Laboratory Directed Research and Development

FY2009 ANNUAL REPORT

Lawrence Livermore National Laboratory

About the Cover:

A time-integrated photograph of a laser shot at the OMEGA facility at the University of Rochester to study diamond melt under high pressure. This ground-breaking research was an outgrowth of Livermore Laboratory Directed Research and Development project 09-SI-005, “Physics and Chemistry of the Interiors of Large Planets: A New Generation of Condensed Matter,” in which researchers measured the melt curve of diamond up to 11 Mbar—the highest pressure ever achieved for a solid in the laboratory. The diamond target is at center-right, and the bright white light is ablated plasma. This research focuses on establishing a new generation of experiments accessing the unexplored regime of ultrahigh compression, with applications that range from understanding the origin and evolution of planets to testing and significantly extending fundamental theories of condensed matter. Results have appeared in 2008 and 2009 articles in *Physical Review B: Condensed Matter and Materials Physics*, a peer-reviewed journal of the American Physical Society.

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Acknowledgments

The Laboratory Directed Research and Development Program extends its sincere appreciation to the principal investigators of fiscal year 2009 projects for providing the content of the annual report and to the publications team. The program also thanks the following members of the Institutional Science and Technology Office for their many contributions to this publication: Nancy Campos, database manager; Steve McNamara, computer specialist; and Cathleen Sayre, resource manager.

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Director's Statement

The Laboratory Directed Research and Development (LDRD) Program, authorized by Congress in 1991 and administered by the Institutional Science and Technology Office at Lawrence Livermore, is our primary means for pursuing innovative, long-term, high-risk, and potentially high-payoff research. The LDRD Program supports the full spectrum of national security interests encompassed by the missions of the Laboratory, the Department of Energy, and National Nuclear Security Administration. The accomplishments described in this annual report demonstrate the strong alignment of the LDRD portfolio with these missions and contribute to the Laboratory's success in meeting its goals.

The LDRD budget of $85 million for fiscal year 2009 sponsored 168 projects. These projects were selected through an extensive review process to ensure the highest scientific quality and mission relevance. Each year, the number of deserving proposals far exceeds the funding available, making the selection a tough one indeed.

Our ongoing investments in LDRD have reaped long-term rewards for the Laboratory and the nation. Many Laboratory programs trace their roots to research thrusts that began several years ago under LDRD sponsorship. In addition, many LDRD projects contribute to more than one mission area, leveraging the Laboratory's multidisciplinary team approach to science and technology. Safeguarding the nation from terrorist activity and the proliferation of weapons of mass destruction will be an enduring mission of this Laboratory, for which LDRD will continue to play a vital role.

The LDRD Program is a success story. Our projects continue to win national recognition for excellence through prestigious awards, papers published in peer-reviewed journals, and patents granted. With its reputation for sponsoring innovative projects, the LDRD Program is also a major vehicle for attracting and retaining the best and the brightest technical staff and for establishing collaborations with universities, industry, and other scientific and research institutions. By keeping the Laboratory at the forefront of science and technology, the LDRD Program enables us to meet our mission challenges, especially those of national security in an evolving global context.

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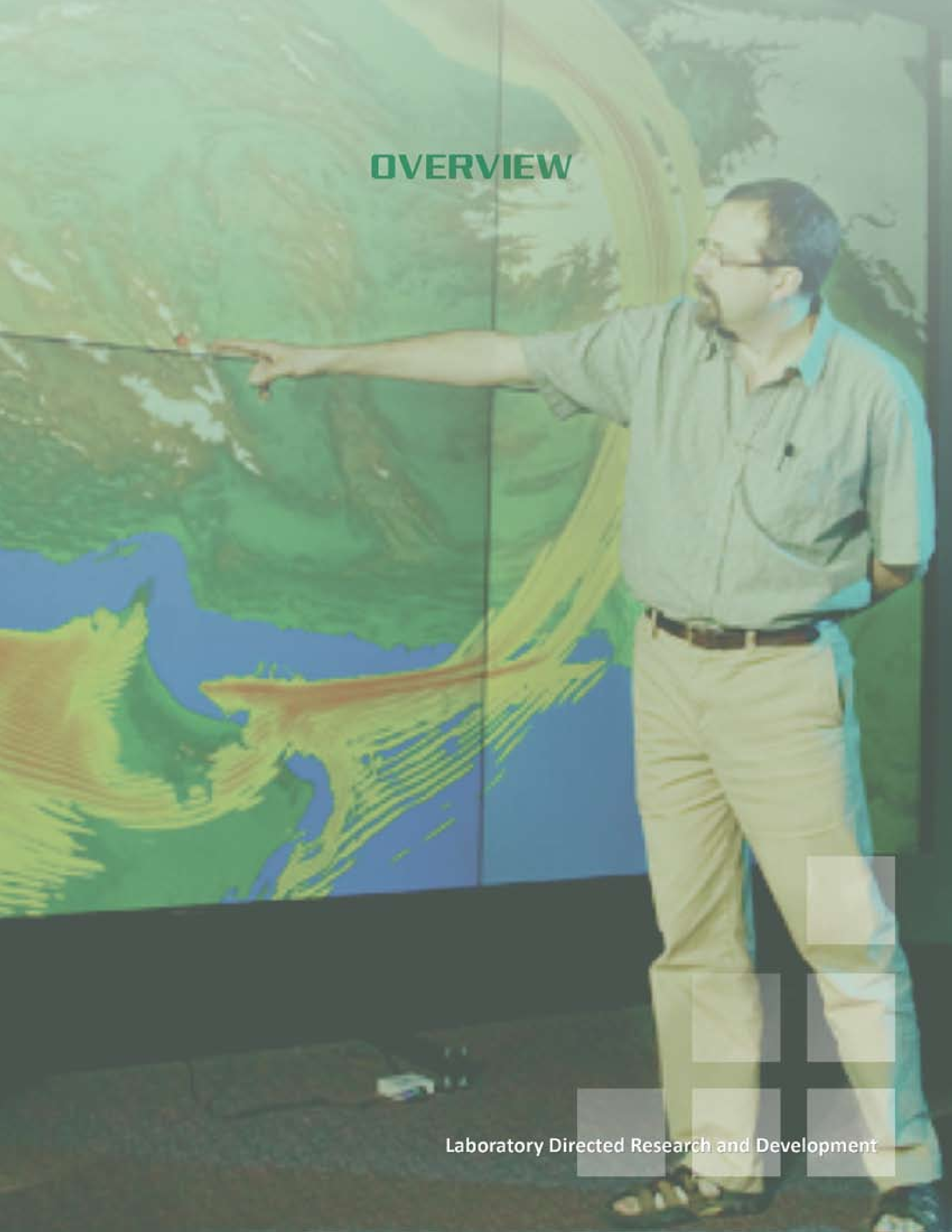


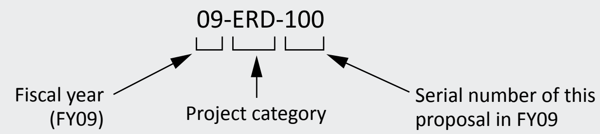
About the FY2009 Laboratory Directed Research and Development Annual Report

The Laboratory Directed Research and Development (LDRD) annual report for fiscal year 2009 (FY09) provides a summary of LDRD-funded projects for the fiscal year and consists of two parts:

Overview: A broad description of the LDRD Program, the LDRD portfolio-management process, program statistics for the year, and highlights of accomplishments for the year.

Project Summaries: A summary of each project, submitted by the principal investigator. Project summaries include the scope, motivation, goals, relevance to Department of Energy (DOE)/ National Nuclear Security Administration (NNSA) and Lawrence Livermore National Laboratory (LLNL) mission areas, the technical progress achieved in FY09, and a list of publications that resulted from the research.

LDRD projects are organized into four categories including Strategic Initiative (SI), Exploratory Research (ER), Laboratory-Wide Competition (LW), and Feasibility Study (FS). Each project is assigned a unique tracking code, an identifier that consists of three elements. The first is the fiscal year the project began, the second represents the project category, and the third identifies the serial number of the proposal for that fiscal year. For example:



Program Overview—Innovation for Our Nation

About Lawrence Livermore National Laboratory

A premier applied-science laboratory, LLNL has at its core a primary national security mission—to ensure the safety, security, and reliability of the nation's nuclear weapons stockpile without nuclear testing, and to prevent and counter the spread and use of weapons of mass destruction: nuclear, chemical, and biological.

The Laboratory uses the scientific and engineering expertise and facilities developed for its primary mission to pursue advanced technologies for other important national security needs—homeland defense, military operations, and missile defense, for example—that evolve in response to emerging threats. For broader national needs, the Laboratory executes programs in energy security, climate change and long-term energy needs, environmental assessment and management, bioscience and technology to improve human health, and breakthroughs in fundamental science and technology. With this multidisciplinary expertise, the Laboratory serves as a science and technology resource to the U.S. government and as a partner with industry and academia.

One of three DOE/NNSA laboratories, LLNL is managed by the Lawrence Livermore National Security, LLC. Since its inception in 1952, the Laboratory has fostered an atmosphere of intellectual freedom and innovation that attracts and maintains the world-class workforce needed to meet challenging national missions.

Laboratory Directed Research and Development Program

To fulfill its missions, LLNL must continually invest in the science and technology that form the foundation of its signature capabilities. The LDRD Program, which was established by Congress at all DOE national laboratories in 1991, is LLNL's most important single resource for fostering excellent science and technology for today's needs and tomorrow's challenges.

According to its Congressional mandate,[1] the purpose of LDRD is to foster excellence in science and technology that (1) supports the DOE/NNSA and LLNL missions and strategic vision, (2) ensures the technical vitality of the Laboratory, (3) attracts and maintains the most qualified scientists and engineers and allows scientific and technical staff to enhance their skills and expertise, (4) helps meet evolving DOE/NNSA and national security needs, and (5) enables scientific collaborations with academia, industry, and other government laboratories.

By enabling LLNL to fund creative basic and applied research activities in areas aligned with its missions, the LDRD Program develops and extends the Laboratory's intellectual foundations and maintains its vitality as a premier research institution. The present scientific and technical strengths of LLNL are, in large part, a product of LDRD investment choices in the past.

At LLNL, Laboratory Director George Miller and Chief Research and Development Officer Tómas Díaz de la Rubia are responsible for the LDRD Program. Execution of the program is delegated to the director of the Institutional Science and Technology Office, Judith Kammeraad. The LDRD Program at LLNL is in compliance with DOE Order 413.2B and other relevant DOE orders and guidelines.

Strategic Context for the LDRD Portfolio

The FY09 LDRD portfolio-management process at LLNL was structured to ensure alignment with the DOE, NNSA, and Laboratory missions. This process involved (1) a top-level strategic planning process to identify strategic science and technology areas for LDRD investment, (2) a call to the Laboratory scientific and technical community for innovative and relevant proposals within the DOE/NNSA mission areas, and (3) a scientific peer-review process to select the highest quality LDRD portfolio from these proposals.

In FY09, the Laboratory director called for the development of a new strategic roadmap that sets institutional strategic goals and identifies science and technology needs in selected mission focus areas, in fundamental research, and in critical science, technology, and engineering capabilities. *The Roadmap to the Future* was developed by multidisciplinary teams under the guidance of Chief Research and Development Officer Tomás Díaz de la Rubia. This document set the strategic context for the LDRD competition for five years, starting in 2009. It will be updated annually to respond to our ever-changing mission needs. Further strategic context is provided by the *2006 U.S. Department of Energy Strategic Plan*[2] and by *The National Nuclear Security Administration Strategic Planning Guidance for FY2010–FY2014*[3], released in April 2008. The DOE strategic plan articulates strategic themes for achieving the DOE mission of discovering solutions to power and secure America's future. In FY09, the Laboratory's LDRD Program strongly supported the DOE strategic themes:

1. **Energy Security**—Promoting America's energy security through reliable, clean, and affordable energy.
2. **Nuclear Security**—Ensuring America's nuclear security.
3. **Scientific Discovery and Innovation**—Strengthening U.S. scientific discovery, economic competitiveness, and improving quality of life through innovations in science and technology.
4. **Environmental Responsibility**—Protecting the environment by providing a responsible resolution to the environmental legacy of nuclear weapons production.

[1] *U.S. Department of Energy Order 413.2A, Laboratory Directed Research and Development* (January 8, 2001).

[2] *2006 U.S. Department of Energy Strategic Plan*. <http://www.cfo.doe.gov/strategicplan/strategicplan.htm> (retrieved April 1, 2008).

[3] *The National Nuclear Security Administration Strategic Planning Guidance for FY 2010–FY2014* <http://nnsa.energy.gov/about/documents/NSPG-FY10-14_04-08-08.pdf> (retrieved March 12, 2009).

The Laboratory's *Roadmap to the Future* guides the LDRD portfolio planning process. This five-year strategic roadmap describes institutional strategic goals and science and technology needs in selected mission focus areas and in critical science, technology, and engineering pillars:

Mission Focus Areas

- Stockpile Stewardship Science
- Nuclear Threat Elimination
- Cyber Security, Space Security, and Intelligence
- Biosecurity
- Energy and Climate
- Laser Inertial Fusion Energy
- Advanced Laser Optical Systems and Applications

Science, Technology, and Engineering Pillars

- High-Energy-Density Science
- High-Performance Computing and Simulation
- Materials and Chemistry at the Extremes
- Information Systems
- Measurements and Experimental Science
- Energy Manipulation

The DOE and NNSA oversee the Laboratory's LDRD Program to ensure that it accomplishes its objectives. This oversight includes field and headquarters reviews of both the technical content and management processes. The value of LDRD to DOE as well as to the country is evidenced in the 2010 Energy and Water Development and Related Agencies Appropriations Act:

> LDRD is the national labs' most important tool for maintaining the vitality of the national labs in support of other national security missions. LDRD enables the labs to hire the "best and brightest" young scientists and engineers and allows them to seek innovative science and technology solutions for current or emerging national security issues, including those of energy security.[4]

Structure of the LDRD Program

Project Categories

The LDRD Program at LLNL consists of three major project categories: Strategic Initiative (SI), Exploratory Research (ER), and Laboratory-Wide (LW) competition. During the year, the LDRD Program also funds a few projects in a fourth category, Feasibility Study/Project Definition (FS).

Strategic Initiative

The SI category, which is open to all Laboratory scientific, engineering, and programmatic staff, focuses on innovative research and development activities that address major specific science and technology challenges of high potential strategic impact for the *Roadmap to the Future*, and significantly enhance the Laboratory's science and technology base. Projects in this category are usually larger and more technically challenging than those in the other categories. All new and current SIs must be aligned with at least one of the mission focus areas or underlying science, technology, and engineering capabilities (pillars).

Exploratory Research

The ER category is designed to help fulfill the strategic R&D needs of a Laboratory directorate (ERD) or institute (ERI) and must also support and be aligned with the Laboratory's roadmap. As with all the LDRD project categories, ER proposals must meet the criteria for intellectual merit used across the scientific community, such as importance of the proposed activity to advancing knowledge, capability, and understanding within its own field or across different fields, as well as ensuring the proposed activity explores creative and original concepts.

Laboratory-Wide Competition

Projects in the LW category emphasize innovative research concepts and ideas and undergo limited management filtering to encourage creativity of individual researchers. The LW competition is open to all LLNL staff in programmatic, scientific, engineering, and technical support areas. Direct alignment with the Laboratory's strategic roadmap is not required for LW proposals. However, to be funded, all LW proposals must be relevant to one or more missions of the DOE and NNSA.

Feasibility Study/Project Definition

This special project category, FS, provides researchers with the flexibility to propose relatively small, short-term projects to determine the feasibility of a particular technical approach for addressing a mission-relevant science and technology challenge. To increase its responsiveness to Laboratory scientists and engineers, the LDRD Program funds FS projects throughout the year.

Project Competency Areas

Although LDRD projects often address more than one scientific discipline, each project is classified into one of ten research categories established by DOE that is relevant to NNSA and Laboratory missions. The ten categories are:

- Advanced Sensors and Instrumentation
- Biological Sciences
- Chemistry
- Earth and Space Sciences
- Energy Supply and Use
- Engineering and Manufacturing Processes
- Materials Science and Technology

[4] "Title III," *Energy and Water Development and Related Agencies Appropriations Act, 2010,* S.1436 (July 9, 2009), The Library of Congress <http://thomas.loc.gov/cgi-bin/cpquery/?&dbname=cp111&sid=cp111b23IJ&refer=&r_n=sr045.111&item=&sel=TOC_403428&> (retrieved March 25, 2010).

- Mathematics and Computing Sciences
- Nuclear Science and Engineering
- Physics

The LDRD 2009 Portfolio

Portfolio Overview

The FY09 LDRD portfolio was carefully structured to continue the LDRD Program's vigorous support for the strategic vision and long-term goals of DOE, NNSA, and LLNL. The projects described in this annual report underwent a stringent peer-reviewed selection process and received ongoing management oversight.

In FY09 the LDRD Program funded 168 projects with a total budget of $85 million. The distribution of funding among the LDRD project categories is shown in the pie chart at the bottom of this page.

Strategic Initiative

In FY09, the LDRD Program funded 12 SI projects. Although the SI category represented only a little over 7% of the total number of LDRD projects for FY09, it accounted for over 36% of the budget. SI projects ranged in funding from $900K to $3M.

Exploratory Research

The LDRD Program funded 131 ER projects for FY09. The largest project category, ERs accounted for 78% of the number of LDRD projects and over 57% of the budget for the fiscal year. Projects in this year's ER category ranged in budget from $70K to $2.24M.

Laboratory-Wide Competition

In FY09, 21 LW projects were funded, which represent just over 12% of the LDRD projects for the year and over 6% of the budget. The LW projects for FY09 ranged in funding from $154K to $352K.

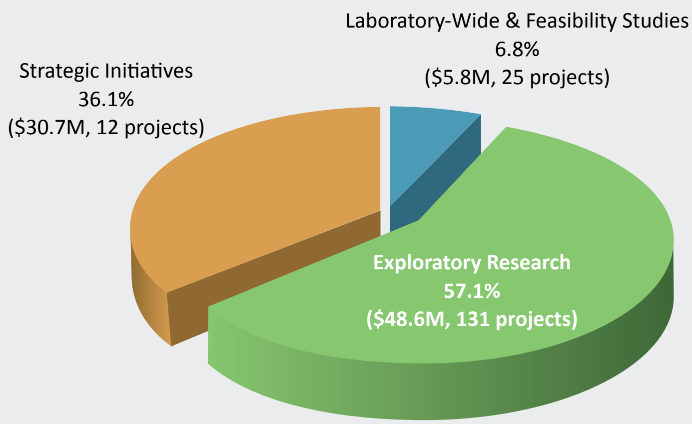
Feasibility Study

The LDRD Program funded just 4 FS projects in FY09, which represent slightly over 2% of the LDRD projects for the year and less than 0.5% of the budget. The FS projects for FY09 ranged in funding from $80K to $125K.

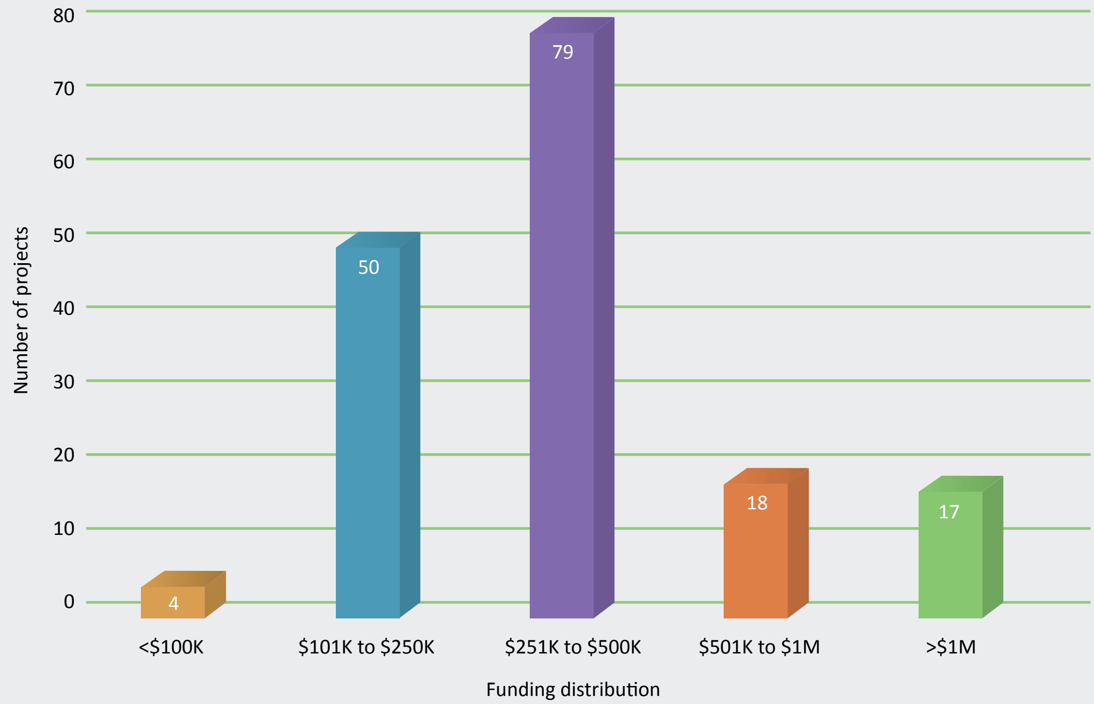
LDRD Statistics

The top bar chart on the next page shows the funding distribution by dollar amount for the 168 FY09 projects—77% of the projects were in the $101K to $500K range, with about 2% falling below $100K. Projects in the $501K to $1M funding range accounted for about 11% of the total, and another 10% of the projects received more than $1M. The average funding level for the 168 projects was $506K.

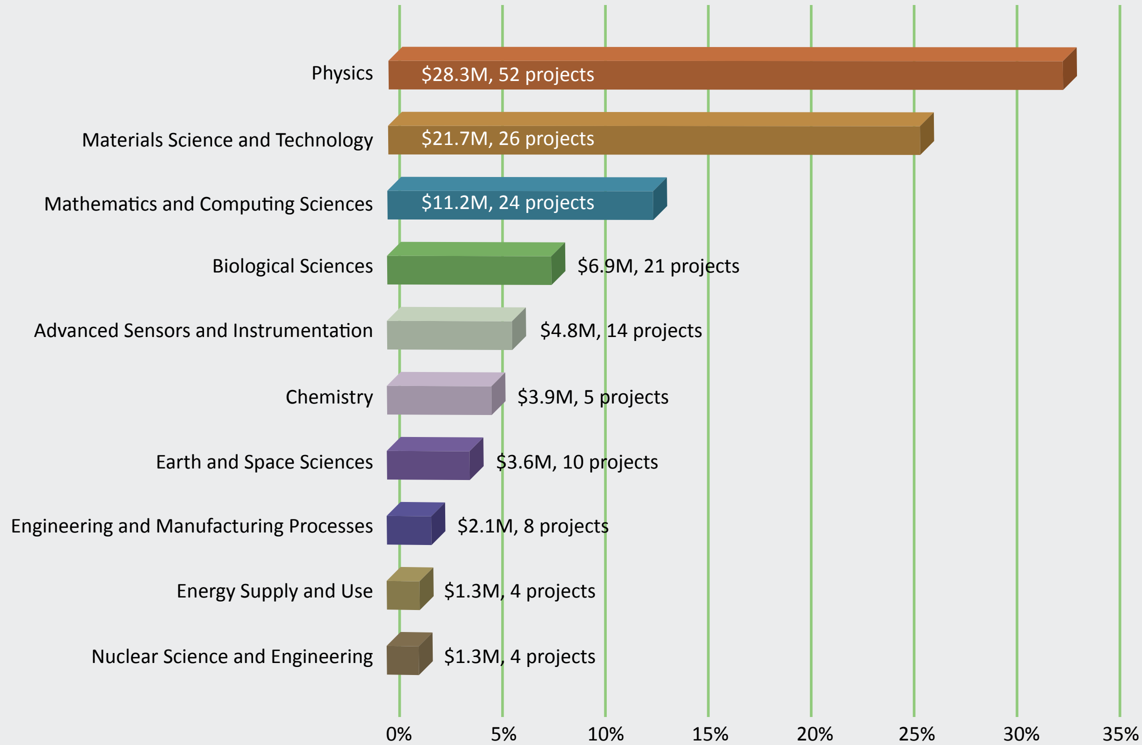
The percentage of LDRD funding and number of projects in each research category for FY09 are shown in the bottom bar chart on the next page.



Distribution of funding among the LDRD project categories. Total funding for FY09 was $85M.



Number of projects and levels of funding. The average funding level for an LDRD project in FY09 was $506K.



Dollar amount and percentage of LDRD funding and number of projects in each research category in FY09.

Highlights of 2009 LDRD Accomplishments

In FY09, the LDRD Program at LLNL continued to be extremely successful in achieving its goals of scientific discovery, providing new concepts for core missions, and creating an exciting research environment that attracts outstanding young talent to the Laboratory. Below is a selection of highlights that exemplify LDRD's noteworthy research results and timely support for the Laboratory's five-year strategic *Roadmap to the Future*, as well as for critical national needs.

Quantum Properties of Plutonium and Plutonium Compounds—
Michael Fluss, Principal Investigator (07-ERD-048)

Mission Focus Area	Stockpile Stewardship Science
Science, Technology, and Engineering Pillars	Materials and Chemistry at the Extremes; High-Performance Computing and Simulation

Plutonium is arguably the most complex element known and one of the least well understood. In the solid form, it exhibits six material phases that vary considerably in density. Plus, a seventh phase may appear when the radioactive metal is under pressure. Experiments over the years have demonstrated other anomalous properties, including an almost complete absence of magnetism and highly unusual resistivity.

One of the most important components of a nuclear weapon is the core or pit, a sphere of plutonium that is compressed by conventional explosives to create a nuclear chain reaction. Understanding the performance of plutonium pits is crucial to Lawrence Livermore scientists and engineers who must ensure the safety and reliability of the nation's nuclear stockpile. Planning the future needs of the U.S. nuclear weapons complex also depends on confidence in the long-term stability of the pit and credible estimates for pit lifetimes.

According to principal investigator Mike Fluss, "gaining a better understanding of the electrons in plutonium will lead to a greater understanding of correlated electron systems in general. And as a monoatomic material, plutonium is relatively simple compared to some of the compounds that also exhibit highly correlated electron behavior." These systems are at the root of many important puzzles within the condensed-matter physics community, including high-temperature superconductivity, heavy fermions, and colossal magnetoresistance.

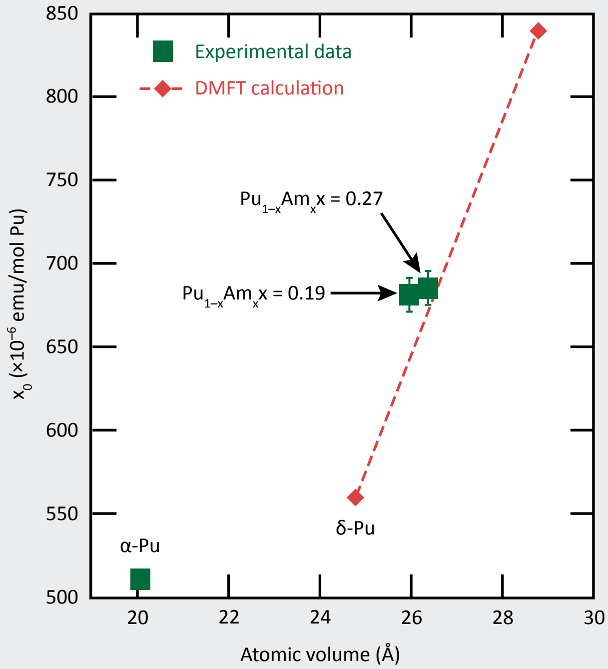
LDRD investigators seek to understand the physics of the 5f orbital shell electrons, which define the properties of plutonium, to help determine why plutonium exhibits such unusual behavior. The team has worked to

- Characterize plutonium at ultralow temperatures
- Probe plutonium compounds to understand electron pairing mechanisms
- Determine why magnetism is not observed in plutonium
- Better understand effects of defects, impurities, and radiation products in plutonium and plutonium alloys

The most significant accomplishments of this project, explains Fluss, "were based on expanding the lattice of plutonium and observing the resulting changes in its physical properties. These changes were created experimentally by alloying americium into plutonium, which has the effect of expanding the distance between atoms throughout the lattice." One change observed was a significant increase in the magnetic susceptibility of plutonium—that is, the change in a sample's sensitivity to an applied magnetic field.

"For decades theorists have predicted magnetic moments in plutonium while experimentalists have been unable to observe them," says Fluss, "and the changes observed experimentally show a clear increase in the magnetic susceptibility and hint at localization at slightly larger lattice expansions." While these measurements were being performed experimentally, a computational technique known as dynamical mean field theory (DMFT) was implemented to calculate the properties of plutonium with an expanded lattice. Remarkably similar results came out of the calculations for similar lattice expansions. But more importantly it indicated, says Fluss, "that these moments do exist on the more closely spaced plutonium lattices, but that they are effectively screened by the large number of conduction electrons in the metal."

