad national security mission," says Koonce, who leads Livermore's effort to develop the open campus. "DOE and NNSA recognize that many national security issues are too important and complex to leave out broader participation by the talented scientists and engineers in universities and industries. We need their contributions to expand and deepen basic research related to national security in areas such as transportation, energy, cybersecurity, high-performance computing, and nonproliferation. We're confident the open campus will attract new partnerships and innovative teams to take on these issues."

LVOC will capitalize on the intellectual and industrial resources of the San Francisco Bay Area, including University of California campuses, Stanford University, the California State University system, and other academic institutions currently working with the two laboratories as well as businesses in the surrounding community and Silicon Valley. In addition, nearby federal laboratories, such as Lawrence Berkeley National Laboratory, SLAC National Accelerator Laboratory, and NASA Ames Research Center, are expected to play important roles in the new campus.

Campus to Cover 110 Acres

The campus is being built on 110 acres (less than 0.5 square kilometers) of contiguous land adjoining the southeast corner of Lawrence Livermore's main site and the northeast corner of the Sandia site. The campus extends from an area adjacent to the National Ignition Facility (NIF) at Livermore to the Combustion Research Facility (CRF) at Sandia. Over the next several years, the exact boundaries will be adjusted as necessary to accommodate mission and program needs.

NNSA Administrator Tom D'Agostino and DOE Under Secretary for Science Steve Koonin formally authorized development of LVOC in 2009, following several years of discussion centered on ways to more fully exploit the resources and talents of Livermore and Sandia. "A Livermore Valley Open Campus will maximize the return on our nation's investment in nuclear security," said



An artist's concept of the future Livermore Valley Open Campus (LVOC) depicts a bustling center of collaborative research. (Courtesy of Flad Architects.)

Secretary of Energy Steven Chu in announcing the new campus. "By leveraging the groundbreaking research of our nuclear security labs through private sector collaborations, we will bring breakthroughs to the market faster and find new solutions to the energy problem."

Camille Bibeau, who leads program development for LVOC, says the campus will enhance Livermore's and Sandia's abilities to execute their missions. It also will help both laboratories remain at the forefront of science, technology, and engineering and ensure that they have the talented workforce they need for the future. "Having an open campus will expand opportunities to engage with the broader international research and academic community in a modern high-tech environment," says Bibeau. "Those kinds of partnerships will help the laboratories recruit and retain talented scientists and engineers and keep our staffs at the leading edge of their fields."

In 2010, Livermore and Sandia engaged Flad Architects, a Madison, Wisconsin, firm with extensive DOE experience, to study development options and create a master plan with different scenarios. For example, one scenario offers a design for expanding the campus over 30 years until it eventually provides 2.5 million square feet (over 230,000 square meters) of laboratory and office space and accommodates up to 4,000 people. Another Flad option features a "village center," which could offer amenities such as conference space, a visitor's center, and food services, while ensuring compliance with security requirements and maximizing the available acreage In the first phase of LVOC construction, from late 2009 through 2011, the two laboratories created a general access area, a new entrance to CRF with more convenient visitor access, and an interim High-Performance Computing Center.

This artist's rendering shows one vision of a completed LVOC circa 2040. Several design plans are being considered for expanding the campus over the next 30 years. (Courtesy of Flad Architects.)

Reducing Partnership Barriers

To fully implement the LVOC concept, Livermore and Sandia must maintain the appropriate level of security and access controls in areas that perform sensitive work while maximizing access to the open campus for research partners and visitors. A critical aspect to LVOC success will be to streamline existing business and operating procedures to enhance scientific collaboration. Toward that end, the laboratories are studying ways to accelerate and accommodate new research.

Koonce points to the Hyperion project as a model for LVOC collaborations. In this pioneering cooperative venture, which began in 2008, Livermore has teamed with 15 companies to develop a realistic high-performance computing environment that industrial partners can use to test new products. Hyperion allows developers to improve technologies and decrease the time required to bring new products to market. The financial benefits offered by this collaboration are also proving to far outweigh the partners' initial investments. (See *S&TR*, December 2009, pp. 15–17.)

LVOC planners have identified two classes of programs to attract collaborations: anchors and candidates. Anchor programs draw on core institutional competencies, well-established expertise, and renowned facilities.

According to Koonce, the LVOC team has initially established three anchor programs. The Transportation Energy Center will engage CRF and associated resources, expanding on Sandia's current efforts with hundreds of industrial collaborators researching combustion science. The International High-Energy-Density Science and Inertial Fusion Energy Center will capitalize on the capabilities offered by NIF, the world's most energetic laser, and Livermore's expertise in high-energy-density science.