This result is exceptionally intriguing because it suggests that selectively removing atoms should also lead to magnetic



The magnetic susceptibility of plutonium increases with atomic volume, showing a trend towards local moment magnetism. The red symbols, values calculated from dynamical mean field theory (DMFT), are in excellent agreement with experimental data (green symbols).

moments arising in plutonium. "And this is precisely what has been observed in our experimental studies of radiation damage," according to Fluss, where the radioactive decay of plutonium atoms results in large damage cascades of vacancies (lattice positions missing an atom) and interstitials (atoms between lattice positions).

Fluss relates that this research "has suggested that a wealth of unexpected properties may arise from radiation damage, and not just in plutonium. This insight has evolved from work on this LDRD, and has spurred interest in probing radiation damage with novel experiments."

Mesoscale Studies of Hydrodynamic Instability Growth in the Presence of Electric and Magnetic Fields—

Peter Amendt, Principal Investigator (08-ERD-062)

Mission Focus Area	Stockpile Stewardship Science
Science, Technology, and Engineering Pillars	High-Energy-Density Science; High-Performance Computing and Simulation

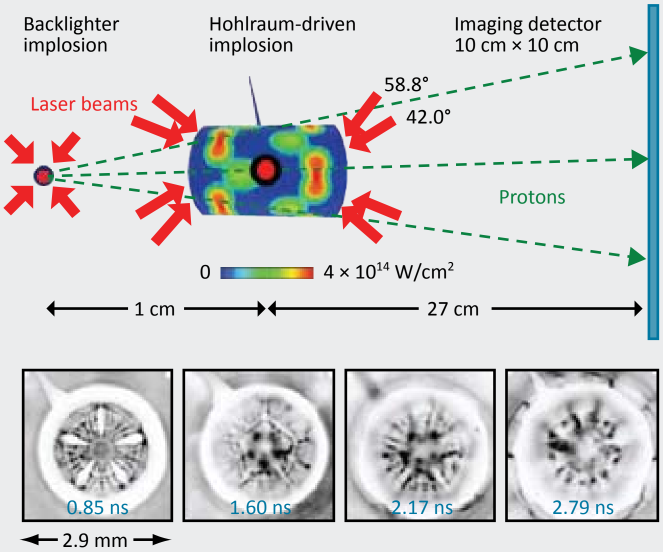
Decades of research and development have been undertaken with the goal of achieving laser ignition—the implosion in a laboratory environment of a small, hydrogen-isotope-filled target capsule by laser beams of sufficient energy and quality to create, for a micro-instant, inertially confined fusion—a process comparable to that at the center of the sun. Laser ignition will represent the first step towards inertial fusion energy, a low-cost, inexhaustible supply of electric power without radioactive by-products through repeated, sustained laser ignition and fusion energy gain.

Understanding hydrodynamic (fluid-like) instabilities in a plasma, both in terms of fundamental physics and computational modeling, is critical to achieving inertial-confinement fusion and other dynamic laser-driven plasma phenomena. To date, it has largely been assumed that the effects of electric and magnetic fields in the plasma are insignificant to these instabilities in the time scales of interest. But if these fields contribute to the instabilities significantly, they may affect the target capsule implosion, which in turn affects the ability to achieve fusion ignition energy.

For this LDRD project, Peter Amendt and his co-investigators are working to understand and model electric and magnetic field effects in imploding systems created by laser-generated x-rays in a gold target case, called a hohlraum, that holds the hydrogen-isotope-filled target. They are developing an understanding of the origin and magnitude of these fields and determining remedial measures if the effects are deemed significant. The team is interpreting the growing database of experimental results to elucidate the underlying physics and benchmark their computational models. This research will have an impact not only on ignition for fusion-class lasers, but also many high-energy-density studies.

"The most significant technical accomplishment of our research was successfully explaining the consequences of observed large electric fields in hohlraum-driven imploding capsules," according to Amendt. A number of anomalies observed from experiments at the OMEGA Laser Facility at the University of Rochester over the past ten years may be explained by the presence of electric fields and their direct impact on ion diffusion in the presence of strong pressure gradients. A recent example, as reported by Amendt and his collaborators in *Science*, was particularly striking. A radiographic image of an x-ray driven implosion in a holhraum, obtained with 14.7-MeV protons emitted by a nearby imploded deuterium and helium-3 capsule, showed five "spokes" that could only be explained by very strong (~300 MV/m), short-lived, local electric fields, and other transient features that are evidence of even stronger (gigavolt/meter) electric fields.

"Our LDRD research succeeded in tailoring the classical fluid-based concept of diffusion to include critical plasma physics effects such as self-generated electric fields and the average ionization states of the fuel ions," Amendt says. In other words, the project has developed a scientific basis for modeling and understanding magnetic and electric fields in plasmas in detail. Applying this new, diffusion-based model to several OMEGA implosion campaigns, where a significant deficit of thermonuclear neutrons was seen, has resulted in good agreement without the need for invoking higher levels of hydrodynamic instability growth.



Schematic of the OMEGA experimental setup for observing an imploding capsule (top), as given by C. K. Li, et al. in the March 5, 2010 *Science* article, "Charged-Particle Probing of X-ray–Driven Inertial-Fusion Implosions." Fifteen laser beams (red arrows) entered each end of the cylindrical hohlraum target case with two different incident angles. The colors shown on the hohlraum wall (center) indicate the computer-modeled predicted laser intensity distribution. The backlighting protons (green arrows) pass through the hohlraum interior, sampling the plasma conditions and capsule implosion at four different times (bottom images). Within each image a darker exposure means higher proton transmission.

The key impact of this research on ongoing Livermore missions is that a new physics-based explanation of previously unexplained observations in the implosion database helps better prepare the Laboratory for upcoming ignition campaigns on the National Ignition Facility, the world's largest and highest-energy laser system. The principal goals of the facility are to achieve thermonuclear fusion of a deuterium–tritium fuel capsule and provide the high-energy-density physics regimes needed for experiments related to national security, fusion energy, and broader scientific discovery.

Amendt states, "This LDRD-sponsored exploratory research has demonstrated the value of pursuing high-risk investigations that can achieve significant and unforeseen payoffs to the core Laboratory missions." Furthermore, the fundamental ideas developed in this research "underscore the value of the Laboratory's scientific environment in developing breakthroughs and offer a vivid example to potential recruits of why Livermore remains a recognized center for world-leading science."

Detection, Classification, and Estimation of Radioactive Contraband from Uncertain, Low-Count Measurements—

James Candy, Principal Investigator (07-ERD-019)

Mission Focus Area	Nuclear Threat Elimination
Science, Technology, and Engineering Pillar	Measurements and Experimental Science

Each year, some 48 million cargo containers move among the world's ports. More than 6 million of these enter the U.S., but only about 2 percent are opened and inspected when they arrive at U.S. seaports. The West Coast ports of Los Angeles–Long Beach, Oakland, and Seattle alone process 11,000 containers per day, or about 8 containers per minute.

Because of this high traffic volume, U.S. seaports are especially vulnerable to a terrorist attack. Illicit radioactive materials could be hidden in any one of the cargo-filled containers that arrive at U.S. ports. Yet, searching every shipment would bring legitimate commercial activities to a halt. Improving security at U.S. ports is thus one of the nation's most difficult technical and practical challenges because the systems developed for screening cargo must operate in concert with ongoing seaport activities.

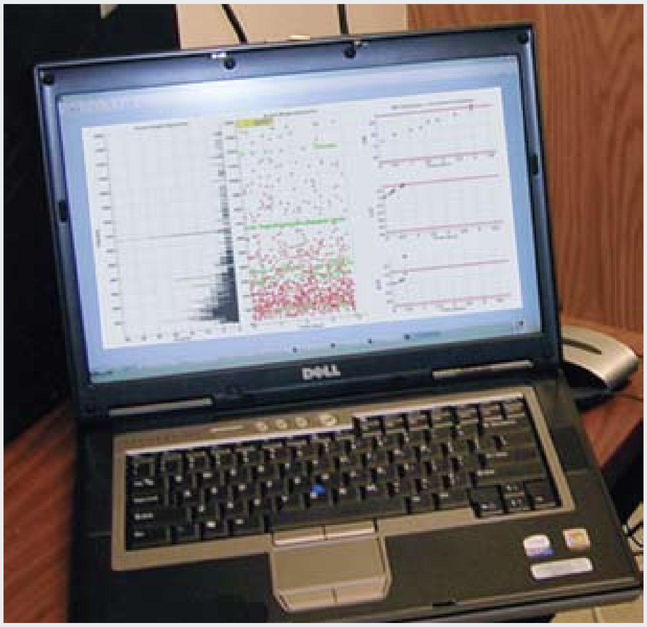
Working at this intersection of commerce and national security, Livermore LDRD researchers are applying their expertise in radiation science and detection to develop improved technologies for detecting hidden radioactive materials. This project is focused on detecting, classifying, and identifying illicit special nuclear materials from highly uncertain, low-count radionuclide measurements. This technology is more important than ever, especially for scenarios requiring timely detection and involving low-count data and a source such as a cargo container and a detector that are both moving.

According to the principal investigator James Candy, the LDRD research "enabled not just me but the entire team to grow by cross-fertilizing the areas of statistical signal processing with radiation transport physics, making possible a unique, breakthrough solution to a long-troubling problem, especially in today's climate of terrorist threats." The result was a novel software solution that nonexperts can use to rapidly and reliably detect radionuclides when accurate identification of radioactive material is required, especially when measurement time is short and demand for confidence is high.

The Statistical Radiation Detection System (SRaDS) applies a Bayesian (accumulated evidence) detection scheme using both simulated and controlled experimental data, a signal-processing transport model based on point-to-point modeling by incorporating transport physics and validating the results with full-physics simulations, and the first implementation of sequential detection incorporating photon–electron (Compton)-scattering physics into the signal processor.

This physics-based solution provides the framework for a wealth of solutions to many radiation-detection problems, including:

- Large stationary radiation monitors used at inspection stations, customs, border crossings, and limited-access areas
- Portable gamma detectors used by first responders
- Surveillance equipment for marine inspections and harbor patrols
- Cargo-container inspections
- Hazardous material management
- Verification of nonproliferation treaties
- Manufacturing and tracking special nuclear material



A notebook computer implementation of Statistical Radiation Detection System software showing statistically significant results obtained from a radiation detector.

- Field operations at uranium mines, weapons facilities, and nuclear power plants
- Medical and research activities involving radioactive material

Candy notes that with this project, “We encouraged many of our younger researchers to take leadership roles for a variety of tasks throughout the project. For example, some presented our approach to NNSA program leaders, while others acted as liaisons with potential industrial partners.”

For Candy, “the successful research allowed for my technical growth in nuclear physics signal processing.” In collaboration with another senior LDRD investigator, he is currently applying this new expertise to enhanced baggage inspection using x-rays at airports.

Developing a First-Principles Computational Toolkit for Predicting the Structural, Electronic, and Transport Properties of Semiconductor Radiation-Detection Materials—

Vince Lordi, Principal Investigator (07-ERD-13)

Mission Focus Area	Nuclear Threat Elimination
Science, Technology, and Engineering Pillar	Measurements and Experimental Science; High-Performance Computing and Simulation

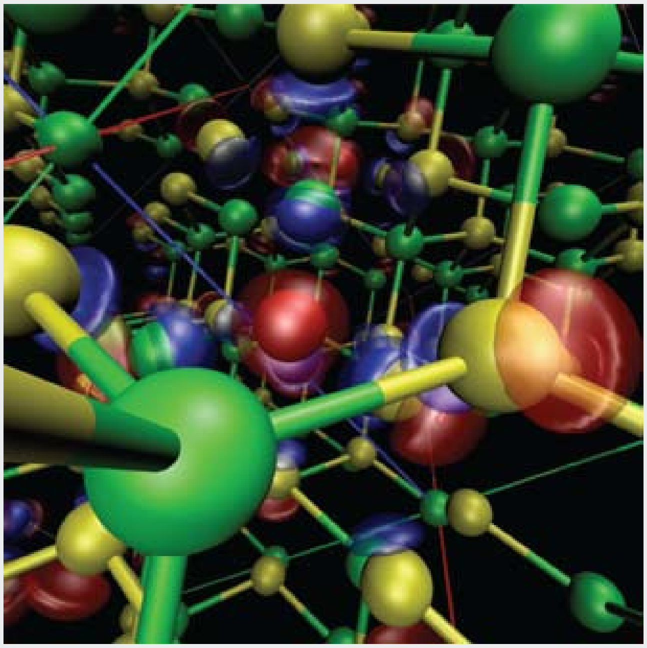
Ensuring that the country remains safe from a nuclear or radiological attack is driving the search for more definitive radiation detection and identification technologies. Detecting illicit sources of plutonium and highly enriched uranium is a priority for first responders, airport security personnel, and U.S. port and border inspectors. Both plutonium and highly enriched uranium are typically identified by using a combination of devices to detect their invisible gamma and neutron radiation emissions. For many years, these existing detection technologies were deemed adequate. However, in 2005 the Department of Homeland Security called for development of significantly more effective materials to detect gamma and neutron radiation emissions. New materials for smaller, faster, and more accurate sensors could improve the nation’s ability to unambiguously identify radiation from illicit sources.

For field applications, radiation detectors must be inexpensive and robust, operate at ambient temperature, provide high efficiency, and be small enough for use in covert operations. They must also provide unambiguous identification of a material. Early work at Livermore on new detector materials for low-energy neutrons from radioactive sources was funded by LDRD. As that project and others demonstrated success, outside funding for new detector materials followed, first from the NNSA and later from the Department of Homeland Security and the Defense Threat Reduction Agency.

LDRD researchers for this project are motivated by the search for new or improved semiconductor materials required for room-temperature radiation detectors. Their goal is to develop tools to predict structural and transport properties of semiconductors, enabling acceleration of material development efforts. As principal investigator Vince Lordi explains, “the task is particularly daunting because in real devices, the semiconductor materials have defects and do not behave ideally. Accurately predicting the distribution and effects of these defects is critical to computational design of electronic devices with optimum performance.”

The team is calculating the formation of defects for candidate materials and their impact on the ability of a semiconductor to carry a charge and its lifetime. In addition, they are determining the intrinsic limits of candidate materials. This project has led to the development of new predictive computational methods—including “computational combinatorial chemistry”—for rapidly screening semiconductors for detrimental and beneficial defects and impurities, enabling the design of materials with optimal transport properties for a given application, particularly radiation detection. A noteworthy success was an order-of-magnitude improvement in the performance of aluminum antimonide detectors based on their predictions.

The team has successfully developed techniques to rapidly and accurately predict the effects of defects on the electrical and optical properties of semiconductor materials, using only simulations with no free parameters. The framework improved the speed of the calculations by several orders of magnitude, enabling concerted efforts between theorists and experimentalists to successfully optimize device performance by engineering the defect distributions in the material. As Lordi explains, “our techniques enabled demonstrated improvements of an order of magnitude in material performance for radiation detectors compared to the prior experimental state-of-the-art.”



The atomic structure of a semiconductor containing a defect is shown, with red and blue regions indicating scattering centers that impede the flow of current through the material. Green and yellow spheres represent aluminum and antimony atoms, respectively.

According to Lordi, “This LDRD project absolutely had a positive impact on my professional career at LLNL. It enabled me to gain valuable experience leading a team, while also advancing the state-of-the-art of a scientific discipline not tied directly to a large Laboratory program.” He goes on to say, “At the same time, this project allowed me opportunities to share the new work our group was performing with other scientists at the Laboratory to make the connections to other Livermore needs.”

Based on the success of this project, the NNSA Office of Nonproliferation Research and Development will support continued research efforts in applying predictive first-principles modeling of defects and transport in semiconductors to help optimize new materials for room-temperature gamma radiation detectors.

Microarrays + NanoSIMS: Linking Microbial Identity and Function—

Jennifer Pett-Ridge, Principal Investigator (07-ERD-053)

Mission Focus Areas	Biosecurity; Energy and Climate
Science, Technology, and Engineering Pillars	Measurements and Experimental Science

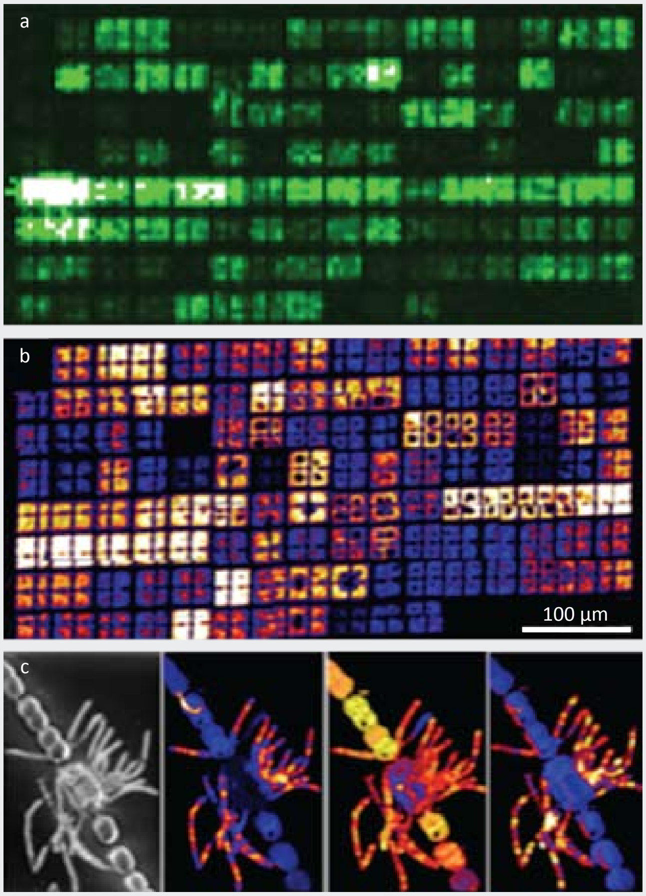
What technology is necessary to simultaneously address issues in bioterrorism, energy generation, human disease, and bioremediation science? The Department of Homeland Security, for example, is interested in rapid identification of bioagents and better methods to distinguish a natural disease outbreak from an intentional release. The production of alternative fuels from renewable, non-food, biological feedstocks is an important component of any future alternative energy strategy and for addressing climate change emissions. The future of biology and medicine depends on the development of technologies and research approaches that embrace the high degree of complexity in biological systems. And conditions for effective bioremediation of chemicals in the soil or groundwater must be correct or the cleansing microbes may grow too slowly, die, or worse, create more harmful chemicals.

This LDRD effort is focused on addressing all of these issues. Researchers are developing a next-generation microarray for rapid genetic identification of biothreat agents. A microarray is a massively parallel way to survey the genetic expression of thousands of genes, from different populations of cells, using microscopic spots of genetic material arrayed on a grid that are labeled with fluorescent dye and scanned by a laser. The team re-engineered the microarray through optimized slide surface preparation and coating procedures to create an indium tin oxide array on a plastic, unbreakable chip with an improved, high signal-to-nose background. They then combined the re-engineered microarray with nanoscale secondary-ion mass spectrometry (NanoSIMS) analysis by leveraging LLNL’s mass spectrometry capability. The technology has resulted in a patent application as well as publications in the *Proceedings of the National Academy of Science of the United States of America* and *Applied and Environmental Microbiology*.

Against a background of non-enriched genes, the team is identifying isotopically enriched rRNA in carbon-13-labeled bacteria extracted from cellulose-degrading biofilms, human tissues, and contaminated soils. They then compare these data to the standard fluorescence analysis of an array.

As principal investigator Pett-Ridge explains, “approaches that we developed in this LDRD project enabled two novel technologies that allow us to link microbial metabolism to phylogenetic identity.” She elaborates that “connecting the composition of a microbial community to its function has been the ‘Holy Grail’ of microbial ecology for the past decade, and the methods we developed are already being used to better understand cellulose degradation, terrestrial and marine carbon cycling, and microbial symbioses.”

The advanced approaches developed with this project have enabled analysis of complex biological communities such as nitrogen-fixing bacteria derived from a dihydrogen-producing beetle as well as seawater-carbon-fixing bacteria. In addition, researchers are developing the ability to identify organisms metabolizing carbon dioxide or nitrogen using NanoSIMS analysis.



Re-engineered microarray showing fluorescence signal following rRNA hybridization of soil bacterium (a). Nanoscale secondary-ion mass spectrometry (NanoSIMS) carbon-13 images, indicating distribution of isotopic enrichment across the same array region (b). In situ, single-cell fluorescence and NanoSIMS images of a microbial consortium consisting of filamentous cyanobacteria and alphaproteobacteria attached to heterocysts (c).

This research provides applications to address a variety of broad issues, including:

- An improved array methodology for biosecurity research
- Development of biofuels, fuel cell bioreactors, and secure energy sources
- Environmental remediation with microbial degradation of contaminants
- Modeling of microbial roles in carbon sequestration and global climate change

According to Pett-Ridge, "the positive attention we've received for spearheading these techniques has illustrated the important role LLNL can play at the intersection of biology and isotope chemistry." For her personally, "the research projects are extremely rewarding, and I hope to build upon them to make significant scientific discoveries in the coming years." The DOE Office of Biological and Environmental Research will support follow-on research using techniques developed with this project to study biofuel and dihydrogen-producing microbial systems, particularly the wood-eating beetle hindgut and microbial mats.

Chemical and Structural Modification and Figure Control During Glass Polishing—Tayyab Suratwala, Principal Investigator (08-ERD-055)

Mission Focus Area	Advanced Laser Optical Systems and Applications
Science, Technology, and Engineering Pillar	Materials and Chemistry at the Extremes

The laser, invented just over 50 years ago, has become a transformative technology with immense scientific, commercial, industrial, and societal importance. It is now a multi-billion dollar industry and plays a pivotal role in everyday life, with uses in optical storage devices, fiber-optic communications, materials processing, medicine, and weapons. Perhaps most importantly, the laser is now an indispensable scientific tool for advanced measurements, allowing researchers to further understand nature's fundamental building blocks and properties of the universe. Lasers are also essential to the Stockpile Stewardship Program's ability to understand weapons physics and materials under extreme conditions of temperature, pressure, and strain rate. In addition, the laser holds the promise of ignition and a self-sustaining elemental fusion burn, which could create an inexhaustible source of clean energy.

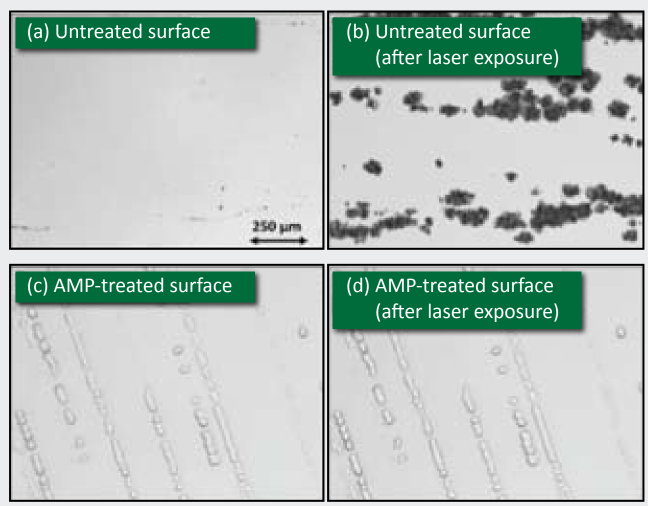
The maximum output energy or power available from high-energy laser systems used for scientific research is typically limited by laser-induced damage to the optical system that transports the laser beam. LDRD investigators are forming a science-based physical picture for understanding and preventing one of the most insidious sources of laser-induced damage to high-quality fused silica optical components: damage caused by "rogue" particles that scratch the surface in the optical polishing process.

According to principal investigator Tayyab Suratwala, "we have found that the primary issue is surface fractures generated during the polishing and shaping process." To address this problem, Suratwala and his team subjected fused silica optical components to a series of controlled etching experiments in the laboratory, followed by laser irradiation. The team found that laser damage resistance was strongly process-dependent and scaled inversely with scratch width—a result that was further explained with a detailed mass transport model of the process.

With the optimized etch process, the resistance of fused silica to laser damage increased dramatically. For a 30-µm wide scratch, the material could withstand about 6 times more laser fluence (41 J/cm^2) before damage was initiated. Also with the new etch process, the statistical probability that an ensemble of scratches will initiate damage at 12 J/cm^2 decreased by a factor of about 100,000. The optimized etch process is now being used to treat fused silica optics at the National Ignition Facility to improve laser damage performance.

"For those who work in Laboratory programs, LDRD projects are a wonderful way to obtain a more fundamental and scientific understanding of key problems," says Suratwala. "It is even more fulfilling to see that our understanding later undergoes technology transfer to solve real-world problems." In addition to extending the capability of fusion-class lasers by significantly extending the useful lifetime of expensive optical components, this project advances scientific knowledge in glass finishing and polishing. It will also be of general interest both to the precision optical and semiconductor industries because it

- Achieves greater control of glass surface profiles



Optical micrographs of scratches on fused silica surfaces before (left images) and after high-energy laser shots (right images) for an untreated sample (a, b) and a sample treated with the Advanced Mitigation Process developed in this project (c, d).

- Enhances the understanding of chemical interactions that occur on the glass surface during polishing
- Alters or removes the chemically or structurally modified surface layer of glass
- Increases the damage threshold of glass surfaces

In addition to publications in *Applied Physics Letters* and the *Proceedings of SPIE* (the journal of the International Society for Optical Engineering) the LDRD team has submitted a patent application for methods to treat silica optics to reduce optical damage.

Role Discovery in Dynamic Semantic Graphs—
Tina Eliassi-Rad, Principal Investigator (09-ERD-021)

Mission Focus Area	**Cyber Security, Space Security, and Intelligence**
Science, Technology, and Engineering Pillar	**Information Systems**

With today's intelligence community facing massive amounts of data to analyze for a wide range of complex national security applications, the automation of intelligence analysis is imperative. Computational tools are needed to sift through vast quantities of surveillance data, for example, to find patterns, entities, and relationships that can then be brought to the attention of a human analyst.

One such tool is the dynamic semantic graph, which can uncover relationships hidden in streams of data from multiple sources—one of the most challenging data-analysis scenarios. Essentially, dynamic semantic graphs help analysts to literally "connect the dots" by determining the paths that connect the many entities, such as the roles and relationships of individuals in a clandestine organization. Consequently, this analytical tool is used widely in cyber security, counterproliferation, counterterrorism, and other national security applications involving networks of people, machines, or both.

Role discovery—identifying what function a particular entity performs in the network of entities being examined—is an essential component of graph analysis. This technique allows analysts to uncover hostile elements in collected data by modeling behavior or detecting anomalies, for instance. In the cyber security domain, this technique could model the function of computer hosts over time to detect suspicious activities such as an abrupt role change. The two types of models currently used for role discovery both have significant shortcomings: predictive models tend to focus on predictions of a single aspect in a static graph, while process models tend to yield general properties from a dynamic but homogeneous graph.

An LDRD team led by principal investigator Tina Eliassi-Rad, along with collaborators from universities and industry, are working to combine both prediction and process-based models. They are developing algorithms that infer the roles and functions of entities hidden in dynamic semantic graph data and track how these roles evolve over time. According to Eliassi-Rad, "the project allowed them to investigate fundamental questions in network science for which they received recognition in the external research community." Their approach to role discovery comprises three steps:

- Data "cleanup," in which attributes and relationships are predicted
- Group discovery, which also looks at how groups change over time
- Information diffusion, in which multifaceted information is diffused through the groups identified

The team has discovered that commonly used statistical tests can result in unacceptably high levels of false positives for graph classifiers. The team has determined that up to 40% of the time, learning algorithms will appear to be different when they are not. Using theoretical analyses of the sources of this bias, they developed a new statistical test that limits false positives while providing reasonable levels of statistical power.

A second major accomplishment concerned searching graph data, such as a social network, to find communities (groups of nodes with common interests). They found that frequently used community-discovery algorithms do not offer all of the desirable characteristics, such as effectiveness in terms of link prediction performance, or the ability to find the appropriate number of communities automatically. To fill this gap, the team developed the probabilistic Hybrid Community Discovery Framework, which was shown to effectively incorporate hints from a number of other community-detection algorithms and produce results that outperform its constituent parts. The approach was presented at the 2010 SIAM International Conference on Data Mining and as an invited seminar at Google.

"This LDRD project makes a positive difference in my career goals," says Eliassi-Rad. She expects the team's work "to have widespread impact in the network science community. Our work on the correct way of evaluating network classifiers to compare their differences is applicable throughout the field." Furthermore, "Our work on community-discovery algorithms not only introduces new ways of evaluating such algorithms but also provides a systematic way of combining multiple algorithms."

Members of the role discovery project for analysis of intelligence data include (left to right): Tina Eliassi-Rad (principal investigator), Brian Gallagher, and Keith Henderson.