Ed Moses, principal associate director for NIF and Photon Science, sees a bright future for the open campus. "LVOC is encouraging leading researchers from around the world to collaborate on NIF experiments that explore matter under extreme temperatures and pressures," he says. "Those studies will lead to important new discoveries. We expect the field to change dramatically in the years ahead."

The third anchor program will be the High-Performance Computing Center, designed to provide significant computational resources to LVOC collaborations. According to Bibeau, the

The Combustion Research Computation and Visualization building was completed in 2010. This facility complements the existing Combustion Research Facility at Sandia, one of the key anchors for LVOC. Both buildings are located within a newly designated general access area.

permanent facility, when constructed, will provide researchers with supercomputing power equivalent to the resources already available for Livermore's classified nuclear weapons program.

Candidate programs are smaller research efforts that can start up more quickly in an open environment compared with the current configuration of the laboratories. These efforts offer a wide range of opportunities for collaborations with academia and industry. Potential programs include the Hydrogen Materials in Extreme Conditions Institute, Applied Antineutrino Physics Program, Joint Microscopy Center, Cyber Science and Security Institute, Bay Area Biosecurity Center, and Climate and Energy Center.

Large Role for High-Performance Computing

Mark Seager, assistant department head for Advanced Technology in Livermore's Computation Directorate, has been meeting with California business executives to discuss how working with LVOC's computational resources could significantly reduce the time required to advance from concept to manufacturing prototype. "We want to bring high-performance computing to California businesses, especially small and medium-size companies, so they can test new products in simulations—a process called virtual prototyping," says Seager, who spearheaded the Hyperion project. With virtual prototyping, manufacturers can design, build, test, and "break" new technologies before they devote time and money to manufacturing and testing a physical prototype. Seager adds, "Virtual prototyping helps them bring products to market far sooner than they can with traditional methods."

Koonce reports enthusiastic response from local, state, and federal officials and strong support from DOE and NNSA. Alice Williams, manager of NNSA's Livermore Site Office, says, "The new campus is an exciting concept with enormous potential, and we're working hard to expedite its realization."

"LVOC represents a new way of doing business with the national labs," says Koonce. "Everyone we have spoken to is very excited, especially because of the potential to expand our partnerships both locally and internationally."

—Arnie Heller

Key Words: Combustion Research Facility (CRF), high-energy-density science, Hyperion, Livermore Valley Open Campus (LVOC), National Ignition Facility (NIF).

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In this section, we list recent patents issued to and 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

Biological Sample Collector
Gloria A. Murphy
U.S. Patent 7,789,246 B1
September 7, 2010
In this biological sample collector, a filter plate with multiple wells is mounted on a manifold plate, and a hollow slider in a slide case is used for positioning a tube. Once the tube is aligned with a selected well, it is pushed through the slider into the well and forms a seal. The tube then deposits a biological sample onto a filter in the bottom of the well. The biological sample collector may be portable.

Electrostatic Generator/Motor Having Rotors of Varying Thickness and a Central Stator Electrically Connected Together into Two Groups
Richard F. Post
U.S. Patent 7,834,513 B2
November 16, 2010
In this module, two outer sets of stationary fan-blade-shaped sectors made with conductive material are maintained at ground potential. Midway between the two is a set of stationary sector plates, each of which is electrically insulated from the other. In one example, the inner sector plates are connected alternately, forming two groups of parallel-connected condensers. These condensers are then separately connected through high-charging circuit resistances to a source of direct-current potential with respect to ground. Each group has an additional lead that connects output as an alternating current output to a load. When connected to a driver circuit, these same leads can be used to produce motor action.

Durable Silver Mirror with Ultra-Violet thru Far Infra-Red Reflection
Jesse D. Wolfe
U.S. Patent 7,838,134 B2
November 23, 2010
A highly reflective silver mirror designed for environmental durability is characterized by high reflectance in a broad spectral range, from about 300 nanometers in the ultraviolet to the far infrared (about 10,000 nanometers). A high-absorptivity metal underlayer prevents a galvanic cell from forming with the silver layer while increasing the layer's reflectance. Overcoat layers enhance mechanical and chemical durability and protect the silver layer from corrosion and tarnishing. With this design, the mirror can be used in various surroundings or climates, including harsh or extreme environments.

Processing a Printed Wiring Board by Single Bath Electrodeposition
Michael P. Meltzer, Christopher P. Steffani, Ray A. Gonfiotti
U.S. Patent 7,846,317 B2
December 7, 2010
With this method, initial processing steps can be implemented in a printed wiring board. Copper is plated in a printed wiring board from a bath containing nickel and copper. Nickel is also plated on the board from a bath containing nickel and copper, and final processing steps are then implemented on the board.