LDRD Metrics

Intellectual Property

Projects sponsored by LDRD consistently account for a large percentage of the patents issued for LLNL research, especially considering that the program represents a small portion of the Laboratory's total budget. In FY09, LDRD costs at LLNL were $85M, which is 5.76% of the total Laboratory costs, yet LDRD generated 43% of Laboratory patents. The number of patents resulting from LDRD-funded research since 2005 and the percentage of total patents that were derived from LDRD research and development is shown in the table below. LDRD investment in a technology is typically made several years before the technology is actually patented. Furthermore, although an LDRD-sponsored project makes essential contributions to such technologies, subsequent programmatic sponsorship also contributes to a technology's further development.

Notably the number of patents decreased significantly over this time period, most likely because from 2005 through 2007, patents were not an institutional priority. In December, 2007, a functional management assessment of the patenting and licensing processes at LLNL was conducted by the new contractor. The findings and recommendations pointed to an immediate need to transform the manner in which intellectual properties were selected for patenting and actually patented. Starting in 2008, patents again became a priority, and the Industrial Partnerships Office at LLNL took significant steps to encourage and submit new patent applications. The number of patent applications per year at LLNL is now increasing, and early indications suggest that the patents will increase in 2010. Despite the recent downturn, LDRD projects continued to generate 40% or more of Livermore's total patents.

Patents	2005	2006	2007	2008	2009
All LLNL patents	93	63	62	57	46
LDRD patents	51	29	32	23	20
LDRD patents as percentage of total	55%	46%	52%	40%	43%

Patents resulting from LDRD-funded research as a percentage of all LLNL patents for the last five years. Year shown is the year patent was granted.

As with patents, records of invention submitted by LDRD researchers account for a significant percentage of the total for the Laboratory. Overall, LDRD records of invention for 2005 to 2009 account for approximately 43% of the 719 total. In 2009, Livermore submitted 145 records, with 56 (39%) of those attributable to LDRD-supported projects. The general trend in the number of records of invention, which showed a notable decrease in FY08, has recovered more rapidly than the trend for patents. While records of invention arise readily from active research, the number of those that become patent applications and eventually patents is strongly limited by the high cost of that process, which typically takes several years.

Record of Invention	2005	2006	2007	2008	2009
All LLNL records	145	157	162	110	145
LDRD records	63	74	69	44	56
LDRD records as percentage of total	43%	47%	43%	40%	39%

Records of invention resulting from LDRD-funded research as a percentage of all LLNL records for the last five years.

Finally, LDRD also plays a role in producing Laboratory copyrighted material. From 2005 to 2009, LDRD-supported projects accounted for over 23% of the 336 Livermore copyrights. In 2009, LLNL had 47 copyrights, with 12 (26%) that could be attributed to LDRD research.

Publications in Scientific Journals

LDRD publications in scientific journals demonstrate that research and development under LDRD furthers the progress of the broad scientific and technical community by contributing new scientific results and innovative technologies, sometimes marking fundamental breakthroughs. In a typical year, Laboratory scientists and engineers collectively publish more than 1,000 papers in a wide range of peer-reviewed journals. In 2009 there were 1,001 such articles, of which at least 161 (16%) resulted from LDRD projects. The downward trend in recent years is in part related to a decrease in the size of the scientific and engineering workforce at LLNL. During FY08 this population at Lawrence Livermore decreased by 15% (from 3,412 to 2,891), and the number of postdoctoral researchers declined by 19% (from 147 to 119). Since that year, the total population of scientists and engineers at LLNL has remained relatively constant at the lower number (~2,900), and the postdoctoral population has not recovered to pre-FY09 levels. Further, because most of LLNL's postdoctoral researchers are sponsored by LDRD and represent a substantial component of the Laboratory's publishing scientists and engineers, this decline in the number of postdoctoral researchers is an important contributing factor to the lower number of publications from 2007 through 2009. The decrease in publications in 2009 is also attributed, in part, to the time lag between manuscript submission and actual publication. An additional reason for the decline in publications for the last two years is that a few highly productive international collaborations that included LLNL were drawing to a close. The following table shows the number of journal articles per calendar year resulting from LDRD-funded research since 2005 and the percentage of total articles that were derived from LDRD research and development.

Journal Articles	2005	2006	2007	2008	2009
All LLNL articles	1,296	1,237	1,162	1,097	1,001
LDRD articles	241	223	237	212	161
LDRD articles as percentage of total	19%	18%	20%	19%	16%

Peer-reviewed journal papers resulting from LDRD-funded research as a percentage of all LLNL papers for the last five years.

Collaborations

External collaborations are absolutely essential to the conduct of research and development in LDRD. By collaborating formally and informally with other national laboratories, academia, and industry, LDRD investigators are able to access world-leading facilities and knowledge—both in the U.S. and abroad—and serve as active and prominent members of the broad scientific and technical community. External collaborations are also key for assembling the best teams for pursuing many research and development activities, complementing LLNL's capabilities and expertise. In addition, LDRD collaborations create strong relationships that are valuable for the Laboratory's pipeline for recruiting scientific and engineering personnel.

The FY09 portfolio included 75 formal LDRD-funded collaborations involving 57 LDRD projects (34% of the total projects funded). Collaborating institutions included the University of California (27% of total collaborations), other academic institutions (51%), DOE sites (13%), and other collaborators (e.g., other government agencies and industry, 9%). These statistics do not include the numerous informal collaborations that PIs pursue in the course of their LDRD projects.

Postdoctoral Researchers

Because LDRD funds exciting, potentially high-payoff projects at the forefront of science, the program helps recruit top talent in new and emerging fields of science and technology. In FY09, the LDRD Program supported over 80% of the Laboratory postdoctoral researchers. Of the 119 postdoctoral researchers at the Laboratory, 97 were supported by LDRD projects. The Laboratory continues significant recruitment efforts to increase the total number of postdoctoral researchers.

Awards and Recognition

A primary goal of LDRD is to foster excellence in science and technology that will attract and maintain the most qualified scientists and engineers, and allow scientific technical staff to enhance their skills and expertise. Laboratory LDRD principal investigators and research teams receive numerous prestigious honors, awards, and recognition for LDRD-funded work. These recent honors attest to the exceptional capabilities, talents, and performances of these researchers, as well as serve as another indicator of the success of the LDRD Program at Livermore.

American Geophysical Union Fellow

Frederick (Rick) Ryerson was named a fellow of the American Geophysical Union in 2009 for his "contributions to our understanding of transport processes in minerals, magmas, and crustal rocks at all scales." Ryerson has been the principal investigator for numerous LDRD projects spanning more than 20 years, including a high-pressure apparatus for geophysical and geochemical research (87-DE-007), the physics and chemistry of Earth materials (93-ERI-049), and tectonic changes of the San Andreas Fault (03-ERI-001). He is currently a member of the scientific team for an integrated response to nuclear incidents using nuclear forensics (10-SI-016).

Frederick Ryerson

American Physical Society Division of Plasma Physics Vice Chair

Steve Allen has been elected the 2009 vice chair of the American Physical Society's Division of Plasma Physics. Allen has led several LDRD projects related to the tokamak reactor concept of producing controlled thermonuclear fusion power with the use of a magnetic field to confine a plasma. Specific projects included development of a new tokamak divertor to reduce the peak heat load (92-SR-025), measurements to facilitate advanced tokamak science in burning plasma experiments (06-ERD-024), and critical enabling issues for burning-plasma diagnostics (09-ERD-030).

Steve Allen

American Physical Society Fellows

Andrew MacKinnon and Per Söderlind were elected as 2008 fellows of the American Physical Society, and Christine Orme and Steve Wilks were recognized as two of five LLNL 2009 fellows. Election is limited to no more than one half of one percent of the association's membership for a given year.

- Andrew MacKinnon was honored "for pioneering experimental studies of interactions

Andrew MacKinnon

of intense laser pulses with matter and in particular, the physics and applications of short-pulse laser-driven proton beams." He has served as a principal investigator for proton radiography investigations of laser–plasma interactions with picosecond time resolution (02-ERD-012) and developing the physics basis of fast-ignition experiments at future large fusion-class lasers (05-ERI-001), and is currently a co-investigator for fast-ignition proof-of-principle experiments (08-SI-001).

- Per Söderlind was cited "for important contributions in electronic-structure theory for transition and actinide metals, particularly plutonium." He has participated in a variety of LDRD projects such as investigation of electronic phase transitions occurring in metals at high pressures and temperatures (04-ERD-0200) as well as a current project on the thermodynamic and kinetic modeling of advanced nuclear fuels (10-ERD-059).

Per Söderlind

- Christine Orme was honored for her "outstanding contributions in understanding the fundamental physics of crystallization and materials assembly with application to biomineralization, biomimetic synthesis, and shape control of nanostructures." She has served as a principal investigator for research into understanding shape control in the synthesis of nanoparticles (06-LW-090) and engineering titanium for improved biological response (00-ERI-006).

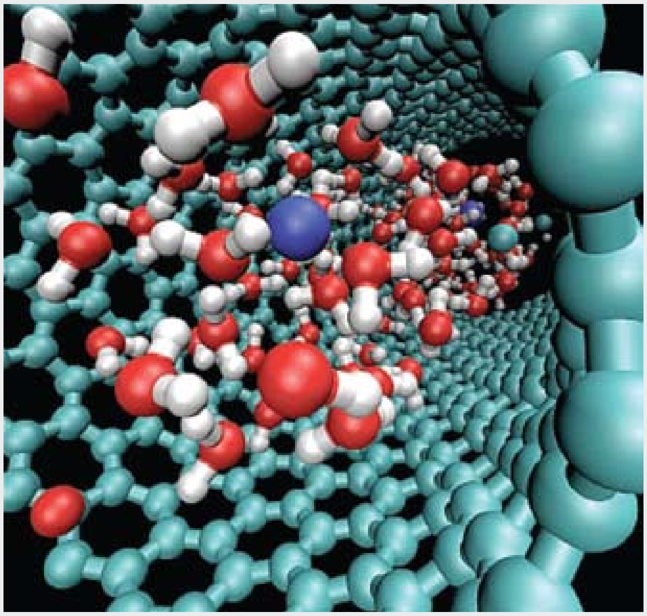
Christine Orme

- Scott Wilks has been a principal investigator for several projects, including research on creating relativistic antimatter plasmas and electron–positron jets with ultra-intense lasers (04-LW-020 and 07-LW-016), and micro-targets for high-energy-density physics (08-ERI-001). He was honored for "pioneering contributions to the understanding of intense and ultra-intense laser plasma interactions and their applications to high-energy density science, including fast ignition, ion acceleration, and positron generation."

Scott Wilks

Breakthroughs in Computational Science

Eric Schwegler and Giulia Galli, a former LDRD researcher now at the University of California at Davis, produced computer simulations of interfaces between aqueous and other materials that were called out as one of the "Breakthroughs in Computational Science" by a DOE Scientific Discovery through Advanced Computing (SciDAC) panel. The groundwork for this research came from several LDRD projects, including properties of confined water and fluid flow at the nanoscale (06-ERD-039).



Simulation of fluid flow through a nanometer-sized tube.

Cozzarelli Prize

The *Proceedings of the National Academy of Sciences* (PNAS) recognizes the most outstanding contributions in each of the scientific disciplines represented by the National Academy of Sciences with the Cozzarelli Prize. Papers receiving the Cozzarelli Prize were chosen from nearly 3,500 research articles published by PNAS in 2008 for demonstrating scientific excellence and originality. In the physical and mathematical sciences, "Fluid Helium at Conditions of Giant Planetary Interiors," was the prize recipient, authored by two university collaborators working on an LDRD project concerning the physics and chemistry of the interiors of large planets (09-SI-005).

DOE Outstanding Mentor Award

Nine scientists and engineers, seven of whom are LDRD researchers, received the DOE's Outstanding Mentor Award for the summer of 2008 for their work with DOE-sponsored summer students. Outstanding mentors provide well-defined research projects that match the student's research interests and demonstrate practices that go above and beyond the normal responsibilities to students in the mentoring relationship. The awards are unique because the recipients are nominated by the students from the previous summer. Recipients include Nerine Cherepy, who is developing advanced rare-event detectors for nuclear science and security (10-SI-015); Sergei Kucheyev, currently examining radiation-tolerant materials (09-SI-003); Joshua Kuntz, studying transparent ceramics optics and advanced armor with nanostructured materials (09-ERD-029); Stephan Letts, investigating high-performance polyimide coating technology (97-ERD-016); Brent Segelke, currently studying virulence mechanisms of the plague bacterium (08-LW-025); Michael Stadermann, examining the structure and transport of water and hydrated ions within hydrophobic, nanoscale channels (07-LW-056); and Ross Williams, a past LDRD researcher on projects spanning several categories of work including the biogeochemical cycling of iodine-129 from nuclear fuel reprocessing plants (02-ERD-058).

Federal Laboratory Consortium Award for Excellence in Technology Transfer

Noninvasive pneumothorax detection has been awarded a Federal Laboratory Consortium Award for Excellence in Technology Transfer for 2009. The handheld device can quickly detect pneumothorax, a medical condition caused by air trapped in the space between the wall of the chest cavity and the lung. John Chang was the principal investigator on two different LDRD projects that led to the diagnostic device: impulse radar application for cardiac monitoring (01-ERD-088) and concealed threat detection (02-ERD-061).

Handheld noninvasive pneumothorax detector.

Federal Laboratory Consortium Far West Regional Awards

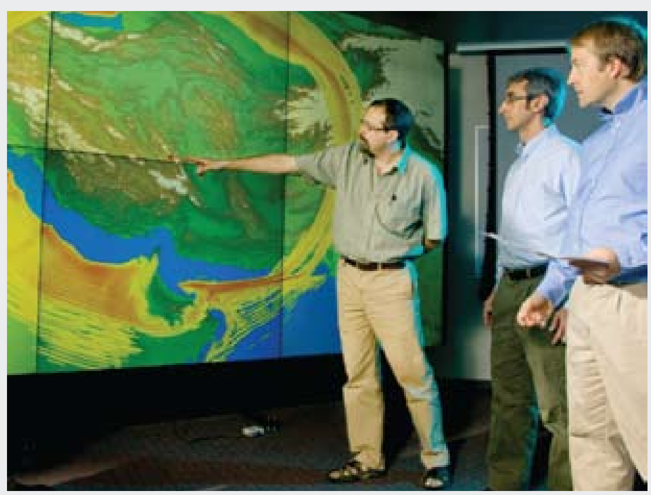
The large-area imager for long-range radiation detection received an Outstanding Partnership award from the Federal Laboratory Consortium's Far West Region competition. The technology was the result of a collaborative research effort involving Lawrence Livermore, University of California at Berkeley, and Oak Ridge National Laboratory. Investigators developed a radiation-sensing device mounted in a truck that pinpoints illicit nuclear material with total insensitivity to variations in an area's radiation field. The early development of this imager was supported by Lorenzo Fabris' LDRD project on the long-range passive detection of fissile material (03-ERD-048).

Lorenzo Fabris, Thomas Karnowski, and Klaus Ziock (left to right) and the large-area imager.

Carbon nanotube technology for water desalination and filtration received a Federal Laboratory Consortium Far West Regional Award for outstanding technology development. During their research, the team found that carbon nanotube membranes demonstrated permeability that is significantly higher than conventional membranes, despite having smaller pore sizes. Members of the carbon nanotube team include Olgica Bakajin, Aleksandr Noy, Jason Holt, Hyung Gyu Park, and Francesco Fornaseiro, most of whom are LDRD researchers that have laid the groundwork for this technology, along with other LDRD investigators, with numerous nanotube projects including carbon-nanotube permeable membranes (03-ERD-050), properties of confined water and fluid flow at the nanoscale (06-ERD-039), and transport of water and hydrated ions within hydrophobic, nanoscale channels (07-LW-056).

Fulbright Scholarship

Laboratory geophysicist Artie Rodgers received a Fulbright Scholarship to study the relationship between topography and seismology at Laboratoire de Géophysique Interne et Tectonophysique, Université Joseph Fourier in Grenoble, France. The Fulbright program is the most widely recognized and prestigious international exchange program in the world, and actively seeks out individuals of achievement and potential who represent the full diversity of their respective societies and selects nominees through open, merit-based competitions. European seismologists have studied earthquake motions in alpine valleys and demonstrated that there are important effects due to topography. Rodgers will study this research and hopes to apply it to San Francisco Bay Area and Laboratory programs. He is currently a co-investigator for an LDRD project to develop computational

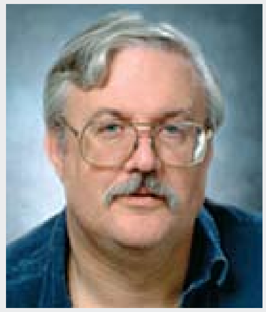


Fulbright Scholar Artie Rodgers, left, points out an earthquake region in the Middle East to his colleagues.

technology for subsurface facility detection and geophysical explorations, as well as earthquake or explosion source characterization (10-ERD-018).

Glenn T. Seaborg Award for Nuclear Chemistry

Kenneth Moody is a 2009 winner of the American Chemical Society award for his work in heavy elements and nuclear forensics. An LDRD researcher for over 10 years, Moody has participated in over 15 projects, including the discovery of element 114 (98-ERD-050), new fragment separation technology for superheavy element research (04-ERD-085), and a current project on an integrated response to nuclear incidents using nuclear forensics (10-SI-016).



Kenneth Moody

Innovator Award

Paul Hoeprich received an Innovator Award from Battelle for work performed under the LDRD project to develop and integrate novel technologies for the production and characterization of membrane proteins (06-SI-003). This award recognizes an innovation that may lead to a game-changing approach for rapid drug development.

Journal Covers

In FY09, several LDRD-supported projects were featured on the covers of peer-reviewed journals. Principal investigator Jennifer Pett-Ridge entered the successful image selected by delegates at the 12th International Symposium on Microbial Ecology that appeared on the cover of each 2009 issue of the *ISME Journal*. The research is a result of her project linking microbial identity and function using microarrays and nanoscale secondary ion mass spectrometry (07-ERD-053). The discovery of a method to dissolve the explosive TATB to improve its quality once it reverted back to a solid, an effort initially funded by LDRD as part of the Transformational Materials Initiative (06-SI-005), was featured on the January 2009 cover of the *New Journal of Chemistry*. In October 2009, the cover of *Meteoritics and Planetary Science* featured images from Lawrence Livermore of comet samples using scanning electron microscopy, part of an LDRD project that performed the first-ever study of cometary material collected by the Stardust space mission (03-ERI-007).

Journal covers of LDRD projects to combine a next-generation microarray for rapid genetic identification of biothreat agents with nanoscale secondary-ion mass spectrometry (left), reprocessing of explosive bulk material by crystallization (middle), and creating an integrated analytical capability for analyzing nanoscale samples using multiple instruments simultaneously to maximize the science yield (right).

Materials Research Board

Christine Orme has been elected to the board of directors of the Materials Research Society, which promotes communication and technical information exchange across the various fields of science affecting materials. The society has 15,000 members from the United States and over 80 other countries. Orme has served as a principal LDRD investigator for research into understanding shape control in the synthesis of nanoparticles (06-LW-090) and engineering titanium for improved biological response (00-ERI-006).

National Leaders in Environmental and Clean Energy Fields

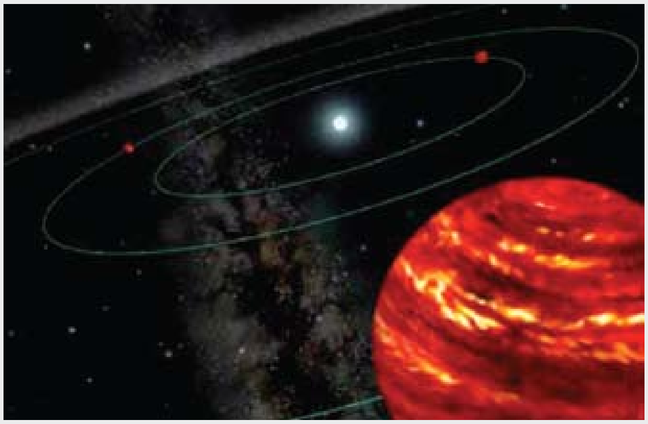
Julie Lundquist was one of ten Bay Area residents selected by *The San Francisco Chronicle* as a national leader in environmental and clean energy fields. Lundquist was a co-investigator for projects on dynamic data-driven event reconstruction for atmospheric releases (04-ERD-037) and improving atmospheric flow prediction at intermediate scales (09-ERD-038), and is currently a collaborator on two projects developing simulation tools for water resources and wind power (10-ERD-011 and 10-ERD-027).

Julie Lundquist

Newcomb Cleveland Prize

The American Association for the Advancement of Science's oldest award, the Newcomb Cleveland Prize, is awarded to the author or authors of an outstanding paper published in the Research Articles or Reports sections of *Science*. LDRD researcher Bruce Macintosh was one of the lead authors of the paper, "Direct Imaging of Multiple Planets Orbiting the Star HR 8799." A number of LDRD projects over 10 years led to the paper that earned Macintosh and his collaborators the award, including exploring primitive planetary systems via the Keck Telescope

(99-ERI-003), direct imaging of warm extrasolar planets (02-ERI-005), probing other solar systems with current and future adaptive optics (05-ERD-055), and tracing the shadows of planetary systems (08-ERD-043).



Artist's conception of the multiple planet system HR 8799, initially imaged by Gemini North adaptive optics and confirmed with W. M. Keck Observatory imaging. Gemini Observatory artwork by Lynette Coo.

Presidential Early Career Awards for Scientists and Engineers

Lynford Goddard, a former postdoctoral researcher in the Laboratory's Engineering Directorate, was named by President Obama as a recipient of the Presidential Early Career Awards for Scientists and Engineers (PECASE). Goddard was nominated for this award for his ongoing collaborations with LLNL researchers, including a new LDRD project developing embedded sensors for monitoring the nation's nuclear weapon stockpile (10-ERD-043). He is now an assistant professor of electrical and computer engineering at the University of Illinois at Urbana-Champaign.

Lynford Goddard

R&D 100 Awards

In 2009, LDRD-supported technologies garnered four of the eight R&D 100 awards presented to the Laboratory by *R&D Magazine.*

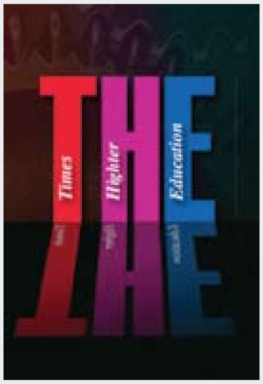
- **FemtoScope.** To meet the emerging need for greater dynamic range and temporal resolution in high-energy-density-physics and fusion-energy research diagnostics, researchers developed the FemtoScope—a "time microscope" that is attached to the front end of a conventional recording instrument to dramatically improve its performance. Initial efforts for this project were funded by LDRD, specifically development of ultrafast transient recording enhancements for optical-streak cameras (04-ERD-025). The FemtoScope—developed in collaboration with colleagues from Stanford University, the University of Southampton, and the University of California at Davis—improves the performance of an oscilloscope or streak camera much in the same way that a high-performance lens improves a camera's output. When combined with an oscilloscope, the FemtoScope produces an instrument capable of recording 100-ps frames at 155 million frames per second, and when combined with an optical streak camera, produces an overall improvement of 600 times compared with the performance of the streak camera alone.
- **Precision Robotic Assembly Machine.** Historically, building laser fusion targets required a significant amount of handcrafting skill and technique involving microscopes and manually driven fixtures. Now, Livermore scientists, along with collaborators from General Atomics in San Diego, California; Aerotech, Inc., in Pittsburgh, Pennsylvania; and Indicate Technologies, Inc., in Santa Clara, California, are transforming the way fusion targets are manufactured with a new device called the precision robotic assembly machine. Early investments from LDRD provided roots for the expertise in precision engineering needed to take on this challenge, including an extremely high-bandwidth diamond tool axis for weapons physics target fabrication (02-ERD-008). The precision robotic assembly machine can manipulate tiny fusion target components with unprecedented precision in an operating arena the size of a sugar cube.

Systems engineer and LDRD investigator Richard Montesanti operates the precision robotic assembly machine. The inset shows an assembled fusion ignition target.

- **ROSE Compiler Infrastructure.** ROSE is an open-source customizable compiler infrastructure that gives all computer programmers easy access to complex, automated compiler technology and assistance. ROSE accepts code in today's most common programming languages, including C, C++, and Fortran. Compiling is converting human-friendly source code into the machine-friendly binary code a computer needs to execute a program (i.e., executable files). The conversion of source code into binaries is performed by specialized software applications called compilers. Because ROSE has full knowledge of common programming languages, it can be used to optimize code performance and find errors. Additionally, ROSE returns these improvements to the user in revised source code rather than in the form of machine-readable binaries. Initial funding was partially provided by LDRD through projects such as software security analysis that focused on binary analysis and the development of tools for analyzing source code (07-ERD-057).
- **Land Mine Locator.** The *Landmine Monitor Report 2008*, published by the International Campaign to Ban Landmines, revealed that many thousands of square kilometers of land are contaminated by up to 100 million mines and other explosives. Furthermore, the pace of mine removal is far slower than the rate at which new mines are being placed. Livermore, together with colleagues at First Alliance Technologies, LLC, in San Ramon, California, and Hystar Aerospace Corporation in Vancouver, Canada, has developed the land mine locator, an aerial detection system equipped with Livermore's LANDMARC (land mine detection advanced radar concept), which features an ultrawideband radar-sensing technology called iRadar and tomographic algorithms that provide three-dimensional subsurface images. Groundwork for this technology was supported by LDRD with projects that included radar mine detection with LANDMARC (97-SI-013). For the land mine locator, LANDMARC is deployed on the remotely operated Hystar aerial platform, thereby reducing the time and cost of demining while significantly improving the safety of personnel and equipment. Other potential applications include the detection of roadside bombs and improvised explosive devices.

Top 20 Institutions in Engineering Based on Impact

LLNL was named one of the "Top 20 institutions in engineering based on impact" in 2008 by *The Times Higher Education*, published by TSL Education Ltd. Because LDRD funds exciting research and development projects, the program helps recruit and retain top talent in new and emerging fields of science and technology. The many world-class LDRD researchers and projects at Livermore helped the Laboratory become a "top-20 institution."



LDRD provides cutting edge research and development to enhance the Laboratory's scientific vitality.

Engineers Christine Paulson and Kique Romero demonstrate the iRadar array at Livermore's inert mine test pit.

ADVANCED SENSORS AND INSTRUMENTATION

Laboratory Directed Research and Development

Biophysical Characterization of Pathogen Invasion— Amy Hiddessen (06-ERD-013)

Abstract

A fundamental understanding of pathogen infection and host response is needed to develop new treatments for infectious disease. A comprehensive description of key processes is needed to meet this challenge, including data on the spatiotemporal expression of molecular regulators of signaling cascades. We will develop a pathogen mimic system, with well-characterized pathogen ligands and host receptors, to quantitatively characterize the real-time dynamics of a single pathogen's entry into a single, living host cell. We will achieve this using a unique suite of tools in our laboratory, including fluorescent subcellular reporters to visualize signal transduction, atomic force microscopy, and advanced optical imaging and trapping methods.

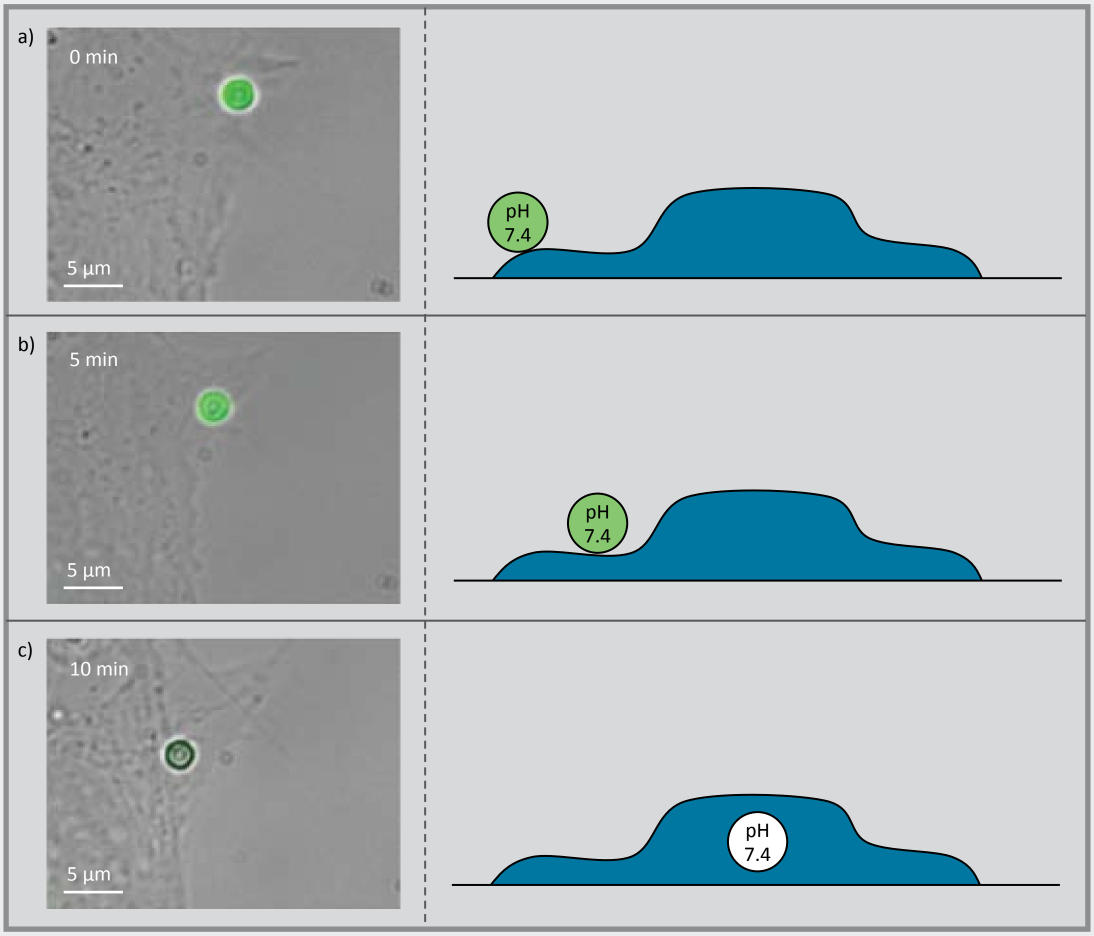
Investigations of the complex phenomenon of pathogenesis will provide valuable knowledge about the molecular causes of infectious disease, as well as new insights into cell-regulatory machinery and signaling pathways in host cells. Successful completion of this project will provide the first detailed, quantitative picture of the initial process of infection with high spatiotemporal resolution. Moreover, this research will develop a novel single-cell platform for studying signal transduction in cellular systems and presymptomatic responses in the host cell. The results and tools generated in this work will be published and used to develop new capability for a high-throughput, multiplexed pathogen-characterization system.

Mission Relevance

By combining synergistic experimental techniques to better understand pathogen–host interactions, this work will support Lawrence Livermore missions in biosecurity, homeland security, and bioscience to improve public health. This project also supports LLNL missions to stay at the forefront of research in nanosciences and bionanotechnology.

FY09 Accomplishments and Results

In FY09 we (1) developed a novel method to track, in real-time, pathogen entry using a pathogen mimetic; (2) used this novel method to track the dynamic process of pathogen entry in a single host cell in real time and to measure the effect of density of the pathogen ligand (InlA); (3) measured the step-wise biophysical process of entry—pathogen internalization, phagosomal acidification, and phagosomal–lysosomal fusion—novel fluorescence assays; and (4) measured the binding between a



Real-time tracking of the binding and internalization of InlA beads (a pathogen mimetic) using a pH-sensitive fluorophore (FITC) at 0 minutes (a), 5 minutes (b), and 10 minutes after the start of binding (c).

pathogen mimetic and live cells using atomic force microscopy. The successful conclusion of this project has resulted in the development of novel methods to study the dynamic processes that precede and follow pathogen entry into host cells, allowing for real-time quantification of these processes. We anticipate interest in this new capability from the National Institutes of Health, in particular the National Institute of Allergy and Infectious Diseases.

Publications

Artyukhin, A., et al., 2007. *Visualization of pathogen invasion dynamics and mechanisms at a single cell level using ligand coated microspheres and a FRET reporter.* 47th Ann. Mtg. American Society for Cell Biology, Washington, DC, Dec. 1–5, 2007. UCRL-ABS-236840.

Blanchette, C. D., et al., 2009. "Decoupling internalization, acidification and phagosomal–endosomal/lysosomal fusion during phagocytosis of InlA-coated beads in epithelial cells." *PLoS ONE* **4**(6), e6056. LLNL-JRNL-409584.

Lordi, V., P. Erhart, and D. Aberg, in press. "Charge carrier scattering by defects in semiconductors." *Phys. Rev. B.* LLNL-JRNL-421054.

Woo, Y.-H., et al., 2008. *Visualization of pathogen invasion dynamics and mechanisms at the single cell level using ligand coated microspheres and a FRET reporter.* 235th Am. Chem. Soc. Natl. Mtg., New Orleans, LA, Apr. 6–10, 2008. LLNL-PRES-402545.

Serrated Light Illumination for Deflection-Encoded Recording (SLIDER)—John Heebner (07-ERD-017)

Abstract

Fast, high-fidelity, single-shot diagnostics are critical to performing credible experiments in high-energy-density (HED) physics. Conventional oscilloscopes and streak cameras are fundamentally limited in that they trade dynamic range for temporal resolution and do not scale well into the picosecond regime. We propose to demonstrate a novel technique—serrated light illumination for deflection-encoded recording (SLIDER)—for high-fidelity recording in a temporal regime (1–500 ps) that currently does not have any technology base. Our technique avoids the conventional performance tradeoff by implementing a novel, solid-state, ultrafast optical deflection technique mated with well-established high-fidelity camera technology.

If successful, we will demonstrate the world's first all-optical streak camera capable of picosecond temporal resolution with a dynamic range in excess of 14 bits. Such a device would enable measurement of fusion burn histories and the characterization of ultrashort petawatt, advanced radiographic capability pulses with heretofore unrealized dynamic range. This work continues LLNL's long history of innovation in single-transient measurement techniques.

Mission Relevance

Single-shot measurement on a fast scale is crucial to experiments that support stockpile stewardship and HED physics. Fundamental questions in weapons design and HED physics have remained outstanding for decades because the technology required to record such data does not exist. The SLIDER technique, when coupled with technologies for imprinting x-ray signatures onto optical carriers, would help uncover these answers.

FY09 Accomplishments and Results

In FY09 we continued to optimize our novel concept for deflecting an optical beam at a sweep rate one order of magnitude faster than ever reported. Implementing this deflection mechanism in a recording geometry, we demonstrated a single-shot dynamic range in excess of 3000:1 at a 2.5-ps resolution and in another device demonstrated resolution as low as 1.1 ps. We also tested a means of extending the record length to 200 ps. Finally, we integrated the optical recorder with an x-ray-to-optical transcoder to demonstrate the novel capability for recording x-ray-imprinted optical signals. In summary, this successful project delivered the world's fastest light-beam deflector and a novel capability for the ultrafast measurement of transient waveforms with a high dynamic range and at picosecond time scales. The Laboratory is now using our novel optical measurement technique, mated with x-ray-to-optical transcoders, to construct a fieldable x-ray diagnostic.

Publications

Heebner, J. E., and C. H. Sarantos, 2008. *All-optical streak camera.* 2008 Conf. Lasers and Electro-Optics, San Jose, CA. May 4–9, 2008. LLNL-PRES-403381.

Heebner, J. E., and C. H. Sarantos, 2008. *Ultrafast optical beam deflection in a GaAs planar waveguide by a transient, optically-induced prism array.* Integrated Photonics and Nanophotonics Research and Applications, Boston, MA, July 13–16, 2008. LLNL-PROC-405170.

Sarantos, C., and J. Heebner, 2009. *Progress towards the all-optical streak camera.* Conf. Lasers and Electro-Optics, Baltimore, CA, May 31–June 5, 2009. LLNL-PRES-413544.

Sarantos, C., and J. Heebner, in press. "Solid-state ultrafast all-optical streak camera enabling high-fidelity picosecond recording." *Opt. Lett.* LLNL-JRNL-411016.

Sarantos, C., and J. Heebner, 2008. *Ultrafast optical beam deflection in a planar waveguide for high dynamic range recording at picosecond resolution.* IEEE Photonics Soc. Ann. Mtg., Newport Beach, CA, Nov. 9–13, 2008. LLNL-PROC-405170.

Ultraviolet-Visible Resonance Raman Studies of High Explosives, Impurities, and Degradation Products for Enhanced Standoff Detection—Jerry Carter (07-ERD-041)

Abstract

Improvised explosive devices (IEDs) used by terrorists have proven a difficult weapon to counter. Our objective is to understand the fundamental resonance Raman spectroscopic properties of high-explosive (HE) materials with the ultimate goal of forming the science basis for a new IED standoff-detection technology. Our specific aims include characterizing and understanding the resonance Raman spectral signatures of HE materials, impurities, and degradation products and determining the optimal resonance Raman conditions, sensitivity, enhancement factors, and best target analytes for IED detection. We also will demonstrate the standoff resonance Raman measurement of HE materials at safe distances (tens of meters) and with improved detection limits compared to normal Raman spectroscopy.

We expect to (1) determine optimal conditions for the resonance Raman detection of HE materials; (2) develop a method for determining enhancements relative to normal Raman technology; (3) determine resonance Raman sensitivity, selectivity, and response time for HE materials; (4) evaluate signatures from laser-induced sample degradation; (5) understand time scales and pathways of sample degradation for select HE materials; (6) understand background interference issues; and (7) demonstrate standoff resonance Raman HE identification at tens of meters.

Mission Relevance

This project supports LLNL's national security mission by developing the basis for a new standoff HE detection technology—an important capability needed to fill gaps in our ability to detect and mitigate the effects of IEDs and other terrorist-related threats. Furthermore, this technology also has potential applications in standoff aging and degradation studies of nuclear and conventional weapons. This work will create external strategic partnerships and help recruit new talent to LLNL.

FY09 Accomplishments and Results

We (1) conducted multiwavelength measurements of HE materials, compared spectral measurements, and calculated the difference caused by resonance Raman signals, achieving, among other results, the first quantification of resonance enhancement for HE materials; (2) conducted a study of imaging versus non-imaging approaches and identified several experimental approaches for improving the signal-to-noise ratio over conventional detection methods; (3) conducted HE degradation studies focused on TNT, including determining wavelength-dependent degradation thresholds and damage as a function of pulse width and laser power density; and (4) developed a standoff resonance Raman system and conducted limited testing. Follow-on work would include completing the standoff measurements. We anticipate interest in our resonance Raman results from the Department of Defense Joint IED Defeat Organization.

Salicylic Acid Derivatives: A New Class of Scintillators for High-Energy Neutron Detection—Natalia Zaitseva (07-ERD-045)

Abstract

The preferred method for detecting high-energy neutrons in the presence of strong gamma-radiation background is pulse-shape discrimination (PSD) using organic scintillators. However, single-crystal stilbene, the most effective PSD material, is not only toxic but also has a very limited availability because of crystal growth difficulties. We propose to develop a new class of materials based on salicylic acid derivatives for the detection of high-energy neutrons. We will first identify nontoxic organic crystals as alternatives to stilbene that offer improved performance and are easy to grow. Low-cost solution-growth techniques will be used to survey the properties of many candidates to identify and develop new efficient neutron-detector materials with improved discrimination between gamma radiation and high-energy neutrons.

Our main deliverable will be identification and development of new efficient, readily available, and low-cost scintillator materials that offer the sensitive neutron-detection and effective gamma-discrimination qualities needed for monitoring fissile materials. Systematic studies of many single crystals grown by solution techniques will produce scientific results important for developing a deeper understanding of the physics of scintillation processes, especially the composition, physical state (liquid or solid), crystallographic structure, and quality of materials. We also will apply our results to the development of technologies for production-scale growth of the crystals. Studies of growth mechanisms and optical characterization will generate publications and intellectual property.

Mission Relevance

By developing new compact, sensitive, low-cost, and efficient scintillator materials for the detection and monitoring of fissile materials, this project supports LLNL's national and homeland security missions.

FY09 Accomplishments and Results

In FY09 we (1) grew additional compounds as single crystals, bringing the total number of surveyed materials to 150; (2) measured and analyzed PSD in relation to chemical composition, impurity, and structure; (3) conducted experimental and computational analysis showing that the main factors influencing PSD in organic crystals are the degree of exchange coupling between aromatic molecules in a crystal lattice and impurities; and (4) determined that the absence of PSD in certain crystallographic structures results from triplet migration that is too slow for triplet–triplet collisions or from a specific relation with triplet excitation energies such that an impurity with a smaller triplet energy may act as an excitation trap that quenches PSD in the host crystal. This successful project has opened the path to the engineering of new organic scintillators—solid and liquid—that can be used for the efficient detection of and discrimination between different types of radiation. The results are being applied to research into large-scale neutron detectors by NNSA's Office of Nonproliferation Research and Development and the Department of Homeland Security's Domestic Nuclear Detection Office.

Publications

Hull, G., et al., 2008. *New organic crystals for pulse shape discrimination.* 2008 Symp. Radiation Measurements and Applications, Berkeley, CA, June 2–5, 2008. LLNL-ABS-401363.

Hull, G., et al., 2009. "New organic crystals for pulse shape discrimination." *IEEE Trans. Nuc. Sci.* **56**, 899. LLNL-JRNL-411978.

Zaitseva, N., et al., 2007. "Germanium nanocrystals synthesized in high-boiling-point organic solvents." *Chem. Mater.* **19**, 5174. UCRL-JRNL-226844.

Zaitseva, N., et al., 2009. "Growth and properties of lithium salicylate single crystals." *Cryst. Growth Des.* **9**, 3799. LLNL-JRNL-410824.

Zaitseva, N., et al., 2009. "Neutron detection with single-crystal organic scintillators." *Proc. SPIE* **7449**, 744911. LLNL-JRNL-414904.

Broadband Heterodyne Infrared Spectrometer: A Path to Quantum Noise-Limited Performance—Joseph Tringe (08-ERD-016)

Abstract

The objective of this effort is to demonstrate a new form of infrared spectrometry for chemical detection based on the heterodyne principle of generating new frequencies by mixing signals. Our approach is unique in that a broadband source will be used to enable hundreds of individual spectral channels to simultaneously record a high-resolution infrared spectrum. This approach can potentially achieve quantum noise-limited performance with a room-temperature infrared spectrometer. Previously, the requirement for cooling the spectrometer and detector limited the size, weight, and power, creating a significant impediment to implementation for a number of applications. Room-temperature operation has been a long-sought goal to minimize size, weight, and power and is the only approach capable of achieving that goal.

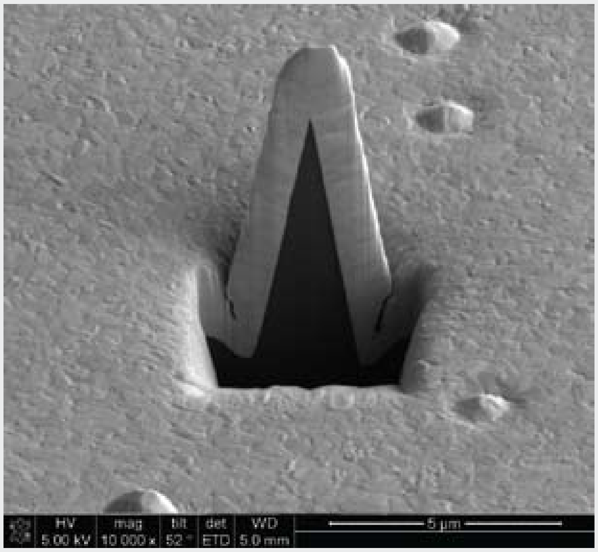
We expect to show that the heterodyne approach will lead to a new spectrometer concept that will allow hyperspectral infrared spectrometry to operate at room temperature with no sacrifice in signal-to-noise performance. This will enable the remote optical detection of chemical vapor effluents with a minimum overhead burden in size, weight, and power. This, in turn, will enable new platform options and applications. At the end of the project we will have demonstrated the key detector components necessary for spectrometer operation at room temperature.

Mission Relevance

By considerably relaxing operational limitations imposed by excessive size, weight, and power, this project will make high-sensitivity hyperspectral infrared information accessible for applications in nonproliferation, homeland security, law enforcement, and the military.

FY09 Accomplishments and Results

In FY09 we (1) successfully synthesized nanostructured antenna-based detectors, integrating carbon nanotube field-emission tips into radiofrequency-compatible quantum-well infrared photodetector chips; (2) performed preliminary characterizations on these devices by testing in vacuum;



Scanning electron microscope image of a cross-sectioned plasmonic infrared condensing lens made from silicon.

(3) successfully established operational temperature limits using our system model—we determined that, with expected improvement in the state of the art for photodetectors, our infrared spectrometer can operate at temperatures in the 250- to 300-K range; and (4) successfully synthesized, characterized, and modeled plasmonic waveguides.

Proposed Work for FY10

In FY10 we will (1) systematically compare the experimentally measured performance parameters of our quantum-well photodetector and carbon-nanotube detector system with parameters from our model to determine ultimate achievable signal levels; (2) improve the antenna design to increase sensitivity and operation frequency, as required for optimum spectrometer performance; and (3) design improved sub-wavelength lensing structures based on the measured performance of the prototype devices tested in FY09. We anticipate these successful results will establish the feasibility of our design to enable room-temperature hyperspectral infrared spectrometry with no sacrifice in the signal-to-noise performance found with cryogenically operated spectrometers.

Tracing the Shadows of Planetary Systems—

Bruce Macintosh (08-ERD-043)

Abstract

The study of other solar systems is driven by the intersection of advanced optical technology and fundamental questions such as, How are solar systems formed? and Are systems like our own common? The next frontier in exploring such systems is their characterization through spectroscopy and polarimetry. We will use Livermore expertise in adaptive optics (AO) and image processing to observe the interplanetary dust that traces the formation and presence of planets and cometary belts. Current AO is limited by the motion of atmospheric turbulence. We propose to develop advanced AO techniques, such as an innovative Fourier-domain predictive controller, that can sharply reduce this effect, leading to AO systems that can detect the giant planets of solar systems outside our own.

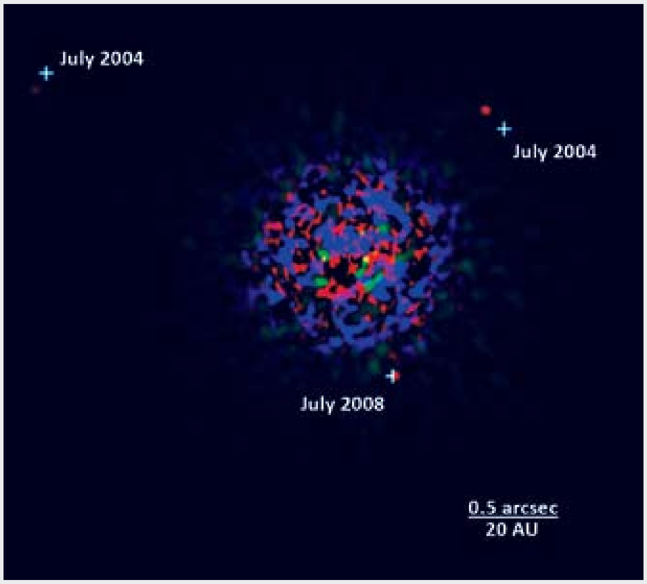
We expect to extract signals from scattered light and infrared emission of dust grains orbiting other stars. These will be compared to numerical models to constrain the location and properties of dust particles and evolution of the system and its planets. We will develop an advanced AO controller that greatly extends the capabilities of the Gemini Planet Imager, automatically identifying moving turbulent wind layers and pre-correcting for their motion in real time. Such a predictive controller can improve AO performance by a factor of two in any case where moving atmospheric turbulence dominates, including non-astronomical applications. Finally, we will prepare techniques and target information to ensure that we lead a proposed large-scale (200-night) survey using the Gemini Planet Imager.

Mission Relevance

A key competency at Livermore, AO is used in applications from astronomy to microscopy and from beam control to surveillance. Advanced techniques benefit all AO areas and can be applied to large optical systems and space optics for remote sensing for counterproliferation and nonproliferation efforts in support of the Laboratory's national security mission. This project also supports the Laboratory's mission in breakthroughs in science and technology and employs collaborations that will lead to new, innovative capabilities for LLNL.

FY09 Accomplishments and Results

In FY09 we achieved a spectacular success, using advanced image processing to produce the first-ever images of another solar system, three giant planets orbiting the massive, dusty star HR8799. We were able to measure the temperature, radius, and luminosity of these planets and thereby constrain their mass. The paper describing these results was featured on the cover of the November 28, 2008 issue of *Science* and was number two on the American Association for the Advancement of Science's list of breakthroughs in 2008. We began follow-up spectroscopic and orbital work to achieve new insights into planet formation and evolution. We also completed the design of a polarimeter mode for the Keck telescope to study circumstellar dust, used our Fourier domain algorithm to identify the motion of independent atmospheric layers in astronomical telemetry, and began to test optimal AO control.



Infrared image, taken with the Keck telescope adaptive optics system, showing three planets orbiting the young, massive star HR8799.

Proposed Work for FY10

Our primary astronomical focus will be on detailed characterization of the HR8799 planets. Specifically, we will (1) use a hyperspectral imager and develop image processing to obtain near-infrared spectra of the outermost planets, which we will use to constrain the planets' composition and atmospheric structure; (2) measure planetary orbits to compare against models for the system's stability and evolution and gravitationally constrain the planets' masses; (3) propose additional observations using the Keck and Hubble telescopes; (4) complete our initial survey of 80 to 100 young massive stars; and (5) implement advanced modal control algorithms on a Livermore AO test bed.

Publications

Cady, E., et al., 2009. "Shaped pupil design for the Gemini Planet Imager." *Astrophys. J.* **698**, 938. LLNL-JRNL-412555.

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Marois, C., et al., 2008. "Direct imaging of multiple planets orbiting the star HR899." *Science* **322**, 5906. LLNL-JRNL-408612.

Poyneer, L., A. Norton, and D. Dillon, 2009. *Open-loop shaping of a 4k MEMS with Fourier-domain pre-compensation.* Adaptive Optics: Methods, Analysis and Applications, San Jose, CA, Oct. 13–15, 2009. LLNL-CONF-413264.

Poyneer, L., M. van Dam, and J. P. Veran, 2009. "Experimental verification of the frozen-flow atmospheric turbulence assumption with use of astronomical adaptive optics telemetry." *J. Opt. Soc. Am.* **26**, 833. LLNL-JRNL-407053.

Poyneer, L., M. van Dam, and J. P. Veran, 2009. *Predictive Fourier wavefront control: Theory and observational results.* Adaptive Optics: Methods, Analysis and Applications, San Jose, CA, Oct. 13–15, 2009. LLNL-CONF-413265.

Point-of-Care Diagnostic for Foot-and-Mouth Disease Virus—Jane Bearinger (08-ERD-044)

Abstract

The timely, effective management of infectious disease—including biothreat agents—requires rapid, scalable, field-operable diagnostics. We will develop a new point-of-care detection capability by designing and characterizing an isothermal assay capable of detecting nucleic acid in clinical samples within 30 minutes and by producing a diagnostic platform with integrated sample preparation, amplification, and detection capabilities. The diagnostic will be field operable, scalable, and disposable. The foot-and-mouth disease virus will be used as an exemplar. We will leverage LLNL's unmatched capabilities and expertise in bioinformatics, assays, instrumentation, and select-agent science, and will collaborate with the Institute for Animal Health in the United Kingdom.

The technology generated by this project will better prepare U.S. first responders to effectively react to infectious diseases and bioterrorism. In the case of foot-and-mouth disease, the technology will reduce the economic impact of an outbreak by (1) providing rapid confirmation of clinical diagnosis, (2) reducing the diagnostic caseload at centralized laboratories, and (3) facilitating the continuity of business. Spin-offs from this work could improve U.S. and global biosecurity against other threats such as pandemic avian influenza.

Mission Relevance

This project supports LLNL's national security mission by providing a fast, inexpensive, scalable, field-deployable disease-detection capability and by laying the foundation for the next generation of technologies for detecting high-consequence pathogens. This project will also help recruit and retain scientific talent in a strategically important, scientifically cutting-edge field.

FY09 Accomplishments and Results

In FY09 we (1) retained our initial optical detection platform after experiencing procurement difficulties with lateral flow materials and reagents; (2) generated full product-requirement and user-needs documentation for the next prototype, which will assist in eventual commercialization; (3) validated our prototype against commercially available systems; and (4) continued to refine our system and reagent design by reducing materials costs and more comprehensively assessing experimental variables.

Proposed Work for FY10

In FY10 we propose to (1) design and fabricate the field-deployable prototype; (2) test and validate the prototype in the United Kingdom, as well as at Plum Island in New York; and (3) integrate Department of Homeland Security validation testing with commercially available technologies.

Cadmium–Zinc–Telluride Sandwich Detectors for Gamma Radiation—Rebecca Nikolić (08-ERD-051)

Abstract

Detectors to sense nuclear and radioactive weapons concealed in transit through borders, airports, and sea ports are crucial for the international struggle against terrorism and proliferation of weapons of mass destruction. Currently, germanium

detectors offer the best performance in detecting gamma rays—however, they must be operated at cryogenic temperatures. A room-temperature detector is greatly preferred because of cost and ease of use, but the only available alternative is based on cadmium–zinc–telluride (CZT) technology, which offers inferior performance. Here we propose a pathway for CZT gamma detectors to achieve the desired energy resolution of less than 1%. We will use a multilayered structure known as a sandwich detector, to allow signal collection while simultaneously rejecting noise. By applying energy bandgap engineering to this discipline, we believe detector performance can be improved.

With this project, we expect to demonstrate a gamma detector with less than 1% energy resolution that will operate at room temperature. To achieve this goal, we will design a novel structure utilizing bandgap engineering concepts that will result in a 90% reduction in leakage current relative to a resistive device. We also will provide leadership to the detector community by providing a technical roadmap for how to demonstrate a 0.5% energy resolution within five years.

Mission Relevance

The solution to the radiation-detector materials problem is expected to have significant impact on efforts to developing detectors that are compact, efficient, inexpensive, and operate at ambient temperature for the detection of special nuclear materials as well as radiological dispersal devices. The multidisciplinary nature of this work and the relevance to national and homeland security align well with LLNL capabilities and missions.

FY09 Accomplishments and Results

In FY09, we (1) benchmarked our models with experimentally gathered data from FY08 and refined them to account for discrepancy; (2) designed and fabricated structures with amorphous layers on CZT and carried out both electrical and radiation characterization, revealing reduced dark current and improved breakdown voltage over structures without amorphous layers; (3) demonstrated an effective resistivity of greater than 1011 ohm-cm (>200 V) in material considered too conductive for typical CZT gamma detectors, which have a resistivity of 109 ohm-cm; and (4) used these structures to characterize the interface and energy barrier between the amorphous material and single-crystalline CZT.

Proposed Work for FY10

In FY10 we propose to (1) utilize x-ray photoelectron spectroscopy to characterize surface Fermi level pinning and add interface physics to our heterojunction detector model, (2) characterize the Schottky barrier height and energy-band offsets in amorphous CZT heterojunctions by measuring current versus voltage over a range of temperatures and measuring capacitance versus voltage, (3) fabricate amorphous layer and CZT heterojunction detectors that have an effective resistivity of greater than 1012 ohm-cm in material that is otherwise too conductive for typical CZT gamma detectors to demonstrate a proof-of-principle detector with improved energy resolution, and (4) prepare a journal paper on amorphous barrier layer results.

Publications

Conway, A. M., et al., 2009. *Amorphous semiconductor blocking contacts on CdZnTe gamma detectors.* Intl. Semiconductor Device Research Symp., College Park, MD, Dec. 12–14, 2009. LLNL-ABS-416278.

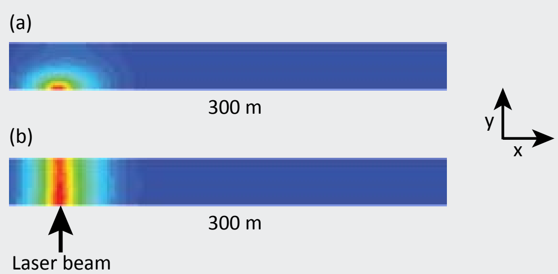
Nelson, A. J., et al., 2009. “X-ray photoemission analysis of CdZnTe surfaces for improved radiation detectors.” *Mater. Lett.* **63**, 180. LLNL-JRNL-414165.

Voss, L. F., et al., 2009. *Amorphous semiconductor blocking contacts on CdTe gamma detectors.* IEEE 2009 Nuclear Science Symp., Orlando, FL, Oct. 26–29, 2009. LLNL-ABS-413003.

Hybridization, Regeneration, and Selective Release of DNA Microarrays—John Dzenitis (08-ERD-064)

Abstract

Microarrays are ideal for studies of the biological component of environmental backgrounds, clinical monitoring of pathogens and hosts, and continuous environmental monitoring. While microarrays identify hybridization patterns and signatures, a critical need exists for methodologies enabling rapid and selective analysis of these signatures. Analysis of DNA sequences from selective spots on an array could quickly yield vital information. This is especially important for countering rapidly mutating



Finite-element simulation of energy deposition that occurs when a laser beam impacts a DNA microarray—for a 10.6-μm laser beam (a) and for a 1.47-μm laser beam (b). The shorter wavelength 1.47-μm beam deposits energy in a more uniform heating profile, which is beneficial for our DNA microarry.

and emerging pathogens. This project will develop a method for selective spot release and analysis. Because microarrays also suffer from long hybridization times (4 to 16 h) and high chip-replacement costs, we will also study hybridization kinetics and mass transfer to enable chip reuse and faster analysis. This work leverages LLNL expertise in optics, microfluidics, and bioinformatics.