Functionalized Apertures for the Detection of Chemical and Biological Materials
Sonia E. Létant, Anthony W. van Buuren, Louis J. Terminello, Michael P. Thelen, Louisa J. Hope-Weeks, Bradley R. Hart
U.S. Patent 7,851,203 B2
December 14, 2010
Nanometer- to micrometer-scale functionalized apertures constructed on a substrate of glass, carbon, semiconductors, or polymeric material allow for real-time detection of biological materials or chemical moieties. Because many apertures can exist on one substrate, numerous chemical and biological molecules can be detected simultaneously. In one design, a macrocyclic ring attached to cross-linkers has a biological or chemical probe extending through the aperture. In another configuration, chemical or biological anchors are attached directly to the aperture walls via cross-linkers.

Micro-Electro-Mechanical Systems Phosphoric Acid Fuel Cell
David A. Sopchak, Jeffrey D. Morse, Ravindra S. Upadhye, Jack Kotovsky, Robert T. Graff
U.S. Patent 7,855,018 B2
December 21, 2010
This phosphoric acid fuel-cell system has a phosphoric acid electrolyte in a porous electrolyte support, with cathode and anode electrodes contacting the electrolyte.

Low to Moderate Temperature Nanolaminate Heater
J. Del Eckels, Peter J. Nunes, Randall L. Simpson, Stefan Hau-Riege, Chris Walton, J. Chance Carter, John G. Reynolds
U.S. Patent 7,867,441 B2
January 11, 2011
A high-temperature energy source has been modified to serve as a heat source that outputs low to moderate temperatures. The high-temperature energy source is positioned between two thin pieces of material to form a close contact sheath. In one configuration, the energy source is a nanolaminate multilayer foil of reactive materials that produce a heating level of less than 200°C.

Explosives Tester
Jeffrey S. Haas, Douglas E. Howard, Joel D. Eckels, Peter J. Nunes
U.S. Patent 7,867,445 B1
January 11, 2011
This explosives tester can be used as a screening tool by nontechnical personnel at any location to determine whether a surface contains explosives. The tester has a heater and two explosives-detecting reagent holders and dispensers.

Awards

Chris Keane, of the Physical and Life Sciences Directorate and a former senior manager for the Department of Energy's (DOE's) fusion energy program, received the **Board of Directors Special Award** from **Fusion Power Associates**. Keane, who led the inertial-confinement fusion program at the National Nuclear Security Administration (NNSA) for many years, was honored "in recognition of and appreciation for managerial contributions to the inertial confinement fusion technical program achievements that occurred during and beyond" his tenure at NNSA and DOE.

Joseph Nilsen, a physicist in the Weapons and Complex Integration Principal Directorate, has been elected a **fellow** of the **Optical Society**, the seventh society fellow currently at the Laboratory. The organization recognized Nilsen for his "pioneering contributions to the development and understanding of X-ray lasers and their applications." Nilsen, who is also a fellow of the American Physical Society, helped develop the prepulse techniques that are now standard worldwide for driving x-ray lasers.

Livermore electronics engineer **Faranak Nekoogar** won the **Best Poster Award** in the Advancements in Containment and Surveillance Session at an **International Atomic Energy Agency** symposium in Vienna. Her presentation, "Advanced Radio Frequency Tags for Safeguards Applications," describes technology that uses radio frequency to detect, remotely monitor, and track cylinders with nuclear materials. The system, which Nekoogar helped develop, substantially improves monitoring capabilities at various stages of the enrichment process.

The **American Physical Society** has selected four Livermore scientists as 2010 **fellows**:

Jon Eggert, a physicist in the Physical and Life Sciences Directorate, was cited in the Shock Compression of Condensed Matter category for significant achievements in linking dynamic and static compression of condensed matter.

In the Plasma Physics category, **Hye-Sook Park**, a physicist in the National Ignition Facility and Photon Science Principal Directorate, was cited for development of seminal experimental techniques to create and probe plasmas with extreme density and temperature.

Ramona Vogt, a staff scientist in the Physical and Life Sciences Directorate, was cited in the Nuclear Physics category for her contribution to the science community's understanding of the dynamics of heavy quark and charmonium production in collisions with nuclei and for providing guidance for using these probes in experimental investigations of hard dynamics in collisions with nuclei.

Olgica Bakajin, formerly a chief scientist at Livermore and now chief technology officer of Porifera, Inc., was cited in the Biological Physics category for her contributions to the development of new instrumentation for studies of protein folding and for fundamental understanding of transport and selectivity at the nanoscale.