This effort will increase by an order of magnitude the information content provided from microarrays. We will do this by investigating (1) chemical and physical changes that occur during in vitro DNA hybridization; (2) stabilities of different chemical couplings between DNA molecules and surfaces; (3) controlling mechanisms between DNA in solution and DNA affixed to a solid support in hybridization experiments; (4) influence of optical, thermal, and fluidic effects on the intrinsic binding or stringency for DNA targets on probes; and (5) individual spots to eliminate the complex background signal. The method we develop will have wide applicability and impact in the DOE complex.

Mission Relevance

This work supports the national security mission areas of nonproliferation and homeland security by enabling the fast and specific detection of, and response to, biological weapons of mass destruction. The capabilities developed will enable efficient, cost-effective, and highly sensitive and specific pathogen detection. With these improvements, microarray technology can be applied to distributed sensors and systems, enabling nonproliferation, counterterrorism, and force protection efforts.

FY09 Accomplishments and Results

In FY09 we (1) extended the alignment capability of the optical selective release system and demonstrated energy deposition to microarrays near the diffraction limit at approximately 100-µm resolution, (2) performed hybridizations integrated with the scanner and proved that the experimental apparatus can provide kinetic data by tracking the hybridization level over time on control spots, and (3) developed a three-dimensional computational fluid dynamics model to characterize the penetration and heating profile of a 10.6-µm laser, and used the code to assess the energy deposition that would result from a 1.47-µm diode laser.

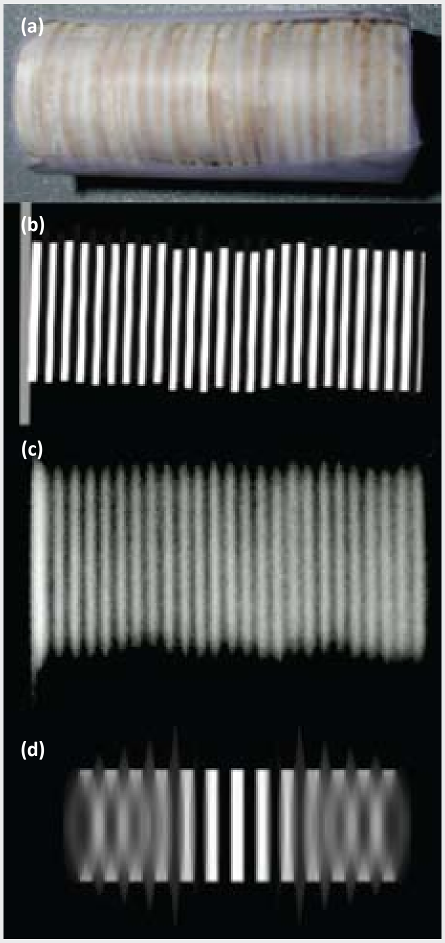
Proposed Work for FY10

In FY10 we will (1) demonstrate selective-release oligonucleotide dehybridization on microarrays with complex samples and confirm sequences on the eluted oligonucleotides; (2) optimize the optical system to reduce wavelength and corresponding spot size by a factor of three, allowing the state-of-the-art high-density microarrays to be targeted by our laser system under single-spot control; (3) apply the microarray flow cell in hybridization studies to quantify and reduce microarray hybridization times; and (4) employ surface chemistries capable of reuse to demonstrate the potential of microarrays for biothreat analysis.

Optimized Volumetric Scanning for X-Ray Area Sources—Sean Lehman (09-ERD-045)

Abstract

The goal of this project is to perform a systematic study to determine optimal scanning geometries for x-ray area sources and provide a roadmap for area-source imaging in the field. Area sources have a much greater spatial coverage than traditional point sources, enabling a more accurate volumetric scanning of an object. This capability is of paramount importance in many



Photograph of an x-ray resolution Defrise phantom (a) compared to our model-based reconstruction (b), ordered-subset expectation maximization reconstruction (c) , and traditional reconstruction (d).

key efforts at Lawrence Livermore. While area sources are a very promising and critical technology, their full potential cannot yet be quantified or exploited because no study has been done to optimize the scanning geometry for area sources. We will carry out this optimization by comparing performances of the possible scanning geometries using simulated and real data.

A successful completion of the project will result in determination of optimal scanning geometries for x-ray area sources, as well as a complete method to perform optimal scanning in the field. Specifically, we will study the feasible scanning geometries and determine which are optimal. A complete methodology for implementing the optimal scan in the field will be developed. Producing such a methodology will greatly advance the use of x-ray area sources, enabling the scientific community to reap full benefits of its greater spatial capabilities than conventional point sources. This is highly significant because the ability to perform imaging with area sources will cause a paradigm shift in x-ray imaging practice.

Mission Relevance

This project supports Laboratory efforts in national and homeland security as well as energy security by optimizing scanning geometries for x-ray area sources used in detectors and diagnostic instruments. Enabling improved x-ray diagnostics for components vital to advanced energy generation systems benefits the Laboratory's mission in pursuit of future clean energy sources. Improved x-ray sources for detecting explosives in luggage at airports is a key counterterrorism tool of interest to the Department of Homeland Security, and greater efficiency in weapons inspection will benefit the nation's nuclear weapons and complex integration program.

FY09 Accomplishments and Results

Two phantoms were used as canonical objects: a cylindrical stack of flat plates with alternating densities, known as a Defrise phantom, and a cylindrically symmetric nested phantom of epoxy, aluminum, and air known as the "as built" phantom. The Defrise phantom, for which data exist, served as a contrast and resolution object. We integrated the LLNL x-ray ray-tracing transmission code CTSIM into the MATLAB programming language and used it to create a stacked-cylinder proof-of-concept model and Defrise data, which were used to create an inversion and compare the reconstructions of pristine and damaged objects. A simulated "defect" inserted in the damaged object was also successfully identified and located.

Proposed Work for FY10

In FY10 we will (1) design data collection methods and techniques, (2) combine single sources to progress to multiple simultaneous sources and develop source- and detector-characterization algorithms and remediation methods, (3) collect data using multiple simultaneous sources and possibly different geometries, (4) develop artifact models and filters, and (5) evaluate system performance and move algorithms to high-performance computers.

Ultrasensitive Rare-Event Detection for Global Nuclear Security—Adam Bernstein (09-ERD-052)

Abstract

We propose to transform two core nuclear security efforts: standoff monitoring of nuclear reactors and detection of non-critical special nuclear material. Success in these closely related areas requires breakthrough research in rare-event detection. Because of remarkable similarities in the underlying physics, we intend to achieve the needed breakthroughs by harvesting world-class technologies and expertise from prominent dark matter and neutrino experiments that Livermore will participate in. While building an enduring foundation for transformational

Collaboration meeting at Brown University for the Large Underground Xenon Dark Matter Experiment.

nuclear security research and design, our work will expand the Laboratory's reputation as a leader in nuclear and particle physics.

This research will create an enduring program in rare-event detection for applied and fundamental nuclear science in the service of global nuclear security. With high confidence, we expect the project will provide the nation with unmatched transformational capabilities in gamma-ray and neutron detection for nuclear security and in antineutrino detection for reactor safeguards. Based on an emerging national consensus among federal scientific, nonproliferation, and intelligence agencies, our research will be relevant to standoff monitoring and discovery of nuclear reactors, with revolutionary implications for global nonproliferation and nuclear security. Finally, the initiative will engage LLNL in world-class dark matter and neutrino research.

Mission Relevance

This work will create transformational capabilities for nonproliferation and homeland and national security, while achieving excellence in fundamental science. This combination is possible because we are operating at a clearly defined nexus between the fundamental science of dark matter and neutrino detection and the applied science of global nuclear security—specifically, the detection of rare, kiloelectronvolt-to-megaelectronvolt gamma rays, neutrons, and antineutrinos emitted by nuclear materials and reactors.

FY09 Accomplishments and Results

In FY09 we (1) completed design of the analog front-end—the system that processes the raw signals emerging from the antineutrino detector—for the Double Chooz experiment in France, (2) tested and delivered prototype front-end cards to the experiment and began work on a simulation of the Chooz reactor, and (3) performed analysis, using data from a predecessor experiment, that set a new limit on inelastic dark matter for the Large Underground Xenon Dark Matter Experiment located in South Dakota. In the single year of this project, which has been converted to a Strategic Initiative for FY10, we contributed to high-profile fundamental physics experiments and advanced our understanding of dual-phase argon technology for use in reactor monitoring in nonproliferation contexts. In addition, the project enabled hiring of three postdoctoral researchers.

Publications

Angle, J., et al., in press. "Constraints on inelastic dark matter from XENON10'." *Phys. Rev. D.* LLNL-JRNL-420707.

Kazkaz, K., et. al., 2009. *Operation of a 1-liter-volume gaseous argon scintillation counter.* LLNL-JRNL-415990-DRAFT.

Advanced Computational Techniques for Improving Space Flight Safety—Scot Olivier (09-ERD-058)

Abstract

More than 80 countries have joined the space community, making Earth orbit an increasingly congested place. Hundreds of active satellites as well as thousands of pieces of space debris orbit Earth. We propose to develop and demonstrate advanced computational techniques for "space situational awareness" that will result in enhanced safety for space operations. In particular, we will develop specific enhancements to the Laboratory's Testbed Environment for Space Situational Awareness (TESSA) that will increase its effectiveness for improving space flight safety. TESSA is an integrated modeling and simulation framework for quantitatively assessing the performance of specific sensor systems, technologies, and data analysis techniques. The proposed enhancements of TESSA capabilities will result in forefront techniques for ensuring our nation's ability to operate freely in space.

This project will help to create a new paradigm for real-time space situational awareness. Specific results will include new operational methodologies, advanced techniques, and new analysis capabilities. These new capabilities can be provided to the government as LLNL resources or transferred to other government agencies for operation. The simulation and modeling capabilities we develop can continue to be used by the government to provide an ongoing basis for selection between different technical options in this area. In addition, some of the techniques developed for this project would be directly applicable to other national problems such as nuclear proliferation and climate monitoring.

Livermore researchers developed advanced modeling and simulation techniques to improve awareness of space satellites and debris.

Mission Relevance

Freedom of operation in a crowded space environment is crucial to U.S. interests, and maintaining space flight safety is a key component of this freedom. Utilizing unique Laboratory technical resources to help address this issue directly supports core LLNL missions in national and global security. Through this project, LLNL has an opportunity to begin to establish a major new business area, to enhance core competencies important for basic scientific research, and to provide leadership for the U.S. in an area of intense national interest and enduring importance.

FY09 Accomplishments and Results

In FY09 we accomplished all proposed project objectives. Specifically, we (1) developed improved techniques for simulating orbital debris generation, (2) modeled and analyzed the ability to detect and track orbital objects with advanced sensors and cueing strategies, and (3) explored advanced approaches for quickly calculating the risk of collisions between orbital objects. The successful conclusion of this project helped to establish a foundation for a new paradigm for real-time space situational awareness. The Space Protection Program, the Air Force Electronics Systems Command, and the DOE Office of Nonproliferation Research and Development are supporting further work to improve space awareness using techniques developed by this project.

Publications

Olivier, S., et al., 2009. "High-performance computer modeling of the cosmos-iridium collision." *Proc. Advanced Maui Optical and Space Surveillance Technologies Conf.*, S. Ryan, Ed., The Maui Economic Development Board, p. E84. LLNL-CONF-416345.

Superimposed Plasmonic and Photonic Detection Platform—Sarah Baker (09-LW-003)

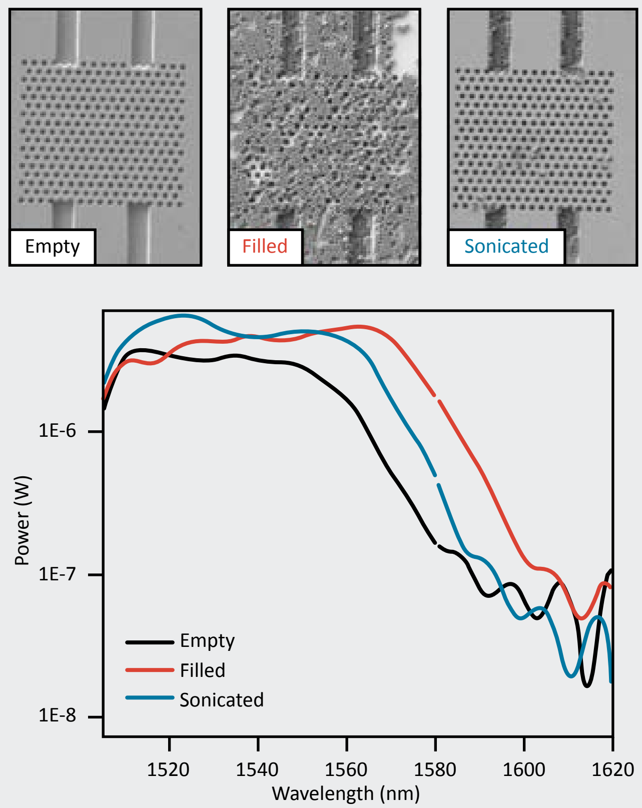
Abstract

Current protocols for detection of pathogenic biological organisms in the environment are time consuming and unreliable, hampering response efforts. Our goal is to design, model, and fabricate a flow-through biosensing platform that will enable collection, concentration, detection, and identification of low concentrations of pathogens using superimposed surface-enhanced Raman spectroscopy and photonic crystal-based transduction methods. This radically new biosensing platform would trap organisms in flow-through pores, detect them via optical measurements of photonic bandgap across the membrane, and identify them at the surface of the membrane.

In addition to enabling rapid and sensitive biological organism detection, this work will provide the first proof of concept for the integration of photonic and plasmonic crystal-based signal transduction and separation. This new class of extremely compact and sensitive flow-through sensors will enable real-time detection of known biological agents for counterterrorism, environmental, and medical applications, and enable future work focused on the generation of fingerprints for detecting unknown organisms. Novel design and nanofabrication approaches for integrating photonics and spectroscopy transduction will also be developed, enabling next-generation multifunctional biosensing platforms and paving the way for new membrane-based devices.

Mission Relevance

This project directly supports Livermore's threat prevention and response mission in homeland security, as well as environmental and biomedical efforts, by developing a novel class of



Scanning electron microscope images of silicon photonic crystals (hole diameter = 280 nm), the pores of which have been infiltrated with polystyrene beads (top). Experimental transmission spectra of the same photonic crystals (bottom).

platforms for rapid collection, detection, and identification of biological agents. Current techniques are based on polymerase chain reaction, which requires amplification and is not easily carried out in the field in real time. The project takes an innovative approach to nanofabrication challenges encountered when creating multifunctional platforms. It will therefore expand the Laboratory's capability and position LLNL as a leader in the areas of functional nanostructures, signal transduction, and biothreat detection, and will be of interest to federal security and health agencies such as the Defense Advanced Research Projects Agency and the National Institutes of Health.

FY09 Accomplishments and Results

In FY09 we (1) used finite-difference time domain simulations to design silicon photonic crystals (PCs) to obtain the desired optical transmission spectrum; (2) fabricated the crystals on silicon membranes at Lawrence Berkeley's Molecular Foundry and at LLNL; (3) built a testing station to measure the photonic crystal infrared transmission spectra, obtaining close agreement between experimental and simulated transmission spectra; (4) detected particles deposited within the crystal pores by measuring a shift in optical band edge; (5) determined that a gold coating on the crystal surface can give rise to localized surface plasmon resonances at visible wavelengths, increasing the electric field around each nanohole, as predicted by simulation; and (6) demonstrated that these enhanced electric fields enable molecular monolayer detection by surface-enhanced Raman spectroscopy.

Proposed Work for FY10

In FY10 we plan to (1) optimize the instrumental setup for measuring PC optical-transmission spectra, and then integrate it with a fluidic assembly for real-time bio-organism simulant-binding studies; (2) perform finite-difference time-domain modeling plasmonics simulations to tune the PC surface plasmonic resonances to optimize surface-enhanced Raman spectroscopy signals at the excitation wavelength of our laser; (3) develop a fundamental understanding of the structural and geometric requirements for integrating fluid flow, sensitive PC transmission measurements, and surface-enhanced Raman spectroscopy; and (4) incorporate these design elements into a prototype device that will be functionalized for selective bio-organism simulant capture and resistance to nonspecific adsorption.

Publications

Baker, S., et al., 2009. *Silicon filtration membranes for organism capture and identification.* Molecular Foundry Users Mtg., Berkeley, CA, Oct. 15–16, 2009. LLNL-ABS-416212.

Antibiotic Heteroresistance in Methicillin-Resistant *Staphylococcus aureus*: Microchemostat Studies at the Single-Cell Level—Frederick Balagadde (09-LW-112)

Abstract

The development of new antibiotics is being outpaced by the emergence of antibiotic-resistant bacterial strains, making it crucial to understand the genetic mechanisms of antibiotic resistance. At the center of this mystery is heteroresistance—the concurrent existence of multiple bacterial subpopulations with varying degrees of antibiotic resistance. We propose to leverage a novel microchemostat technology at LLNL to probe heteroresistance in bacteria, with the ultimate aim of restoring the efficacy of existing antibiotics that have lost potency. We will use a clinically important bacteria—methicillin-resistant *Staphylococcus aureus* (MRSA)—as our test case. The platform we create will be adaptable to study a wide range of clinically relevant antibiotic resistance applications, including the cost-effective, high-throughput screening of microbes against existing antibiotic libraries and novel antimicrobials.

If successful, we will experimentally determine the mechanism of heteroresistance, including constructing protein–protein fusions with other heteroresistance candidates—hmrA, the operon vraSR (already known to be necessary for methicillin resistance), and a global regulator of cell wall biosynthesis that is activated by oxacillin and vancomycin. We expect to publish multiple manuscripts in high-profile journals.

Mission Relevance

By elucidating the genetic mechanisms of antibiotic resistance and potentially helping to restore the potency of existing antibiotics against both clinically significant bacteria and potential bioterror pathogens, this project supports the Laboratory's missions in homeland security and science to improve human health.

FY09 Accomplishments and Results

In FY09 we (1) constructed an MRSA-ready Biosafety Level 2 microfluidics laboratory; (2) constructed, using the microchemostat nano-reactor as the basic building block, a high-throughput screening engine chip that can autonomously start a culture, perform a screening experiment, and sterilize the reactor to prepare for the next cycle; (3) completed all environmental, safety, and health and Institutional Biosafety Committee requirements for this project; (4) fused a mecA bacterial cell gene with green fluorescent protein in *Escherichia coli* using a mecA promoter from a heteroresistant MRSA strain; and (5) performed initial characterization using flow cytometery and cell sorting.

Proposed Work for FY10

During FY10 we will (1) grow MSRA cultures in the microchemostat to a steady state and at a fixed dilution rate, then introduce oxacillin at different concentrations in different reactors and track trends in single-cell-resolved mecA gene expression through fluorescence microscopy with unprecedented temporal resolution; (2) determine a time course of fluorescence distributions of mecA gene expression; and (3) examine the role of mecA in heteroresistance.

BIOLOGICAL SCIENCES

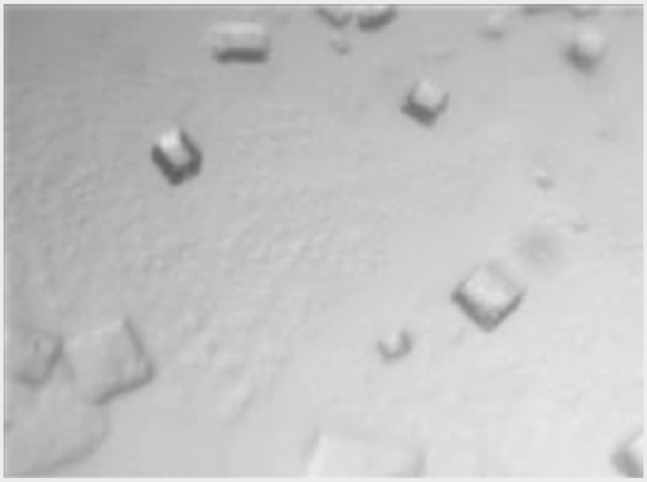
Laboratory Directed Research and Development

Developing and Integrating Novel Technologies for the Production and Characterization of Membrane Proteins—Paul Hoeprich (06-SI-003)

Abstract

Membrane-associated proteins, although essential for mediating cellular processes, have received limited study because they are not amenable to conventional techniques used for isolating and characterizing soluble proteins. This project will develop robust, state-of-the-art methods to produce and characterize membrane proteins. Specifically, we will (1) produce membrane proteins by cell-free methods, (2) capture these proteins in nano-sized (10- to 20-nm) membrane mimetic structures or nanolipoprotein particles (NLPs), (3) optimize NLP production by creating semisynthetic lipoprotein molecules, and (4) characterize NLP constructs demonstrating unambiguous formation of membrane protein–NLP combinations.

This project will result in generally applicable methods for the production, isolation, characterization, and functional reconstitution of membrane-bound proteins and protein complexes in NLPs. Success will significantly benefit life sciences in general and advance biological science at LLNL, contributing towards a better understanding of cell membrane-associated proteins. Following proof-of-principle studies, we will initially produce and capture membrane proteins relevant to biodefense. Subsequent work will focus on proteins that play an important role in DOE's strategies for environmental management. The capabilities we develop for membrane proteins will be adaptable to biodefense and human health and bioenergy research.



Crystals of the nanolipoprotein particles Apo E4 22K and dimyristoyl phosphatidylcholine.

Mission Relevance

This work supports LLNL missions in biodefense, energy security via hydrogen generation, and environmental management through uranium bioremediation. It will also support LLNL efforts in fundamental life sciences and biotechnology to improve human health by providing an understanding of membrane biochemistry, which is essential to the understanding of complex living systems.

FY09 Accomplishments and Results

We (1) used our cell-free protein synthesis technique to prepare the cell membrane proteins Yop B, Yop D, Yop B/D, and GPR109B; (2) successfully captured these target proteins, along with *Pyrococcus furiosus* hydrogenase, in NLPs with the retention of function; (3) made NLPs containing lipids with a chelated nitrogen atom and showed these constructs to be capable of binding histidine-tagged proteins; and (4) determined that conjugating histidine-tagged Env protein from the West Nile virus to a nitrogen-NLP provided mice with a protective immune response to a live viral challenge—80% survival compared to 20% in unvaccinated animals—indicating that these constructs hold potential as vaccines. This project demonstrated our ability to use NLPs to capture, stabilize, and present functional membrane proteins critical to neuro-transmission (GRP109B), energy production (hydrogenase), and the understanding of bacterial pathogenesis (Yop B and D). We also demonstrated the ability to use NLPs as a platform to which antigenic proteins could be conjugated to create, in vivo, a protective viral vaccine. We anticipate funding from the Defense Threat Reduction Agency to continue work on vaccine development.

Publications

Blanchette, C. D., et al., 2009. "Characterization and purification of polydisperse re-constituted lipoproteins and nanolipoprotein particles." *Intl. J. Mol. Sci.* **10**, 2958. UCRL-JRNL-235806.

Cappuccio, J. A., et al., 2008. "Cell-free co-expression of functional membrane proteins and apolipoproteins forming soluble nanolipoprotein particles." *Mol. Cell. Proteomics* **7**, 2246. LLNL-JRNL-401933.

Cappuccio, J. A., et al., 2008. "Cell-free expression for nanolipoprotein particles (NLPs): Building a high-throughput membrane protein solubility platform." *High Throughput Protein Expression and Purification, Methods and Protocols (Methods in Molecular Biology).* Humana Press, New York. UCRL-BOOK-235838.

Coleman, M. A., et al., 2007. “Cell-free protein expression screening and immobilization using protein microarrays.” *Cell-Free Protein Expression.* Landes Bioscience, Austin, TX. UCRL-BOOK-231292.

Fischer, N. O., et al., 2009. “Immobilization of his-tagged proteins on nickel-chelating nanolipoproteins particles.” *Bioconjugate Chem.* **20**, 460. LLNL-JRNL-405192.

Fischer, N. O., et al., 2009. *Nickel-chelating nanolipoproteins particles as platforms for vaccine development.* NSTI 2009 Nanotechnology Conf. and Expo, Houston, TX, May 3–7, 2009. LLNL-AR-415466.

Katzen, F., et al., 2008. “Insertion of membrane proteins into discoidal membranes using a cell-free protein expression approach.” *J. Proteome Res.* **7**(8), 3535. UCRL-JRNL-235799.

Nguyen, T. S., et al., 2008. “Amphotericin B–induced interdigitation of apolipoproteins-stabilized nanodisk bilayers.” *Biochim. Biophys. Acta* **1778**, 303. UCRL-JRNL-226688.

Francisella tularensis: Understanding the Host–Pathogen Interaction—Amy Rasley (06-ERD-057)

Abstract

The highly infectious nature of *Francisella tularensis*—the agent that causes tularemia in humans (also known as rabbit fever)—highlights a need for continued research efforts to understand the interactions of this organism with host immune defenses. Very little is known about how the pathogen defeats host immune responses to cause disease, and no licensed vaccine is currently available. This project will investigate factors involved in the early immune response to *F. tularensis* infection and explore the link between environmental persistence and pathogenesis. Our goal is to uncover global host-response patterns that may be used for both therapeutic development and early detection of exposure.

If successful, this project will identify host genes and gene pathways that are important during *F. tularensis* infection, and define the role that host pattern-recognition receptors play in detecting *F. tularensis* and initiating innate immune responses. In addition, exploring the environmental link between bacterial persistence and pathogenesis may shed light on how virulence evolved in this organism. The proposed research could ultimately lead to the identification of target genes that could be used to develop efficacious therapies to combat tularemia and may help us identify potential early-warning markers for biowarfare agent exposure.

Mission Relevance

Developing the ability to effectively detect and treat exposure to the highly infectious, potential biowarfare agent *F. tularensis* first requires gaining an understanding of how this pathogen interacts with host cells to cause disease. Moreover, by defining this previously unknown pathway of pathogen infection and linking it to the human genomic sequence, we will be advancing the detection of emerging and engineered threats. Consequently, this research directly supports LLNL’s national and homeland security missions in the area of biodefense.

FY09 Accomplishments and Results

We identified seven novel *F. tularensis* proteins, previously uncharacterized, that are hypothesized to be involved in both environmental persistence and pathogenesis. To characterize these proteins, we generated targeted deletion mutants lacking each of these seven genes and screened those mutants in both amoeba and human monocytes; cloned, expressed, and purified each protein and modified those proteins to express His-tags; and crystallized two of the proteins and obtained the structure of one of the proteins. We also finalized gene expression analyses from both mouse and human macrophages infected with a panel of fully virulent *F. tularensis* isolates, observing marked differences between mouse and human cellular responses to infection. The successful conclusion of this project has led to the identification of novel *F. tularensis* proteins involved in both environmental persistence and pathogenesis, and may explain, in part, the ability of this pathogen to persist in nature and cause human disease. Research following from this project will be supported by the National Institutes of Health through the Pacific Southwest Regional Center of Excellence. We also submitted a record of invention that covers the potential use of these seven novel *F. tularensis* genes and the protein products they encode as potential targets for therapeutic or vaccine development.

Publications

El-Etr, S., R. A. Robison, and A. Rasley, 2008. *Environmental amoebae as potential reservoirs for* Francisella tularensis*.* American Society for Microbiology Ann. Mtg., Boston, MA, June 1–5, 2008. LLNL-ABS-400079 and LLNL-POST-403470.

El-Etr, S., et al., 2009. “*Francisella tularensis* type A strains cause the rapid encystment of *Acanthamoeba castellanii* and survive in amoebal cysts for three weeks post infection." *Appl. Environ. Microbiol.* **75**, 7488. LLNL-JRNL-415174.

El-Etr, S., et al., 2009. Francisella tularensis *type A strains preferentially survive and replicate in human monocytes and induce marked secretion of inflammatory chemokines.* American Association of Microbiology Ann. Mtg., Philadelphia, PA, April 2009. LLNL-POST-412958.

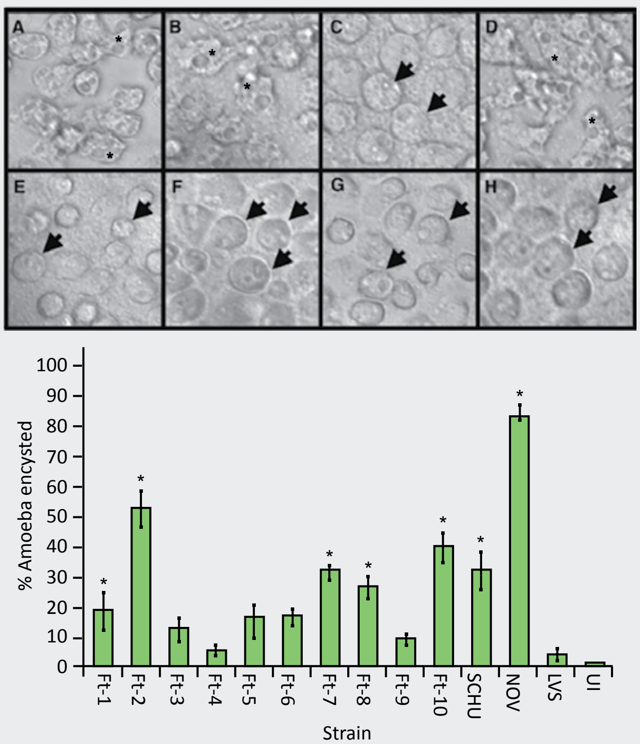
El-Etr, S., et al., 2008. *Prolonged survival of* Francisella tularensis *type A strains in* Acanthamoeba castellanii: *Implications for environmental survival and virulence.* LLNL-PRES-405412.

Characterization and Quantification of Dynamic Robustness in Biological Systems—Eivind Almaas (06-ERD-061)

Abstract

Organisms, even single-celled ones, are extremely complex dynamic systems that must maintain functional stability despite being constantly affected by destabilizing forces. Recent discoveries show that a major destabilizing force lies in the stochastic nature of the cellular machinery itself. The aim of this proposal is to (1) develop analytical and computational methods to identify elements in whole-cell network architectures that increase the robustness of that cellular machinery, (2) analyze weaknesses and failure modes of these robustness-conferring elements, (3) develop new constraint-based approaches to studying cellular networks, and (4) establish and test new metabolic network models that incorporate regulatory programs for *Yersinia pestis*, which causes bubonic plague.

By coupling experimental information on whole-cell organization with analytical and computational predictions and models, we expect to develop a comprehensive understanding of the levels of environmental and inherent internal variation that microbes can tolerate. We hope to infer how individual microorganisms and communities of microorganisms manage both internal and external stochastic variations to avoid potential failure modes. We aim to understand and predict the mechanisms that determine observed failure rates and gain a similar understanding of the dominant failure modalities. For *Y. pestis*, we also expect to identify network-based, new antimicrobial approaches.



Phase-contrast microscopy showing the rapid encystment (arrows) of amoebae in response to *Francisella tularensis* infection. Amoebae may serve as reservoirs for *F. tularensis* in nature.

Mission Relevance

By identifying possible genetic targets for antibiotics to use against *Y. pestis*, this project supports Lawrence Livermore's national and homeland security missions in the area of biodefense, as well as environmental stewardship. More broadly, this project supports LLNL missions in breakthrough science by developing new expertise for the study of stochastic noise propagation in biological networks and the robustness of cellular organisms.

FY09 Accomplishments and Results

We (1) developed models of metabolism for three additional biovars of *Y. pestis* as well as its progenitor *Y. pseudotuberculosis*; (2) used these models to conduct extensive genetic and metabolomic analyses on these organisms' metabolic capabilities; (3) developed a new theoretical tool (GX-FBA) for quantitative combination of genetic expression data with constraint-based models of metabolism; (4) used this tool to study the metabolic response of *Y. pestis* to different kinds of stress, including temperature change and interaction with antimicrobials; (5) developed, simulated, and analyzed a model for a stochastic toggle switch with relevance to synthetic biology, demonstrating that this switch is tunable to ultra-stability, and analyzed the generic mechanism responsible for this stability; and

(6) developed a new approximation method with wide applicability for the stochastic simulation of large genetic circuits. Our constraint-based genome scale model of metabolism in *Y. pestis* (strain 91001) was published in *Molecular BioSystems* and was highlighted in *Nature Chemical Biology* and the Royal Society of Chemistry's *Chemical Biology* journal. The main results of our investigation of stochastic genetic circuits was published in *Physics Review Letters*. This successful project led to the discovery of new regulatory roles for noise in biological organisms and to the development of five new system-level models of metabolism in deadly pathogens and two novel theoretical tools for the analysis of such models.

Publications

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Development of Novel Antimicrobial Proteins and Peptides Based on Bacteriophage Endolysins—

Paul Jackson (07-ERD-025)

Abstract

Antibiotics, the primary tool for fighting bacterial diseases, are limited by microbial resistance and secondary health effects. New antimicrobial agents are needed to address these issues. We will investigate endolysins—bacteriophage-produced proteins that burst bacterial cells—as antimicrobial and detection agents that target specific microbes. We will identify different phage endolysin genes and use these genes and their segments for in vitro production of different endolysins and endolysin fragments. We will measure binding and function of the resulting proteins and peptides to determine specificity and impact on bacterial targets. Based on these initial studies, we will then refine our fragment design to optimize desirable traits.

We will produce antimicrobial proteins or peptides that rapidly lyse (burst) *Bacillus anthracis* (anthrax) and related pathogens. We also will produce antimicrobial proteins or peptides that can

rapidly lyse *Yersinia* species, including *Y. pestis*, which causes plague. In addition, we hope to produce one or more proteins that bind specifically with high affinity to each of these threat agents. The knowledge we gain about the physical and chemical properties of these proteins and peptides, as well as their lytic activity, specificity, binding affinities, and stability under a variety of conditions, will provide insights into whether or not such an approach can be used to control other pathogenic microbes, and will lay the groundwork for producing large quantities of these antimicrobial agents.

Mission Relevance

This project will develop a novel approach to the in vitro production of a new class of antimicrobial and microbe-detection compounds in support of LLNL's national and homeland security missions.

FY09 Accomplishments and Results

In FY09 we (1) continued characterization of endolysins and endolysin fragments, (2) continued production of intact proteins and portions of these proteins, (3) continued study of target-specific portions of the proteins and found that removal of the cognitive portions significantly reduced enzyme activity, and (4) studied the specificity and activity of these proteins on their bacterial targets. In the course of identifying the bacteriophage endolysin genes in phage and prophage genome sequences, we found that all bacteria carry genes encoding similar proteins and that these proteins are probably required for cell wall biosynthesis. The encoded bacterial endolytic proteins were more active and more stable than those isolated from phages and more effective against bacterial targets. In summary, this project resulted in identification and characterization of bacterial muramidases that rapidly destroy *Bacillus anthracis* and other pathogenic microbes. The Centers for Disease Control has taken up the gene encoding of one of these enzymes as well as the procedures for producing the encoded muramidase. They are using the enzyme in newly developed assays to detect antibiotic resistance and are deploying the assays to the Laboratory Response Network laboratories nationwide under a no-cost license with LLNL to produce and use the enzyme. Three additional applications for this class of enzymes have been identified, and support from the Department of Homeland Security for follow-on work is deemed highly likely.

Development of Novel Transgenic Technologies to Study Genome Regulation and Architecture—Gabriela Loots (07-ERD-046)

Abstract

We propose to develop novel transgenic technologies to identify and characterize the biological function of noncoding sequences in genomes. We intend to test some of the known transposable elements including Tol2 and piggyBac for the potential to enhance transgenesis in the frog *Xenopus tropicalis*. The advantage of developing transposon-mediated transgenesis in frogs is that foreign DNA is delivered to a fertilized embryo via microinjection, a procedure that is quick and easy because the fertilized egg is large and tolerant to manipulations. Our approach will blend state-of-the-art computing capabilities with cutting-edge technologies in genomic research. We intend to develop a new set of experimental technologies that will allow us to identify the function of putative regulatory elements in vivo, using the frog as an efficient experimental system. We will establish novel transgenic technologies that will bypass most of the problems associated with current methodologies and develop a universal approach to study genome regulation and architecture on a global scale. Specifically, we will create methods to deliver large fragments of DNA into the frog genome in a site-directed manner. This will permit us to associate regulatory element structure with function and significantly advance the understanding of regulatory mechanisms in complex genomes.

Mission Relevance

This project supports Livermore's mission in biotechnology to improve human health by developing new tools for basic biological research with application to prevention of disease from both natural and bioterrorist threats. This work also supports efforts in outreach and recruitment through its strong potential to attract top-notch university collaborators, students, and postdoctoral fellows to the Laboratory.

FY09 Accomplishments and Results

In FY09 we (1) examined position effects in transgenic frogs having insulator elements and found that the insulators enhance transgene expression level and reduce chimeric expression and position effect, (2) optimized loxP-mediated recombination in vitro and initiated cloning of transgenic constructs to be used in vivo, (3) initiated the engineering of a bacterial artificial chromosome by inserting red fluorescent protein as a reporter and the transposable element Tol2 to create a transgenic construct that would be used in vivo, (4) raised transgenic lines to determine germ-line transmission, and (5) used microarray expression data to generate and test ten predictions of tissue-specific enhancers—we found that 50% of the predictions were faithfully expressed in the tissues. We expect that our development of novel transgenic technologies will continue under a grant from the National Institutes of Health.

Publications

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Pennacchio, L. A., et al., 2007. "Predicting tissue-specific enhancers in the human genome." *Genome Res.* **17**, 201. UCRL-JRNL-216861.

Microarrays + NanoSIMS: Linking Microbial Identity and Function—Jennifer Pett-Ridge (07-ERD-053)

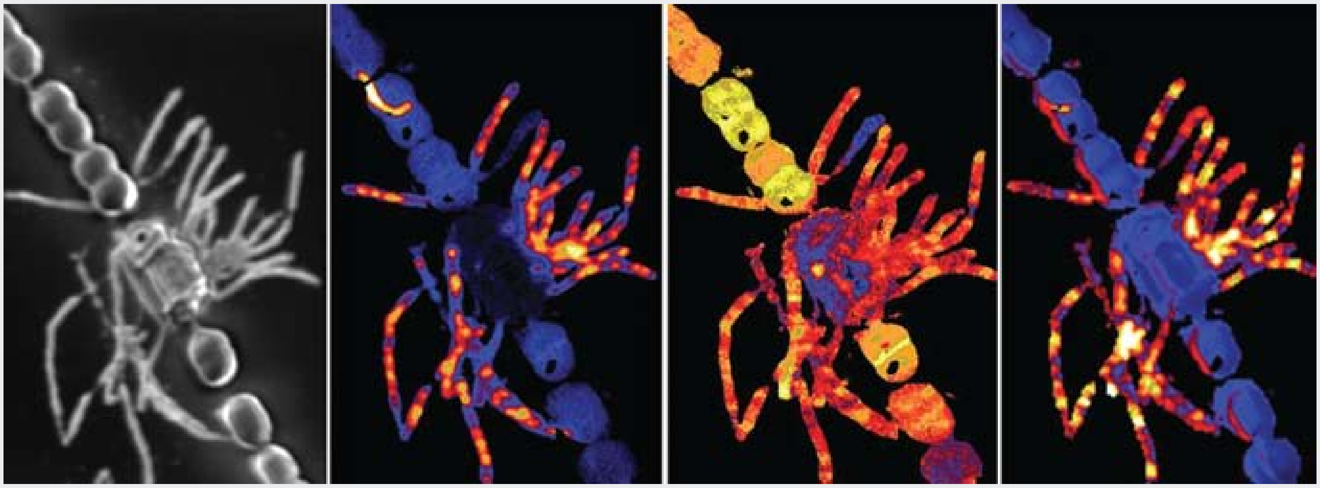
Abstract

This project will develop a next-generation microarray for rapid genetic identification of biothreat agents, then combine this technology with nanoscale secondary-ion mass spectrometry (NanoSIMS) to address issues in energy generation, human disease, and bioremediation science. We will achieve these goals by leveraging LLNL's unique combination of microarray expertise and mass spectrometry capability. Specifically, we will use the high resolution and sensitivity of NanoSIMS to detect isotopic enrichment in ribosomal RNA (rRNA) hybridized in a microarray. This novel technique will allow links between microbial identity and function in multiple applications, and will substantially improve our ability to predict environmental microbial activity and engineer microbes to produce biofuels or treat contaminants by degradation.

Against a background of non-enriched genes, we will identify isotopically enriched rRNA in carbon-13-labeled bacteria extracted from cellulose-degrading biofilms, human tissues, and contaminated soils. Comparing these data to the standard fluorescence analysis of an array, we will identify key microbial phylogenies and their functional roles. This knowledge could enable bioengineering of organisms that efficiently degrade pollutants or produce biofuels such as hydrogen and methane. It also may help define pathways of infection by human pathogens during disease progression, because an understanding of the specific requirements of potentially pathogenic species may enable development of medical treatments. This technique will enable a long-sought means to link structure and function in unculturable microbes.

Mission Relevance

This project supports LLNL's national security mission by delivering an improved array methodology for biosecurity research; supports the energy security mission by furthering development of biofuels, fuel cell bioreactors, and secure energy



Metabolic interactions linked to molecular phylogeny in an *Anabaena* and epibiont association revealed by stable isotope imaging, specifically a combination of nanoscale secondary-ion mass spectrometry and element-labeling fluorescence in situ hybridization. These images were selected for the cover of the *ISME Journal*.

sources; and supports the environmental management mission by furthering remediation of contaminated sites and enabling modeling of microbial roles in carbon sequestration and global climate change.

FY09 Accomplishments and Results

In FY09 we (1) completed pilot tests of the chip stable-isotope probing (ChipSIP) method and began to analyze complex communities—nitrogen-fixing bacteria derived from a wood-eating, dihydrogen-producing beetle hindgut and seawater-carbon-fixing bacteria; (2) continued optimizing our probe design protocol; (3) used NanoSIMS to demonstrate the ability to resolve carbon-12 ribosomal RNA (rRNA) from carbon-13 rRNA probe spots (and nitrogen-14 from nitrogen-15 spots), as well as the ability to identify organisms that have metabolized carbon-13-containing carbon dioxide or glucose or nitrogen-15-containing dinitrogen; and (4) used fluorescence in situ hybridization and SIMS to continue efforts to link phylogeny and metabolism in biofilms, particularly those from hypersaline microbial mats, human oral TM7 bacteria, biofilms growing on medical implant devices, and bacterial epibionts (images of which were selected for the cover of each issue of the 2009 volume of the *ISME Journal*). This project delivered two novel technologies for linking microbial metabolism to phylogenetic identity, both in situ and with high-density oligonucleotide microarrays. The DOE Office of Biological and Environmental Research will support follow-on research using these techniques to study biofuel and dihydrogen-producing microbial systems, particularly the wood-eating beetle hindgut and microbial mats.

Publications

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A New Selectable Marker System for Genetic Studies of Select Agent Pathogens—Brent Segelke (08-ERD-002)

Abstract

The recent ban on use of antibiotics when manipulating bacteria designated as select agent pathogens has severely hampered research in this important area and created an urgent and unaddressed need for molecular genetic technologies involving non-antibiotic selectable markers. The main objective of this project is to advance basic and applied research on bacterial pathogens by developing a genetic engineering technology that will enable manipulation of these pathogens without the use of antibiotics. The specific goals of this project are to develop a novel genetic engineering technology based on plasmid toxin–antitoxin systems to modify bacterial genomes without the use of antibiotic resistance in the mutagenesis process and to assess this technology’s use with select agent pathogens.

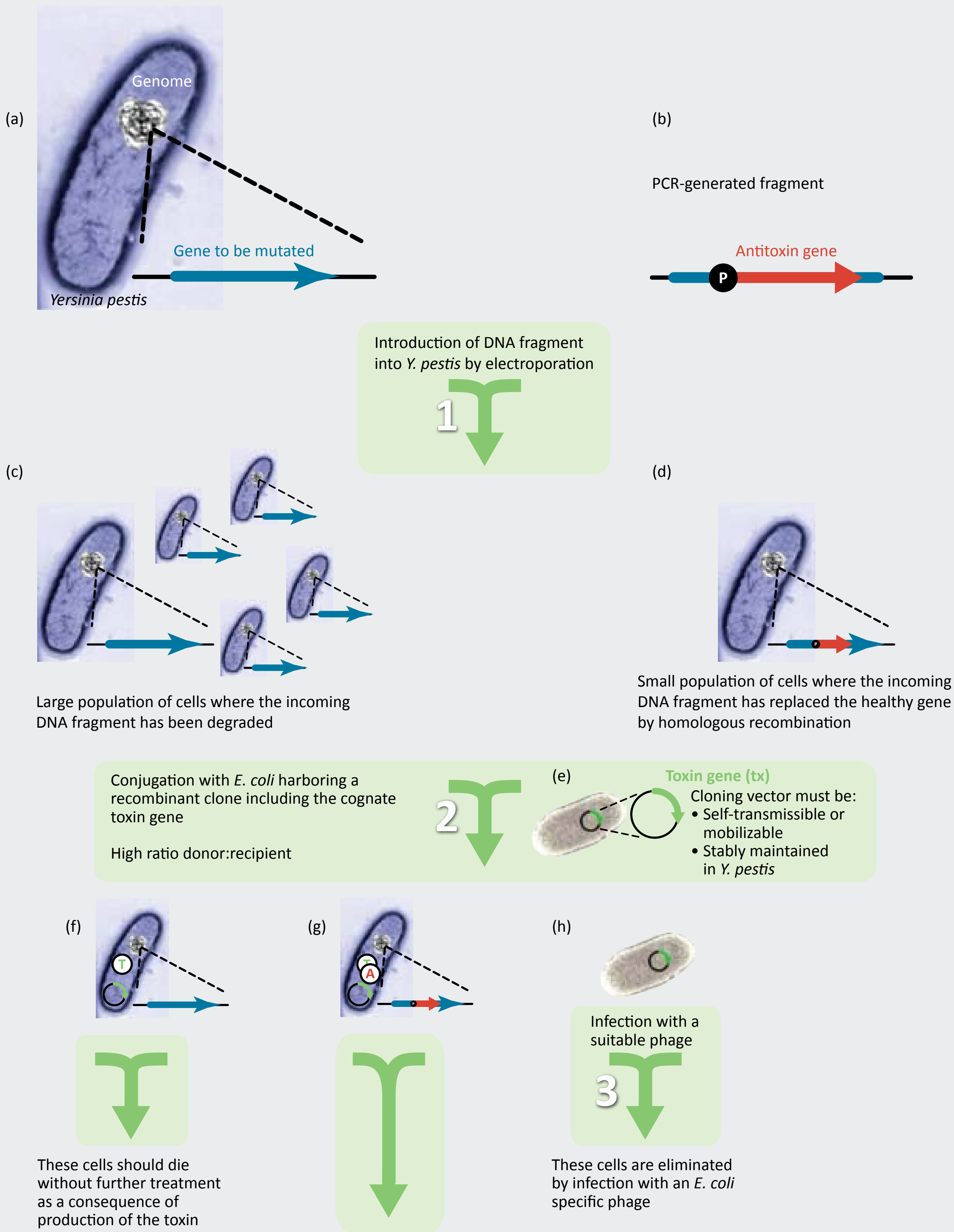
This project constitutes the basic technology development to safely genetically manipulate select agent genomes without the use of antibiotics, allowing the study of these pathogens. Because no methodology for performing such manipulation currently exists, this achievement will advance all areas of select agent pathogen research. In addition, we plan to demonstrate the utility of this novel technology in manipulating the genomes of select agents given top priority by the Centers for Disease Control and Prevention and the National Institutes of Health. Our initial targets for demonstration of this technique will further our understanding of the genes that are involved in virulence and thereby help identify putative vaccine, therapeutic, and detection targets.

Mission Relevance

By developing biodefense capabilities and furthering our understanding of mechanisms of virulence in select agent pathogens, this project supports LLNL’s homeland and national security missions. This work also supports the Laboratory’s mission in bioscience and technology to improve human health by improving disease prevention in general.

FY09 Accomplishments and Results

In FY09 we (1) successfully engineered a toxin-encoding plasmid with the toxin gene under the control of an inducible promoter, transformed the plasmid into *Escherichia coli*, and



Schematic representation of the antibiotic-free methodology for site-directed mutagenesis in select agent pathogens. The wild-type gene to be targeted for mutagenesis is shown (a) and the fragment generated by polymerase chain reaction, where the black circle with a “P” represents a promoter that is functional in *Yersinia pestis* (b). Two types of *Y. pestis* cells are possible after electroporation (c and d). The donor *Escherichia coli* is seen with the toxin gene (also with a promoter functional in *Y. pestis*) (e). Finally, the three possible types of cells resulting from the tri-parental mating (f–h).

validated that the toxin kills *E. coli* without the antitoxin; (2) engineered a mild, or attenuated, version of the toxin encoded in an inducible plasmid and demonstrated that the bactericidal effect can be titrated with an inducer; (3) successfully transformed a plasmid that encodes the mild toxin into an lcr-strain of *Yersinia pestis* and demonstrated that the bactericidal effect of the attenuated toxin is also titratable in that strain of *Y. pestis;* and (4) selected our first gene target in *Y. pestis* to selectively knock out (hmsH), and engineered a clone from which we will amplify recombinant DNA with the *Y. pestis* chromosome.

Proposed Work for FY10

In FY10 we will (1) introduce a single copy of the antitoxin in the *Y. pestis* chromosome and enable selection using either a resident plasmid with the toxin under negative control or a plasmid with the toxin constitutively expressed and introduced afterwards, (2) construct a less lethal toxin that can be negatively controlled, (3) introduce a gene for a red fluorescent protein to allow for easy screening and that could potentially constitute a complementary approach, (4) introduce the antitoxin using either single- or double-recombination techniques, and (5) test the toxin–antitoxin system in other bacterial pathogens to discern the applicability of this selection scheme.

The Elegant Molecular Syringe: Characterizing the Injectisome of the *Yersinia pestis* Type III Secretion System—Brett Chromy (08-ERD-020)

Abstract

Currently, the pharmaceutical industry is not actively pursuing development of antimicrobial compounds from natural products. Reasons include lack of diversity in current synthetic libraries that target bacteria, reduced profitability of the resultant drugs, and low returns in current natural-product discovery from soil bacteria. Moreover, these complex compounds are not being used to target organisms relevant to the biodefense community. For these reasons, we see a tremendous opportunity to screen marine-based natural products for developing countermeasures against biodefense-relevant agents. We will leverage LLNL's large natural-product library, past successes on select agent bacteria research, and expertise in medium-throughput screening.

Specifically, we will (1) better characterize our antibacterial screens that are based on cell viability and induction of the type III secretion system of *Yersinia pestis*—the agent that causes plague—which will test the effectiveness of natural products to kill *Y. pestis* and other select agent bacteria, (2) continue to evaluate our screening assays based on fluorescence, (3) determine the plague injectisome's full complement of protein components and detailed information of its self-assembly, and (4) characterize effective natural products in collaboration with the pharmaceutical or biotechnology industry. Identified proteins will be available for targeting in biodetection and therapeutic strategies.

Mission Relevance

This project supports LLNL's missions in homeland security and bioscience to improve human health by providing new countermeasure targets for plague and new screening technologies, and by improving the understanding of the plague bacterium's key virulence mechanism, the type III secretion system.

FY09 Accomplishments and Results

In FY09 we (1) screened over 450 compounds obtained from the National Cancer Institute for antimicrobial activity against eight human pathogenic bacteria, (2) characterized two natural products that were effective against these bacteria using several different separation techniques, and (3) improved methods for subcellular proteomic fractionation, which is continuing to lead towards injectisome purification.

Proposed Work for FY10

In FY10 we will update our current antimicrobial screen to medium throughput to enable testing of diverse small molecules and natural product compounds, and we will focus more on drug-resistant pathogens, especially multidrug-resistant strains relevant to the military. Specifically, we will (1) test for antimicrobial activity against drug-resistant *Klebsiella* and *Pseudomonas* strains, (2) continue to use comparative proteomics to understand strain diversity in terms of virulence and drug-resistance phenotypes, and (3) examine the temporal and kinetic aspects of type III secretion and examine host–pathogen interaction in real-time.

Publications

Anastasiou, C., et al., 2008. *Sponges: A natural source of antimicrobial compounds.* LLNL-POST-406139.

Carlson, J., et al., 2008. *Analyzing marine natural products for antibacterial properties.* LLNL-POST-405722.

Evans, L., et al., 2008. *Undersea medicine: Screening marine natural products for anti-bacterial properties.* LLNL-POST-406137.

Viability-Based Detection Methods for Pathogens in Complex Environmental Samples—Thomas Bunt (08-ERD-025)

Abstract

The proposed work focuses on detection of viable bacterial pathogens in complex environmental samples relevant to bioterrorism and public health threats. We propose to develop RNA

signatures of pathogens to indicate viability using reverse transcriptase–polymerase chain reaction (RT–PCR), employing novel RNA extraction technology and RNA signatures for detection of viable *Bacillus anthracis* (anthrax) and *Yersinia pestis* (plague). Detection of specific RNA from pathogens has several advantages over DNA-based methods, including low background and more rapid results because little or no cell growth may be needed. We will evaluate and modify RNA-extraction technologies applied to environmental sample types with the goal of developing automated protocols for rapid high-throughput processing and PCR analysis.

If successful, this project will deliver rapid, robust RNA extraction protocols and specific RT–PCR assays to determine presence of viable *B. anthracis* and *Y. pestis* in environmental samples. Results from RT–PCR analysis should be well correlated with culture-based methods and DNA-based, rapid-viability PCR methods. This technology will be transferable to other sample types and pathogens. We expect to produce publications in peer-reviewed journals, form collaborations with government agencies for method validation and application, expand current LLNL biodetection capabilities, and aid the Laboratory in continuing its role in developing next-generation biodetection technologies.

Mission Relevance

The project will enable development of next-generation biodetection technologies in support of Lawrence Livermore's national and homeland security missions of preventing and countering biological weapons of mass destruction. The project leverages LLNL's experience with environmental sample analysis, resources of whole-genome expression and host–pathogen interaction data, capabilities in microarray experimentation and data analysis, bioinformatics tools for assay design and screening, the signature evaluation pipeline, and RNA virus analysis.

FY09 Accomplishments and Results

In FY09, we (1) evaluated RNA extraction methods and identified the optimal technique; (2) evaluated 16 specific *Y. pestis* RNA signatures that target both chromosomal and plasmid RNA, identifying three signatures with the best performance for RNA detection; (3) used dilutions of *B. anthracis* Sterne and *Y. pestis* stocks to compare and evaluate the performance of three RNA amplification kits, and identified the one with the best sensitivity; and (4) optimized RT–PCR assays for *B. anthracis* and *Y. pestis* and correlated their sensitivities to conventional culture, demonstrating the ability to detect as few as 10 viable *B. anthracis* cells and as few as 50 *Y. pestis* cells.

Proposed Work for FY10

In FY10 we will (1) demonstrate *B. anthracis* and *Y. pestis* detection limits and low backgrounds for RT–PCR and nucleic acid sequence-based amplification assays; (2) demonstrate that RNA-based viability methods are accurate compared to traditional culture-based analysis; (3) develop high-throughput protocols for RNA-based detection methods and demonstrate that high-throughput applications are scaleable and provide equivalent sensitivity and specificity to traditional methods; (4) confirm RNA-based detection methods are robust for environmental samples containing debris, complex microbial populations, and dead target organisms; and (5) submit results of our project to peer-reviewed journals.

Important Modes to Drive Protein Molecular-Dynamics Simulations to the Next Conformational Level—

Babak Sadigh (08-ERD-037)

Abstract

Biological action involves dynamic proteins changing between multiple functional states. For example, different states of ion channels have been implicated in a number of neuromuscular and cardiac diseases. Although molecular dynamics based on empirical force fields enables the study of the complex energy landscapes in molecular biology, time scales and transition sizes are subject to local limits. Normal mode analysis can elucidate large conformational changes that are of vital importance to the protein's function, but only in a qualitative fashion. In this project, we will create a new method to use normal mode analysis to remove current limits from molecular dynamics simulations.

We will design a novel Monte Carlo algorithm—the projected importance-sampling Monte Carlo scheme. Integrating this new algorithm into existing molecular dynamics codes, we expect to prove the efficacy of our method by driving a closed ion channel to an open state. This project will provide illustrative predictions of how biological enzymes, receptors, and transmembrane ion channels alter their conformation to perform their function, and determine the atomic structures of transition and active states of these proteins. We expect our results to yield high-profile publications.

Mission Relevance

By creating a tool for predicting membrane protein response to stimuli, this approach could be applied to efforts to counter the effects of biological terrorism in support of national and homeland security.

FY09 Accomplishments and Results

In FY09 we focused on calculating free energy in ligand–protein binding. Specifically, we (1) developed an original, highly efficient free-energy scheme, (2) developed the necessary interface with the NAMD molecular dynamics simulation application, (3) performed a successful simulation of ligand unbinding from a protein, and (4) developed a new technique for calculating the solvation entropy of proteins that can potentially speed such calculations by an order of magnitude.

Proposed Work for FY10

For FY10, we will continue our work on a more efficient algorithm for calculating protein–ligand binding energies. In particular, we will (1) improve the interface to NAMD by extracting forces and momenta on the fly, which will be the basis for determining optimal steering; (2) ready the projected importance-sampling Monte Carlo algorithm for use to guide the reaction in the reduced phase space of the low-energy normal modes; and (3) direct this effort towards simulating binding pathways and determining the kinetic barrier to ligand–protein binding, which is essential for understanding substrate and drug binding. By the end of next year, we expect to have developed a unique capability to routinely calculate the binding energies and kinetic barriers for proteins and their ligands.

New Molecular Probes and Catalysts for Bioenergy Research—Michael Thelen (08-ERD-071)

Abstract

Innovative tools are needed to monitor and catalyze the hydrolysis of plant cellulose, lignin, and other major cell-wall polymers to harness biological systems for energy. Conventional biochemical reagents are not sufficient to meet this demand, and the high cost of converting lignocellulose into fermentable sugars is a serious impediment to generating biofuels. We propose to create novel DNA molecules, or aptamers, that are designed to either detect or hydrolyze key polymers to improve monomer production. This work will provide the basis for future development and patenting of molecular tools that recognize target molecules sought in bioenergy, medicine, and chemical and biological defense applications.