The Laboratory in the News (*continued from p. 2*)

Resolving the High-Pressure Phases of Calcium

Research by Laboratory scientists Amanuel Teweldebrhan, Jonathan DuBois, and Stanimir Bonev is helping to resolve a controversy between theory and experiment about the finite and low-temperature stability of calcium at extremely high pressures, between 0.3 and 1.1 million atmospheres (30 and 110 gigapascals). Because calcium is an important superconducting material, researchers have devoted significant experimental and theoretical work to characterizing its electronic, structural, and superconducting properties at high pressure. However, they have not resolved the structure in which the element becomes superconducting.

Numerous studies have applied density functional theory (DFT) calculations to predict calcium's structures and other properties, most notably its superconductivity. However, the standard exchange-correlation approximations in DFT produce inaccurate energies that do not favor the experimentally proposed phases of dense calcium. By combining quantum Monte Carlo calculations with DFT, the Livermore researchers effectively corrected these discrepancies to more accurately model calcium's properties.

"This finding will be of broad interest to the research community worldwide," says Bonev. "It not only reports important results for calcium but also has more general implications for how DFT methods are applied to study materials under extreme conditions, where electronic changes similar to those found in calcium are common." The team's results were published in the December 3, 2010, issue of *Physical Review Letters.*

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Research Highlights New Glass-Forming System

A molecular-dynamics simulation developed by Livermore researcher Tomas Oppelstrup and colleagues from the Royal Institute of Technology in Stockholm, Sweden, has modeled a novel system in which the glass phase forms via an equilibrium, first-order phase transition from a stable liquid phase. Theoretical studies have predicted that glass can be formed when a first-order phase transition occurs below the material's melting point. However, crystallization has remained a formidable problem. As a result, glasses are typically formed by cooling the liquid phase.

To study the glass-forming process, the team simulated a one-component system with a model metallic pair potential, which represented an ideal glass former—a liquid that does not crystallize under cooling. The only ideal glass formers previously known have been atactic polymers and some electrolytic solutions.

In addition to the intrinsic scientific merit of this work, the result has significant technological implications. In particular, it demonstrates a possible new approach for designing bulk metallic glass formers. The team's results were featured on the cover of the November 7, 2010, issue of the *Journal of Chemical Physics.*

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Abstracts

From Respiration to Carbon Capture

Lawrence Livermore is collaborating with Babcock & Wilcox Company and the University of Illinois to create a molecule that mimics the behavior of carbonic anhydrase—a natural lung enzyme that transports carbon dioxide (CO_2) out of our blood. The team's goal is to make the synthesized molecule rugged enough to function under high pressures and temperatures so it can be used as a catalyst for removing CO_2 from the flue gas of a coal-fired power plant. Replacing current scrubbing processes with such an application could greatly speed up carbon capture. Computational specialists at Livermore are developing a library of candidate molecules, all designed with an outer scaffold of chemical bonds to protect the critical zinc ion at the center of the molecule. Synthetic chemists then test the most promising candidates to determine which ones can be assembled easily and concisely—a key for commercial use. The catalyst's structure must be amenable to further chemical enhancement so that properties such as solubility, thermal stability, surface attachment, and efficiency can be improved when necessary. After synthesis, a molecule goes through a two-step testing process, which ultimately measures the combined rates of all chemical and mass-transfer processes, including the concentration of CO_2 being vented.

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Lending a Hand to an Oily Problem

On April 20, 2010, the Macondo oil well exploded on the seafloor of the Gulf of Mexico and ignited the Deepwater Horizon drilling rig. Eleven members of the drilling crew lost their lives in the explosion, and oil gushing from the well began spreading through the deep waters of the Gulf. In response to the crisis, Secretary of Energy Steven Chu offered the technical expertise and resources from the national laboratories to help in the effort to contain the spill and cap the leak. Engineers and scientists from Lawrence Livermore, Los Alamos, and Sandia national laboratories relied on advanced diagnostics, modeling, and engineering expertise to characterize the underwater structure, quantify the leak, and evaluate plans to cap the well. The laboratories also sent engineers to work at BP's crisis command center in Houston, Texas, until September 19, when the leak was contained. The broad interdisciplinary experience of Livermore personnel enabled them to respond quickly and make a tangible contribution to this international effort.

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Coming Next Issue

Persistent Surveillance

Courtesy of U.S. Department of Defense.

A new video-analysis system promises to help the U.S. quickly detect suspicious activity recorded from drone aircraft.

Also in April/May

• Livermore is creating the brightest gamma-ray light source ever, one that will be able to study the nuclei of individual isotopes.

• An innovative predictive computational tool explains the basic chemistry controlling biofuel processes.

• A Laboratory–private industry partnership is building electromechanical batteries that can store and dispatch energy for integration into the electric grid.

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