Aptamers are short, single strands of DNA that bind specifically to plant cell-wall disaccharide and polymer targets. We will develop aptamers as a new assay tool for deconstruction. This collection of aptamers will recognize each of several polymers and polymer byproducts and therefore will be extremely valuable in biofuel process engineering. We anticipate that the aptamers will be patented and used in other biofuels efforts at LLNL and in our collaborations with both the DOE Joint BioEnergy Institute and with industry. Aptazymes, or nucleic acid enzymes, that hydrolyze carbon–oxygen bonds in polysaccharides or lignins will be selected as deconstruction catalysts, providing completely new tools in the bioenergy arena.

Mission Relevance

Methods to convert plant biomass to transportation fuels as a secure, sustainable, and clean energy resource are increasingly urgent to address both energy security and global warming. This proposal supports LLNL's energy security and environmental management missions by developing new tools for monitoring and catalyzing lignocellulose deconstruction, thereby furthering efforts to deconstruct plant cell walls into saccharide precursors for use in biological generation of ethanol and other fuels. This project also supports the national security mission by developing tools for biosecurity applications in which target molecule recognition is a key technical hurdle.

FY09 Accomplishments and Results

In FY09 we prepared randomized 40-nucleotide DNA libraries (flanked by fixed, 20-nucleotide polymerase chain reaction primer sequences) for each of the three target polysaccharides—beta 1,4 xylan; alpha 1,4 glucuronic acid (pectin); and beta 1,3 glucan. We applied a stringent selection regime using six rounds of binding and polymerase chain reaction amplification, cloning the final round and sequencing 30 aptamers for each target. We then reselected 8 to 12 aptamers each, sequenced and characterized them for binding specificity using biochemical assays, including surface plasmon resonance, fluorescent plate assays, and fluorescence microscopy. The results of these initial experiments were mostly negative, indicating perhaps that the aptamers had been selected based on binding to surface materials and not to the polysaccharides.

Proposed Work for FY10

Because of difficulties in selecting aptamers that bind to cellulose, we will target more soluble polysaccharides. We will (1) design aptamer libraries to bind beta 1,3 glucan (found in both fungi and plants) and alpha 1,4 glucuronic acid (plant pectin); (2) select and characterize, with fluorescent imaging and circular dichroism assays, aptamers that bind to these substrates; (3) sequence and computationally analyze those candidates that bind with high affinity for secondary structures to predict binding interactions; (4) perform confocal microscopic imaging of plant cell walls using glucan- and pectin-specific aptamers; and (5) test the glucan-specific aptamer for nonpathogenic microbes containing this cell wall polymer.

Publications

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Rowe, A., et al., 2008. *Aptamer selection and electrochemical biosensors for small analyte detection*. LLNL-ABS-408636.

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Siebers, A. K., and Thelen, M., 2009. *DNA as a probe for bioenergy research.* LLNL-ABS-408526.

Regulation of *Yersina pestis* Virulence by Autoindicer-2-Mediated Quorum Sensing—Brent Segelke (08-LW-025)

Abstract

We propose to establish a causative link between autoinducer-2 (AI-2) signaling and regulation of *Yersina pestis* virulence. The bacterium *Y. pestis* causes plague, one of the most devastating diseases in human history, and is a recognized biothreat agent. Virulence-factor gene expression and AI-2 quorum sensing are correlated in *Y. pestis*. Other pathogens are known to regulate virulence via AI-2 signaling. However, the causative link between AI-2 signaling and virulence has not been identified. We will establish a causative link and elucidate AI-2 signaling pathways by observing the impact of quorum-sensing gene knockouts on virulence-factor gene expression; by tracking the fate of exogenous, radiolabeled AI-2 taken up by *Y. pestis*; and by identifying AI-2 metabolites for enzymes known to be involved in AI-2 processing.

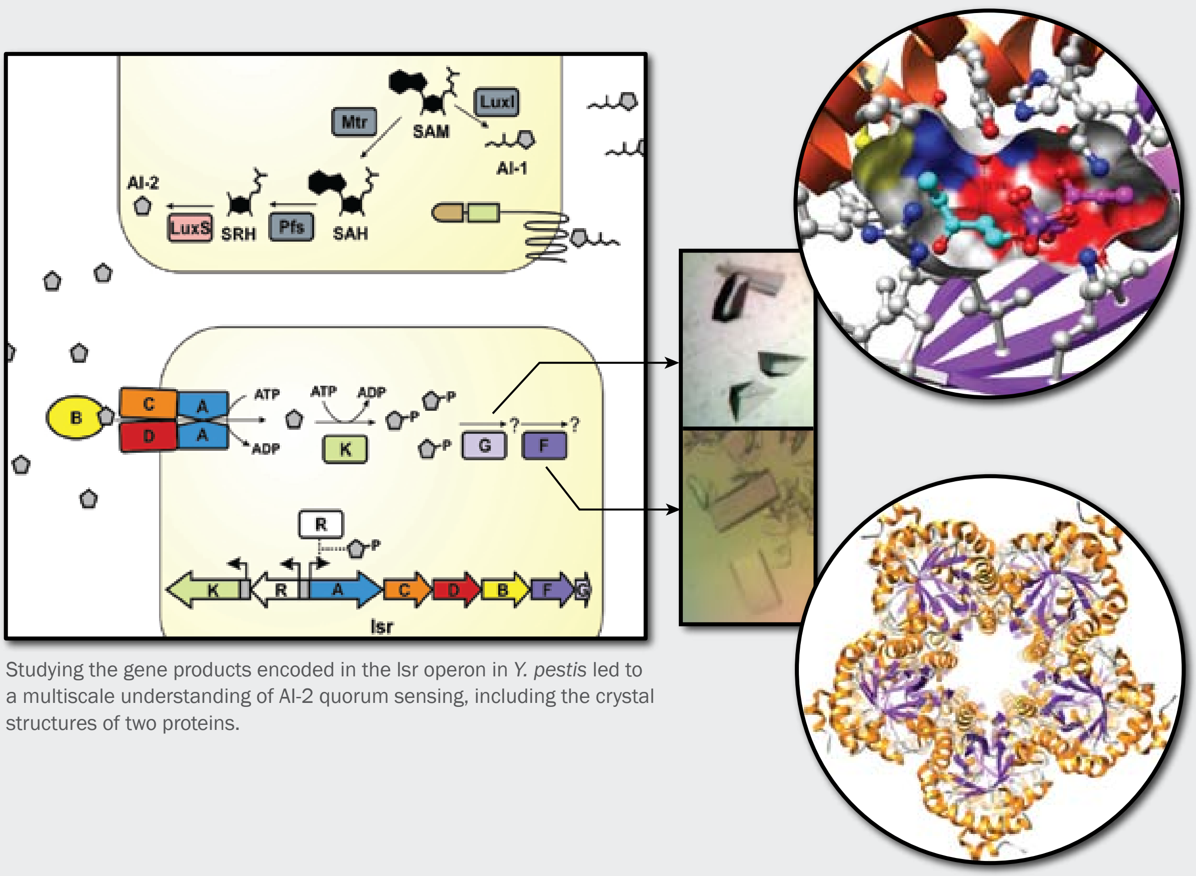
We expect to gain new insights into mechanisms of *Y. pestis* virulence and cell–cell communication. A number of basic research questions will be answered, and new research directions will be enabled. We intend to establish a link between AI-2 quorum sensing and regulation of virulence, and track the fate of AI-2 after uptake by *Y. pestis*. This will enable antimicrobial development designed to poison quorum-sensing mechanisms. In addition, we expect to create genetic knockouts for the AI-2 signaling pathway and produce synthetic AI-2 to enable expression-array experiments.

Mission Relevance

The proposed research will advance national security by supporting Laboratory efforts to counter the spread and use of biological weapons of mass destruction, as well as advance fundamental science and technology. Successful completion of this project will enable a greater understanding of *Y. pestis* virulence mechanisms, which may lead to new strategies for countermeasures or detection, impacting both biodefense capabilities and disease prevention. This will help to build core strengths in biodefense research and leverage the unique research capabilities and facilities at LLNL.

FY09 Accomplishments and Results

We (1) successfully cloned all of the genes in the AI-2 uptake and response network from the CO92 strain of *Y. pestis*; (2) expressed in high yield and purified to near-homogeneity four of the six soluble proteins in the AI-2 network and several sub-domains of a fifth; (3) determined the crystal structure of



Studying the gene products encoded in the lsr operon in *Y. pestis* led to a multiscale understanding of AI-2 quorum sensing, including the crystal structures of two proteins.

two of the proteins (enzymes lsrF and lsrG) and yielded crystals of a third in complex with AI-2; (4) successfully synthesized both unlabeled and labeled AI-2, enabling metabolite studies and in vitro biochemistry studies; (5) identified three novel protein–protein interactions using dual polarization interferometry; and (6) obtained a genetic mutation—the knockout for the gene locus ypo0405. This project has led to new collaborations, and follow-on work is expected to be of interest to the National Institutes of Health, particularly the National Institute of Allergy and Infectious Diseases.

Publications

Gryshuk, A., et al., 2008. *Structure-driven approach to detection and characterization of virulence proteins*. LLNL-POST-402554.

Gryshuk, A. L., et al., 2009. Yersinia pestis *processing of quorum sensing signaling molecule AI-2*. LLNL-POST-403521.

Bacteria–Mineral Interactions on the Surfaces of Metal-Resistant Bacteria—Alexander Malkin (08-LW-027)

Abstract

We propose to combine atomic force microcopy and synchrotron infrared-spectromicroscopy techniques to investigate the surface chemistry, structure, and environmental dynamics of metal-resistant bacteria. We intend to reveal the molecular mechanisms that control formation and mechanical properties of biogenic metal phases on cell surfaces. Currently, definitive models for reduction of toxic metals by bacteria await elucidation. We will characterize the dynamic, stress-induced structural responses of bacterial surfaces and formation of metal-mineral phases on cell surfaces. This work will improve the fundamental understanding of mechanisms of environmental remediation by metal-resistant bacteria, which is of great interest to DOE for in situ, reductive immobilization of toxic metals.

By elucidating relationships between the stress-induced organization, function, and environmental dynamics of protein and polymer complexes at bacterial cell-wall surfaces, and by unraveling the ways they guide the formation of biogenic metal phases on cell surfaces, this work will profoundly enhance insights into molecular architectural, structural, and environmental variability of cellular and microbial systems. We also expect that our proposed work will improve the fundamental understanding of environmental remediation mechanisms by metal-resistant bacteria. Our research will result in a new technical competency for application to Laboratory efforts in environmental biology, as well as published papers and conference presentations.

Mission Relevance

Microbial processes active in the near-surface environment are a critical component of DOE's strategy for site remediation where toxic metals and radionuclides contaminate groundwater or have the potential to do so. This work will contribute towards a molecular-scale understanding of these processes. Additionally, this research will support DOE's broader strategy in environmental biology through development of techniques capable of probing the physical and chemical interactions in cellular systems in their natural state.

FY09 Accomplishments and Results

In FY09, we improved experimental procedures for the in vitro visualization of structural dynamics of single cells in fluid and collected data on the environmental responses of cellular systems to toxic metals, which enhanced insights into the molecular architecture, structural, and environmental variability of cellular systems. This project enabled novel probe microscopy and synchrotron infrared spectromicroscopy techniques to analyze molecular-scale biophysical pathways of cellular systems related to biotransformation, environmental resistance, and remediation processes. The Laboratory will support additional research to evaluate chromium-transformation pathways in metal-reducing bacteria.

Publications

Malkin, A. J., 2009. *Macromolecular assembly: From virus crystallization to structure-function relationships of microbial and cellular systems.* Gordon Research Conference on Thin Film and Crystal Growth Mechanisms, New London, NH, July 12–17, 2009. LLNL-PRES-414599

Malkin, A. J., 2009. *Probing the architecture and structure-function relationships of microbial and cellular systems by high-resolution in vitro atomic force microscopy.* American Chemical Society Natl. Mtg., Salt Lake City, UT, Mar. 22–26, 2009. LLNL-ABS-40789.

Malkin, A. J., 2008. *Unraveling the architecture and structure-function relationships of single pathogens by in vitro atomic force microscopy.* American Chemical Society Northeast Regional Mtg., Burlington, VA, June 29–July 2, 2008. LLNL-ABS-402724.

Malkin, A. J., and M. Plomp, in press. "High-resolution architecture and structural dynamics of microbial and cellular systems: Insights from in vitro atomic force microscopy." *Scanning Probe Microscopy of Functional Materials: Nanoscale Imaging and Spectroscopy.* Springer, New York. LLNL-BOOK-409734.

Malkin, A. J., et al., 2009. *In vitro high-resolution architecture and structural dynamics of bacterial systems.* Physics of Cells:

From the Edge to the Heart, Primosten, Croatia, Sept. 6–13, 2009. LLNL-ABS-415463.

Plomp, M., et al., 2007. *In vitro high-resolution architecture and structural dynamics of single pathogens.* Materials Research Society 2007 Fall Mtg., Boston, MA, Nov. 26–30, 2007. UCRL-ABS-231840.

Prediction of Patient Response to Chemotherapy Using Drug Microdosing—Michael Malfatti (08-LW-100)

Abstract

Platinum-based drugs are the most successful class of compounds for the treatment of cancer. These drugs kill cancer cells through toxic DNA damage. However, many patients are unresponsive to treatment or acquire drug resistance. Using a radiocarbon-labeled anticancer drug (carboplatin) and accelerator mass spectrometry, the most sensitive method for studying long-lived isotopes, we will measure platinum-induced DNA damage sites (adducts) in cancer patients. The goal of the study is to determine which cancer patients will benefit from carboplatin treatment and which will be resistant. This project is being conducted in collaboration with researchers from the University of California Davis Cancer Center, who will help design the study and recruit patients for the clinical trial.

We expect to observe three types of patients: (1) responders, with high DNA adduct levels; (2) those who stabilize with an intermediate level of DNA damage; and (3) nonresponders, who have very low levels of drug-modified DNA and for whom treatment is least successful. We will address: Does drug uptake or DNA repair predominate cellular sensitivity to platinum drugs? Will a single patient dosed several times show the same kinetics of DNA damage and repair each time? Will drug metabolism kinetics differ between patients substantially enough to allow discrimination of responders from nonresponders in a small group of patients? Answering these questions will form a foundation for establishing a database of pharmacokinetic parameters to allow predictive diagnostic testing with accelerator mass spectrometry.

Mission Relevance

The ability to track pharmokinetics at exceedingly low isotopic doses will directly contribute to Livermore's mission in biosciences to improve human health and has potential applications in biothreat detection for LLNL's missions in national and homeland security.

FY09 Accomplishments and Results

In FY09 we (1) developed protocols for filter sterilization and packaging of [^{14}C]carboplatin and [^{14}C]oxaliplatin chemotherapy drugs and submitted them to the Food and Drug Administration (FDA) for a preliminary Investigational New Drug (IND) meeting, (2) developed tumor DNA repair protocols using nude mice and human tumor xenographs, and (3) worked with the FDA and LLNL for approval of a clinical feasibility study of [^{14}C]carboplatin and [^{14}C]oxaliplatin microdosing in bladder cancer patients. The pre-IND meeting resulted in FDA approval for use of [^{14}C]carboplatin and [^{14}C]oxaliplatin in humans without requiring further animal studies. This project has laid the foundation for continued work on a human clinical feasibility study for microdosing with [^{14}C]carboplatin or [^{14}C]oxaliplatin. The work will continue at the University of California at Davis Medical Center in collaboration with LLNL to perform a clinical feasibility study when the requisite certification and approvals are complete.

Publications

Henderson, P. T., et al., 2008. "Towards personalized chemotherapeutics: Exploring variations in DNA damage/repair in cells and tumors treated with carboplatin using accelerator mass spectrometry." *Environ. Mol. Mutagen.* **49**(7), 552. UCRL-POST-228855.

Coupling Advanced Cryo-Electron Microscopy with High-Performance Computing to Resolve Biomolecular Function—Felice Lightstone (09-ERD-009)

Abstract

The objective of our research is to combine advancements in aberration-corrected cryo-electron microscopy with high-performance computing to rapidly solve biomolecular structures and determine their function. Resolving protein structures is currently limited by the small number of proteins that can be crystallized to determine structure. We plan to be the first to use aberration-corrected electron microscopy to image a protein at atomic resolution. Specifically, we will (1) adapt ion-mobility to improve sample preparation and deposit more homogeneous populations of proteins on a clean substrate, (2) obtain aberration-corrected electron microscopy data on protein, (3) develop image-processing techniques to reconstruct the three-dimensional image and model, and (4) apply high-performance computing to simulate the protein to predict its function.

If successful, we will be the first to use aberration-corrected electron microscopy to image a protein at atomic resolution. This demonstration will revolutionize the biological field because there will no longer be a need to crystallize samples prior to structural determination. We ultimately will create a single-molecule method for determining biomolecular structures at atomic resolution. To achieve this, we will make advancements in each of the steps necessary for the imaging and structure

determination of the protein. We will also have predicted protein function through high-performance computing simulations of the protein.

Mission Relevance

The national and homeland security missions of Lawrence Livermore include developing new countermeasures to combat chemical- and biological-warfare threats. Our project success will entail demonstration of proof-of-principle for a new capability to determine structures and functions of unknown proteins in host-pathogen pathways. This will enable rational design approaches that can be applied to development of new therapeutics and pre-treatments. This capability can be applied to all fields of biology and will expand LLNL's reputation in the biological sciences.

FY09 Accomplishments and Results

In FY09, we (1) demonstrated the ability to use ion mobility mass spectroscopy to improve sample preparation by separating out the protein LsrF based on completeness for complex formation and conformation, (2) developed new one-dimensional algorithms to improve the signal-to-noise ratio in signal processing, (3) leveraged LLNL tomography codes to process the data to create three-dimensional models, (4) applied high-performance computing simulations to the homology models of the lsrF complex, and (5) imaged lsrF using cryo-electron microscopy to determine the preliminary overall structure.

Proposed Work for FY10

In FY10 we will continue advancements to atomic resolution imaging of LsrF and LsrG. Specifically, we will (1) improve sample preparation to increase the homogeneity of purified protein deposited on the microscopy grid, (2) use aberration-corrected electron microscopy to collect atomic-resolution images, (3) leverage Laboratory image-processing algorithms to improve the signal-to-noise ratio of cryo-electron microscopy images with a two-dimensional filter while greatly improving the quality of the three-dimensional models generated with novel reconstruction tools, and (4) apply high-performance computing simulations to the newly generated models to predict the protein's function.

Flexible and Rapid Therapeutic Countermeasures for Global Biosecurity—Jane Bearinger (09-ERD-054)

Abstract

Emerging and engineered infectious diseases are a threat to political, social, and economic stability. A robust global biodefense strategy requires anticipation, detection, and rapid response. Currently, biodefense is guided by knowledge of state-sponsored bioweapon programs and a list of the biological threat agents. This strategy is poorly suited to address the rapidly evolving nature of biological threats. Our goal is to create a science and technology base to significantly reduce the development time for antimicrobial drugs. The foundation we lay will help reduce drug development times to months rather than years. This project integrates advanced scientific computing, microfluidics, accelerator mass spectrometry, and select-agent science to create a unique approach for rapid development of new therapeutics.

We expect to develop automated, high-throughput extraction and culturing techniques for processing existing libraries of marine natural products and chemical genomics, which will make it possible to create a huge new library of drug candidates from these compounds. We will develop techniques for rapidly identifying drug candidates using host gene expression, gene knockout libraries, and metallome analyses and model systems to illuminate these pathways and identify factors involved in the early immune response to pathogen infection. In addition, we will accelerate the process for predicting the effectiveness of drugs using ultrasensitive accelerator mass spectrometry.

Mission Relevance

This project supports LLNL's mission to reduce or counter threats to national security by helping enable a flexible biodefense capability to detect and characterize unknown and engineered pathogens, and to rapidly develop new medical countermeasures.

FY09 Accomplishments and Results

In FY09 we (1) characterized samples from the National Cancer Institute and identified novel activity against the bacterial pathogens *Bacillus anthracis*, *Yersinia pestis*, and *Francisella tularensis* that is not toxic in human monocyte cell-lines at concentrations lethal to microbes; (2) completed in vitro metabolism studies of two compounds—the stimulant caffeine and ciprofloxacin —and determined separation parameters for major metabolites for drug interaction studies using accelerator mass spectrometry; (3) optimized infection and qRT polymerase chain reaction expression protocols for host monocyte studies with *Y. pestis* and *F. tularensis* (unique virulence mechanisms); and (4) tested protein-induced x-ray emission analysis protocols developed for metalloprotein expression work.

Proposed Work for FY10

In FY10 we will (1) continue to develop network analysis computational tools—a flux balance model will create a metabolic database incorporating systems biology, structural informatics, and docking studies; (2) generate and prioritize relevant genes and promising drug targets for novel antimicrobials based on pathway analyses and available proteomics data; (3) experimentally identify common and unique mechanisms of virulence and host response for both *F. tularensis* and *Y. pestis* and perform complementary comparative gene-array studies and host-response proteomics; and (4) complete drug–drug interaction with animal-based studies using accelerator mass spectrometry and provide data for physiologically based pharmacokinetic simulations.

Biological Testing of Systems Biology: Validation of Flux-Balance Analysis Predictions—Ted Ognibene (09-ERI-002)

Abstract

Flux-balance analysis can determine metabolic capabilities of cellular systems and growth rates of organisms, but current techniques for measuring metabolite fluxes lack the necessary sensitivity and instead rely on concentration measurements from which flux ratios are calculated. Our objective is to develop a protocol for measuring metabolite fluxes to test, validate, and further constrain flux-balance models. We will use accelerator mass spectrometry to measure the rate of metabolite formation using a carbon-14-labeled tracer and, using these results, improve flux-balance simulation for the yeast *Saccharomyces cerevisiae*. We will also develop a protocol utilizing accelerator mass spectrometry to measure fluxes for amino acid biosynthesis metabolites as a proof of concept to constrain and validate flux-balance models.

Using whole-cell labeling techniques, we will determine the rate of incorporation of glucose metabolism products into cellular pools of DNA, protein, lipids, and small molecules in yeast cells over time. We will also develop an extraction method and high-performance liquid chromatography protocol for separating and quantitating several metabolites and free amino acids along phenylalanine and tyrosine biosynthesis pathways. The extraction and purification protocols will be used to measure the fluxes of metabolite intermediates chorismate, prephenate, and arogenate and the free amino acids phenylalanine and tyrosine. Experimentally derived fluxes will be compared to fluxes predicted by the existing flux model for yeast and used to constrain and validate the model.

Mission Relevance

By developing advanced flux-modeling technology with biodefense and bioenergy applications, this project supports LLNL's missions in national as well as energy security.

FY09 Accomplishments and Results

We grew yeast in media supplemented with 1 nCi of carbon-14 glucose and fractionated the cells using standard protocols to isolate DNA, RNA, and protein. Using accelerator mass spectrometry, we found that the labeling procedure resulted in 0.00443% of the carbon-14 label incorporated into DNA, 0.182% in the RNA, and 0.0138% of the label was incorporated in the protein. These results correspond to 18.45 molecules of carbon-14 label per DNA molecule, 0.00419 per molecule of RNA, and 0.000212 per protein. Negligible amounts of the label were detected in the small molecule and lipid pools. We concluded that the labeling protocol is appropriate for measurement of cellular macromolecules, but may be lower than optimal for measuring the flux of metabolic precursors such as amino acids and nucleotide bases.

Proposed Work for FY10

In FY10 we will develop and apply metabolite extraction and high-performance liquid chromatography techniques to separate amino acids from *S. cerevisiae* cells. Extraction and separation of amino acids will enable quantitative measurement of metabolic fluxes. Specifically, we will (1) extract polar metabolites including amino acids and amino acid precursors, (2) separate individual metabolites by high-performance liquid chromatography, (3) use FY09 results to optimize labeling procedures for measuring amino acid fluxes, and (4) measure fluxes of labeled metabolites using accelerator mass spectrometry. Generated data will be used to test and refine existing yeast flux-balance models.

Publications

Sporty, J., et al., 2009. "Quantitation of NAD+ biosynthesis from the salvage pathway in *Saccharomyces cerevisiae*." *Yeast* **26**, 363. LLNL-JRNL-410719.

The Role of Dendritic Cells in Tularemia Pathogenesis—Sahar El-Etr (09-LW-036)

Abstract

Our objective is to understand the pathogenesis of *Francisella tularensis*, with the ultimate goal of helping to develop countermeasures for the disease caused by it, tularemia (also known as rabbit fever). Hypothesizing that *F. tularensis* disrupts host cellular trafficking pathways upon entry into immune cells, we will identify and localize the stage at which this disruption occurs and identify the bacterial and host genes involved in the process. Using immunofluorescent microscopy and biochemical analysis and a panel of pathogenic and nonpathogenic strains, we will compare the localization of known protein markers along the trafficking pathway of human dendritic cells and localize the stage where *F. tularensis* causes aberrant host-protein localization. We will also identify bacterially secreted proteins involved in the process.

We expect this study to result in the identification of host proteins that are directly disrupted by *F. tularensis*. These findings will have broad impact on identifying potential drug targets for tularemia and possibly other intracellular pathogens that interfere with host immune responses in similar ways. In addition, identifying bacterial proteins involved in the disruption of host cellular functions will help identify bacterial candidates for vaccine development. Our study will be the first ever to compare the behavior of multiple pathogenic and nonpathogenic strains

in human host cells and will have a broad impact on the scientific community and provide critical information on the pathogenesis of tularemia.

Mission Relevance

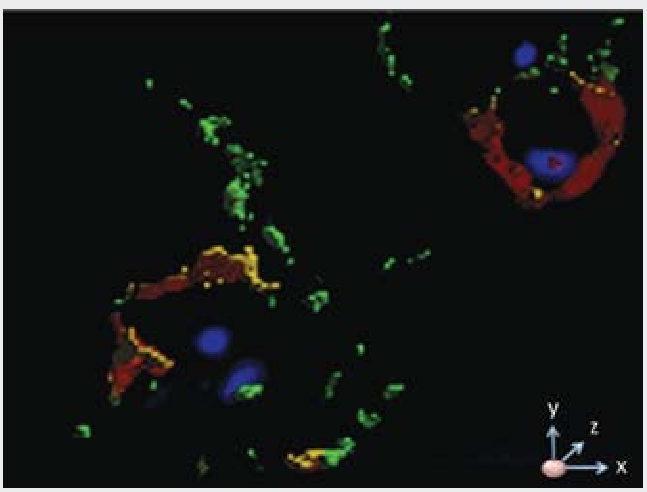
Understanding the mechanisms of pathogenesis of *F. tularensis* and identifying bacterial and host genes involved in the virulence process will contribute significantly to development of countermeasures against tularemia, a serious biothreat agent. This project thus support's LLNL's national security mission of controlling the use of weapons of mass destruction and strengthening homeland security.

FY09 Accomplishments and Results

In FY10 we (1) obtained and successfully optimized the differentiation of dendritic cells; (2) obtained antibodies against virulent *F. tularensis* strains, optimized their use, and successfully optimized infection experiments; (3) successfully conducted and optimized immunofluorescence experiments with nonpathogenic *F. tularensis* strains and conducted experiments with the virulent strains; and (4) optimized the biochemical analyses of cytokines from cell supernatants and begun optimizing conditions for phagosome isolation.

Proposed Work for FY10

Our goals for FY10 are to (1) localize the stage at which pathogenic *F. tularensis* strains disrupt the phagosomal pathway in dendritic cells by comparing trafficking and cytokine profiles of cells infected with pathogenic and nonpathogenic bacteria, (2) isolate bacterial phagosomes from infected cells and identify the bacterial proteins present, (3) isolate and identify host proteins that interact with the bacterial proteins we identified, and (4) analyze the protein pathways containing bacterial and host proteins identified above. Both bacterial and host proteins identified are likely to be involved in pathogenesis and would represent targets for development of countermeasures against tularemia.



Three-dimensional rendered immunofluorescence projections of human dendritic cells infected with *Francisella tularensis* (subspecies *novicida*) and stained with a *F. tularensis* antibody (green), the endosmal marker Rab5 (red), and the nuclear stain DAPI (blue) at two hours post infection. Areas where the bacteria co-localize with Rab5 appear yellow. These regions have been highlighted and quantified using Volocity software.

Publications

El-Etr, S. H., et al., 2009. "*F. tularensis* type A strains cause the rapid encystment of *Acanthamoeba castellanii* and survive in amoebal cysts for three weeks post infection." *Appl. Environ. Microbiol.* **75**(23), 7488. LLNL-JRNL-415174.

Effect of Aging on Chondrocyte Function—

Gabriela Loots (09-LW-072)

Abstract

Age is a risk factor associated with skeletal degenerative disease such as osteoporosis and osteoarthritis. It is estimated that osteoarthritis affects 20 million Americans and incurs over $30 billion in medical costs annually. We hypothesize that age-dependent changes in molecular and biochemical content of skeletal tissue affect the binding of individual cells to the extracellular matrix, resulting in the understimulation of cells and altering the cell's metabolic activity. We will examine mechanisms by which aged cells become less responsive to the stimulus of mechanical loading to determine if the decrease in cell synthetic activity with age is caused by reduced cell–matrix interaction. For this project, we will leverage LLNL's capabilities in molecular biology, bioengineering, atomic force microscopy, and microfabrication.

If successful, we expect to find that aged cells have impaired gene expression and are less responsive to mechanical loading because of weaker adhesion to the surrounding extracellular matrix, such that the weakened interaction shields the cells from the normal physiological loading that healthy young cells experience. These findings would represent a paradigm shift in studies of the loss of cartilage cell (chondrocyte) function with age, and would also help identify target matrix molecules or receptors that are responsible for the decreased sensitivity of aged chondrocytes to loading. Such targets may be amenable to pharmaceutical treatment or gene therapies to retard or reverse the onset of osteoarthritis.

Mission Relevance

This project works toward a better understanding of osteoarthritis in support of LLNL's mission in science to improve human health. The project will develop a unique approach to molecular-level microfabrication that could benefit efforts such as chemical and biological warfare agent detection that utilizes sensors and other such structures.

FY09 Accomplishments and Results

In FY09 we (1) measured the intrinsic compressive stiffness and Poisson's ratio of immature chondrocytes, (2) optimized cell isolation conditions and determined proper storage of isolated cells to minimize variability from experiment to experiment, (3) identified local sources of adult chondrocyte tissues and optimized cell isolation protocols, and (4) examined if carbon nanotubes promote chondrogenic fate using both molecular markers and histology.

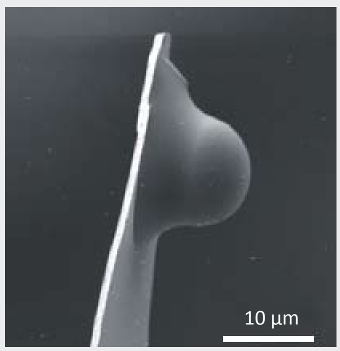
Proposed Work for FY10

In FY10 we will (1) conjugate two bovine proteins (hyaluronan and collagen type II) to beads and glass substrates, (2) measure adhesion forces between proteins attached to beads and both immature and adult chondrocytes, (3) obtain mechanical measurements to determine if young and old chondrocytes have different affinity for extracellular proteins derived from young and old joints, (4) isolate RNA from chondrocytes labeled with green fluorescent protein from young and aged cells from joints and vertebral disks, and (5) carry out microarray experiments.

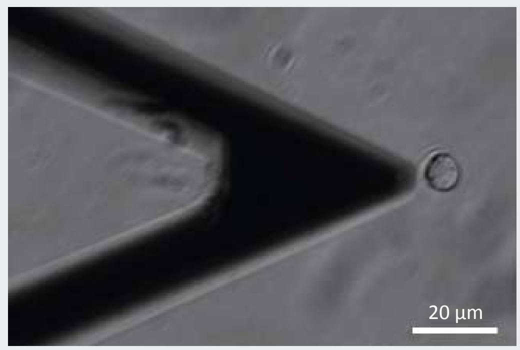
Publications

Blanchette, C. D., et al., 2009. *Characterization of the dynamic mechanical properties of chondrocytes by AFM.* American Society for Bone and Mineral Research (ASBMR) 31st Ann. Mtg., Denver, CO, Sept. 11–15, 2009. LLNL-POST-416718.

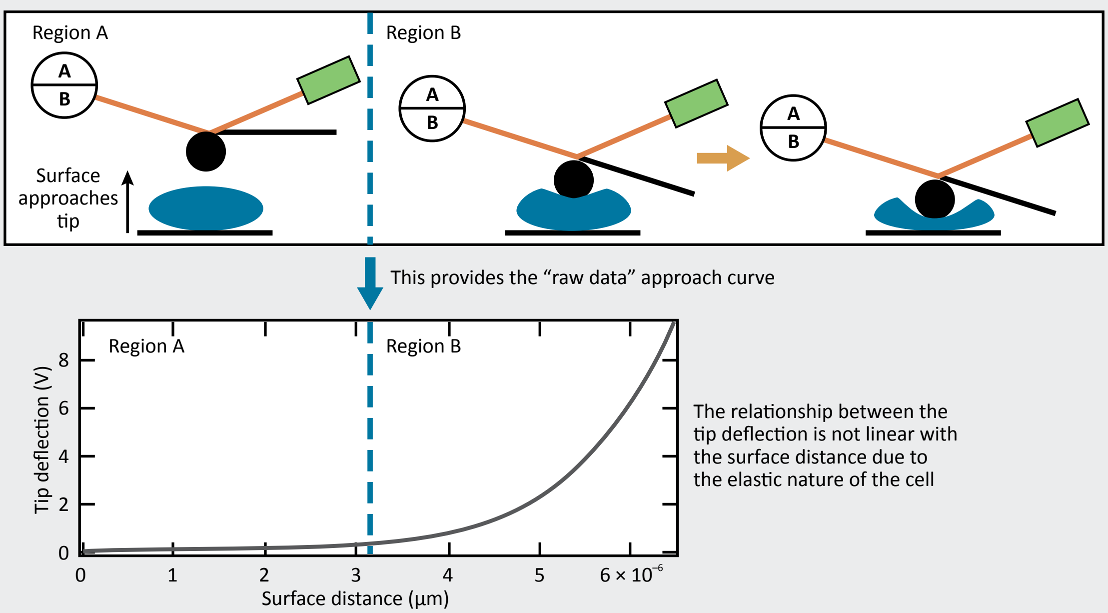
AFM/optical microscope



10-µm PS/AFM tip



Align AFM/10-µm probe over cell



A combined atomic force microscope (AFM) and optical microscope was used to measure the mechanical response of chondrocyte cells to loading.

Versatile Delivery and Immune-Stimulatory Platform for Just-in-Time Vaccine Development—
Craig Blanchette (09-LW-077)

Abstract
The goal of this project is to develop new vaccines in which a versatile and rapidly manufactured platform can be used for efficiently delivering pathogenic antigens. Although traditional whole- or killed-cell pathogens have proven successful in the past, this method is plagued with technical difficulties. Currently, researchers are attempting to use subunit vaccines as a substitute but have had little success in efficiently delivering the recombinant protein to immunogenic cells. We propose using nickel–nanolipoprotein (NiNLP) particles as an antigen delivery vehicle. This method will allow us to combine the delivery vehicle, immune stimulation, and pathogen antigen into a single entity, thus eliminating problems currently facing researchers in this field.

The expected result of our proposed research is just-in-time vaccine production in which a robust and highly effective antigen-platform vaccine is manufactured from a gene of interest and ready for use in a matter of hours. This technology will also greatly enhance the field of disease prevention by helping to develop vaccines against hundreds if not thousands of pathogens. Furthermore, development of this vaccine technology will launch a whole new and unexplored field of vaccine development.

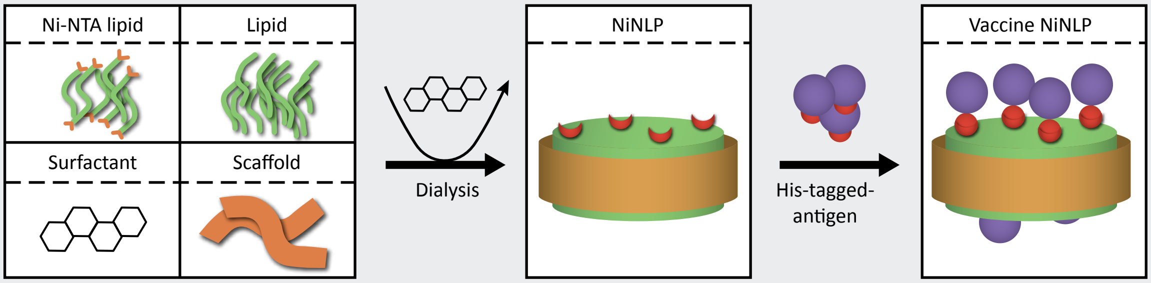
Mission Relevance
Our proposed work is crucial to developing potent vaccines that can be applicable to both disease prevention and increased biodefense capabilities, in support of Laboratory missions in human health and homeland security.

FY09 Accomplishments and Results
In FY09 we (1) identified lipid-to-scaffold protein combinations that resulted in highly stable and uniform NiNLPs and determined the optimal nickel and nitrilotriacetic acid content; (2) used analytical size-exclusion chromatography to extensively characterize polyhistidine-tagged protein binding with optimized NiNLP compositions; (3) quantified, using surface plasmon resonance, the stability of the interaction between the polyhistidine-tagged proteins and optimized NiNLPs; (4) used analytical size exclusion chromatography to assess the stability of the NiNLPs by themselves and when conjugated to polyhistidine-tagged proteins after lyophilization; and (5) completed additional lyophilization studies.

Proposed Work for FY10
For FY10 we propose to (1) test the immune response to the optimized NiNLPs in mice, (2) adapt the NiNLP composition in a reiterative manner based on the animal studies, and (3) include secondary adjuvant lipid A into the NiNLP construct to determine whether secondary adjuvants enhance the immune response. One of the primary objectives of our proposed work is to validate the efficacy of different NiNLP constructs before subjecting them to challenge studies.

Epidemic Disease Response and Impact Simulation—
Carl Melius (09-FS-003)

Abstract
Mitigating the impact of emerging natural infectious diseases and those that might be genetically engineered by bioterrorists is critical to our national security. We propose to determine the feasibility of extending the MESA (Multiscale Epidemiological/



Schematic of the assembly of vaccine-ready nickel–nanolipoprotein (NiNLP) particles.

Economic Simulation and Analysis) model, which was developed to simulate the spread of disease among farm animals on a regional scale, to simulate human disease epidemics at the national level. We will determine the efficacy of treating the spread of disease as fundamental processes that can be modified by appropriate response measures. We intend to identify potential bottlenecks in the model's ability to scale to the national level and arrange for our results to be externally reviewed by a leading expert in the disease control and prevention community.

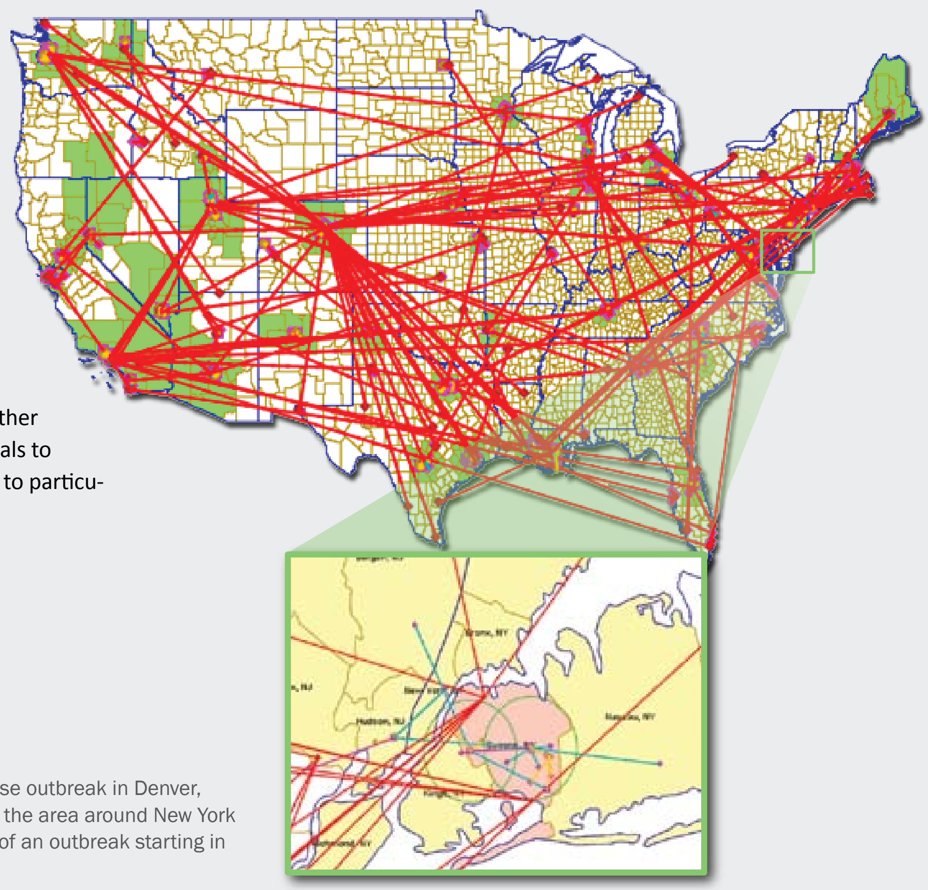
If our approach is found to be feasible, this work will form the basis for a working model that predicts the effect of specific emergency responses (for example, closing airports) on the spread of human disease epidemics at the national level. We will identify key issues of how human epidemics spread across the country—for example, going to school or work or travel by airplane. In addition, the model will help determine the applicability of basic control measures such as vaccination and quarantining, as well as social behavior modifications including washing hands and avoiding crowded public areas such as shopping malls. We will identify potential bottlenecks in the ability of the model to scale to the national level and determine tradeoffs between the level of detail in the disease spread model and computer memory and usage and central processor unit requirements.

Mission Relevance

Our proposed research will support Laboratory efforts in national and homeland security by helping to characterize the threat and develop a response to a bioterrorist contagious disease attack. The resulting model will also help assess and guide LLNL's development of new detection schemes and other countermeasures. The model will enable health officials to treat diseases and create response measures specific to particular situations.

FY09 Accomplishments and Results

We successfully modeled the spread of human disease outbreaks across the United States. The model we created based on spatial–temporal entities—MERSi (Multi-scale Epidemic Response Simulator)—was shown to be capable of handling 280 million people located in 65,000 census tracts, along with 90,000 schools and 2,000 transportation nodes, including airports, train stations, and bus stations. MERSi was used to apply a variety of response measures, including vaccination and school closings. We also modeled the disease states of individuals in a census tract by extending the code SEIR (Suspect Exposed Infectious Recovered), in which schools and transportation nodes are treated as transient entities. We also demonstrated that using entity-to-entity contact lists to represent social networks efficiently reduces the computation time. In summary, this study produced a model capable of efficiently modeling the response to human disease outbreaks at the national level.



The outcome of a simulated disease outbreak in Denver, Colorado (map), and a close-up of the area around New York City two weeks after confirmation of an outbreak starting in Queens (inset).

CHEMISTRY

Long-Time-Scale Shock Dynamics of Reactive Materials—Nir Goldman (06-ERD-037)

Abstract

We propose to study the long-time-scale effects of shocks on highly reactive materials, using a novel shock dynamics technique, the Multiscale Shock Simulation Technique implemented in an ab initio molecular dynamics code. Until recently, existing techniques for quantum simulations of shocked materials have been prohibitively expensive. The combination of Multiscale Shock Simulation Technique with an ab initio molecular dynamics code will elucidate answers to key questions regarding materials decomposition. We propose to conduct shock simulations of simple liquids such as water and simulate shocked astrochemical mixtures of prebiotic molecules that are found in comets and other celestial bodies.

Our studies represent the first use of a state-of-the art quantum mechanical simulations code to study shocked, highly reactive materials. These simulations will allow us to determine the exact kinetic and thermodynamic nature of chemical reactivity at high temperature and pressure. From them, we will gain important insight into how simple molecular systems are influenced by rapid compression and how this pertains to geochemical and planetary processes.

Mission Relevance

Knowledge of highly reactive materials decomposition under conditions of high temperature and pressure is essential for a complete understanding of liquids in the interiors of Earth and large planets, and is central to the Laboratory's stockpile stewardship mission. The quantum-simulations algorithms and codes developed in this project will be applicable to several national security missions. In addition, this high-profile scientific research supports LLNL's mission in fundamental science and technology and will attract new talent to the Laboratory.

FY09 Accomplishments and Results

We successfully determined a mechanism for the synthesis of amino acids in cometary ice impacting the Earth. Our proposed mechanism is driven by the sudden heating and compression from impact and independent of the atmosphere and materials already present on early Earth. In addition, we developed a new methodology for including quantum mechanical corrections to molecular dynamics calculations of shock Hugoniot temperatures. In summary, this project successfully applied novel simulation methodologies to the study of materials under shock compression, including water and cometary ices. The National Aeronautics and Space Administration has expressed interest in this work under its Exobiology and Evolutionary Biology Program.

Publications

Goldman, N., E. Reed, and L. Fried, 2009. *Nuclear quantum vibrational effects in shock Hugoniot temperatures.* 16th APS Topical Conf. Shock Compression of Condensed Matter, Nashville, TN, June 28–July 3, 2009. LLNL-ABS-410214.

Goldman, N., et al., 2007. "Ab initio molecular dynamics simulations of water under static and shock compressed conditions." *AIP Conf. Proc.* **955**, 443. UCRL-PROC-233148.

Goldman, N. et al., 2009. "Ab initio simulation of the equation of state and kinetics of shocked water." *J. Chem. Phys.* **130**, 124517. LLNL-ABS-410224.

Goldman, N., et al., in press. "A microscopic picture of electrical conductivity of H20 in ab initio molecular dynamics simulations of shock compression." *Nat. Phys.* LLNL-JRNL-401364.

Goncharov, A. F., et al., 2007. *Dissociative melting of ice at high pressure.* UCRL-JRNL-227048.

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The Viral Discovery Platform—Christopher Bailey (08-SI-002)

Abstract

A top priority for homeland security is to develop systems and supporting assays for detecting engineered biothreats. This project will integrate existing and new laboratory developments into a comprehensive approach for the rapid identification and characterization of viruses in clinical samples. We will leverage recent developments in microfluidic engineering, highly multiplexed biological assays, and bioinformatics to provide a broad capability for identifying and characterizing known and previously unknown viruses. This project will lead to broadly applicable advances in microfluidic chemistry and detection, the biology of virulence, and computational biology, as well as play an important role in the next generation of technologies for the nation's biodefense.

This project will (1) design and experimentally validate the first-ever bioinformatic system to design multiplexed primer sets for rapid identification of all viruses; (2) provide design parameters and analysis for next-generation microarrays; (3) optimize short primer sets to generate expected family-specific signatures for identifying known and unknown threats; (4) demonstrate

microfluidic isolation of virus particles in complex biological samples; (5) develop systems for precise fluid manipulation, droplet sorting, and polymerase chain reaction; and (6) develop the first-ever comprehensive, automated sample-preparation system for sorting all components in clinical samples.

Mission Relevance

This project supports the Laboratory's national security mission by developing advanced technologies for detecting biological agents.

FY09 Accomplishments and Results

In FY09 we (1) designed, fabricated, and tested the second generation of our viral discovery microarray and collaborated with over a half-dozen groups worldwide, searching for viral pathogens from a number of sources; (2) published our work that has demonstrated single viral-particle detection in high-throughput emulsion analysis, where we analyzed approximately two million droplets per hour; and (3) demonstrated isolation of nucleic acid using transverse isotachophoresis and developed a novel, simplified approach to dielectrophoresis for bacterial isolation.

Proposed Work for FY10

In FY10 we will focus on integrating the separate modules for complete analysis and work with external collaborators who can provide real-world samples. We will (1) develop a next-generation microarray, which will include not just a complete set of viral probes but also bacterial and fungal probes, providing the world's first all-pathogen detection device; (2) increase the throughput of our droplet analysis system while incorporating advanced detection capabilities, including microfluidic bar coding; (3) incorporate additional microfluidic sample preparation steps to separate bacteria and free nucleic acid from viruses; and (4) expand bioinformatic and experimental assay development to include discovery using next-generation, high-throughput sequencing techniques.

Publications

Beer, N. R., K. A. Rose, and I. M. Kennedy, 2009. "Monodisperse droplet generation and rapid trapping for single molecule detection and reaction kinetics measurement." *Lab Chip* **9**, 841. LLNL-JRNL-405725.

Beer, N.R., K. A. Rose, and I. M. Kennedy, 2009. Observed velocity fluctuations in monodisperse droplet generators. *Lab Chip* **9**, 838. LLNL-JRNL-409551.

Gardener, S. N., et al., 2009. "Multiplex primer prediction software for divergent targets." *Nucleic Acid. Res.* **37**(19), 6291. LLNL-JRNL-405234.

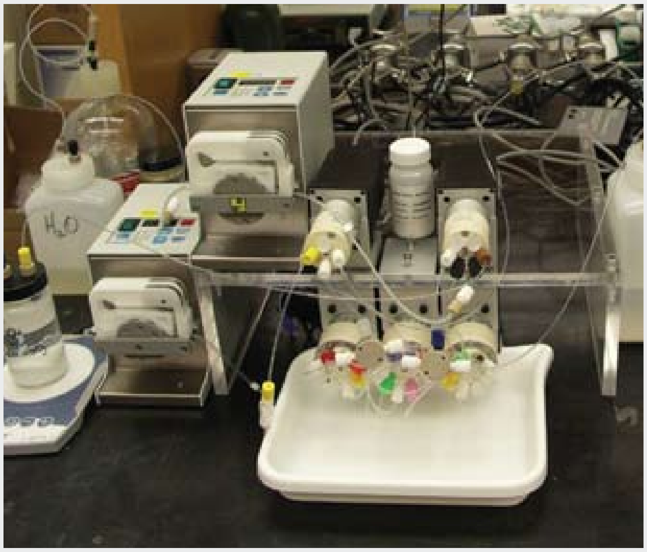
Jung, B., et al., 2008. "Acoustic particle filter with adjustable effective pore size for automated sample preparation." *Anal. Chem.* **80**(22), 8447. LLNL-JRNL-404158.

Kiss, M. M., et al., 2008. "High throughput quantitative polymerase chain reaction in picoliter droplets." *Anal. Chem.* **80**(23), 8975. LLNL-JRNL-403189.

Rapid Radiochemical Separations for Investigating Chemistry of the Heaviest Elements—Dawn Shaughnessy (08-ERD-030)

Abstract

Producing new heavy elements brings us closer to the Island of Stability, where nuclei are postulated to have longer half-lives. Largely unknown are the exact location of the Island of Stability and the chemical properties of the transactinides. We will study both the region stability and the chemical and physical properties of heavy elements. Beginning with elements 104 and 105, chemical separations and automated techniques will be developed, and the results will indicate whether the transactinides follow the lighter homologues in the periodic table, or whether relativistic effects induced by nuclear charge alter predicted chemistries. The combination of physics and chemistry will provide insight into



Prototype automated radiochemistry system developed for heavy-element chemistry.

the chemical behavior of heavy elements and potentially result in discoveries of new elements and isotopes. The possibility exists to produce element 117 using the calcium-48 and berkelium-249 reaction, and then to study its chemical properties.

We expect to develop systematic chemical separations for elements 104 and 105 that will isolate single atoms from large amounts of interfering background material, while identifying the chemical properties of these elements. Through experimentation, we will confirm atomic number assignments of the parent nuclei as elements 114 and 115. The automated chemistry apparatus we develop will be capable of rapid sample processing with minimal dose exposure to personnel, be used in accelerator-based online experiments with elements 104 and 105, and have applications in nuclear forensics and attribution, environmental monitoring, and diagnosis of fusion-laser capsule performance.

Mission Relevance

This project supports the Laboratory's mission in national and energy security by furthering the study of heavy elements, which helps maintain core competency in nuclear chemistry and radiochemistry techniques used in device performance, nuclear forensics and attribution, and environmental monitoring. The project's achievements in automated chemistry will have applications in nuclear forensics and attribution and in fusion-laser capsule diagnostics.

FY09 Accomplishments and Results

In FY09 we (1) continued extraction studies on separations of group IV and V elements using diglycolamide extractants and developed a scheme for intra- and inter-group separations applicable to elements 104 and 105, (2) constructed a prototype of an automated chemical apparatus and tested it with tracers, (3) collaborated with researchers at the University of Nevada at Las Vegas on diglycolamide extractions and mutually performed research required for development of a separation scheme, and (4) participated in a search for element 117 at the Joint Institute for Nuclear Research in Dubna, Russia and provided data analysis and experimental support.

Proposed Work for FY10

In FY10 we plan to (1) irradiate calcium-48 and berkelium-249 and participate in experiments to search for element 117 at the Joint Institute for Nuclear Research and independently analyze the data, (2) develop a chemical separation for lawrencium isotopes designed to identify the decay daughters of element 117, (3) perform online chemistry and deploy the chemical system at the Joint Institute for Nuclear Research, (4) participate in gas-phase studies to investigate the chemical properties of element 117, and (5) independently analyze the data and detail the results for publication. In addition, we hope to finish design and construction of our target chamber for performing online, automated chemical studies at Livermore.

Publications

Henderson, R. A., et al., 2009. *Automated radiochemistry efforts at LLNL.* Periodic Table of D. I. Mendeleev. The New Superheavy Elements, Dubna, Russia, Jan. 20–21, 2009. LLNL-PRES-406833.

Moody, K. J., 2009. *A retrospective on a decade of superheavy elements.* Actinides 2009, San Francisco, CA, July 12–17, 2009. LLNL-ABS-414083.

Shaughnessy, D. A., et al., 2009. *Production and properties of the transactinide elements.* Actinides 2009, San Francisco, CA, July 12–17, 2009. LLNL-PRES-414519.

Probing the Organization of the Cell Membrane—
Peter Weber (08-LW-015)

Abstract

The objective of this research is to provide new insight into the mechanisms by which the cell membrane is organized. This work is fundamental in nature and has broad implications, from host–pathogen interaction to next-generation sensors. Lipid rafts (microdomains) in the cell membrane are believed to play a key role in organizing the membrane, enabling it to carry out essential cellular processes, including protein recruitment and signal transduction. Building on our proof-of-concept experiments, we will provide the first direct evidence for the role of lipids in cell organization, which no method to date has been able to do. Our approach combines molecule-specific stable isotope labeling with nanoscale secondary-ion mass spectrometry (NanoSIMS) to probe membrane organization.

We will be the first to directly image and quantify lipid rafts, which are hypothesized to play a key role in cell membrane organization. We also will image and quantify membrane–protein interactions, such as those known to mediate cell-to-cell signaling. These data are of fundamental importance because they will provide the basis for understanding cell membrane function. Understanding this mechanism has broad implications, from understanding how viruses such as HIV attack cells to creating biosensors that mimic the sensitivity and specificity of a cell membrane. Our proof-of-concept was selected by *Chemical and Engineering News* as one of the top research advances in 2006, and we expect this research will result in high-profile publications in peer-reviewed journals.

Mission Relevance

This work supports Lawrence Livermore's mission in national security to counter the use of biological weapons. Lipid rafts are implicated in cell invasion by pathogens, and therefore are relevant to understanding emerging threats. The mechanism of lipid membrane organization also could potentially be harnessed for producing biosensors that mimic the sensitivity and specificity of the cell membrane and would be applicable to characterizing nano-lipoproteins for such sensors. In addition, the project will advance our capability for NanoSIMS analysis of bioweapon particles.

FY09 Accomplishments and Results

The highlight of our work in FY09 was that, for the first time ever, we visualized heterogeneity in the distribution of lipids in the membrane of a natural cell. Our NanoSIMS images showed that the isotopically labeled sphingosine and fatty acids are incorporated into the cell membrane. As expected, the distribution of the fatty acids was relatively homogenous, whereas the distribution of the sphingolipids was very heterogeneous, which supported the hypothesis that sphingolipids are a component of a compositionally distinct lipid raft. In addition, we imaged lipid heterogeneity in tethered lipid bilayers and characterized nitrogen in graphene and published our work in the peer-reviewed literature.

Proposed Work for FY10

We plan to build on our FY09 results by performing experiments on natural cells. FY10 experiments will include isotopically labeled cholesterol and fatty acids. We propose to (1) integrate time-of-flight SIMS chemical imaging of samples at LLNL into the project to improve our localization of cell membranes for NanoSIMS, (2) perform correlated time-of-flight-SIMS and NanoSIMS analyses of isolated cell membranes and membranes on intact cells, (3) conduct cell experiments with influenza-model cell lines, (4) perform supporting model membrane experiments, and (5) prepare manuscripts of journal articles detailing our results.

Publications

Boxer, S. G., M. L. Kraft, and P. K. Weber, 2009. "Advances in imaging secondary ion mass spectrometry for biological samples." *Ann. Rev. Biophys.* **38**, 53. LLNL-JRNL-408214.

Wang, X., et al., 2009. "N-doping of graphene through electro-thermal reactions with ammonia." *Science* **324**, 768. LLNL-JRNL-411511.

"Day-One" Nuclear Forensics—Ian Hutcheon (09-ERD-056)

Abstract

This project will develop a more robust and responsive nuclear forensics capability to reconstruct a nuclear incident quickly and with high fidelity, even in a crisis situation. We will leverage unique LLNL capabilities in weapon physics, forensic science, laser spectroscopy, multiscale modeling, and radiation detection to achieve scientific and technological breakthroughs in areas critical to nuclear forensics. We will focus initially on debris analysis, with a modest effort in detonation and fallout modeling. Once integrated, these advances will dramatically enhance the nation's current nuclear forensics capability and directly lead to a viable "day-one" forensics capability.

We will develop new capabilities in actinide analysis and predictive modeling with a focus on the rapid return of high-fidelity data. We will (1) investigate actinide behavior, material transformations, and physiochemical properties at the high temperatures relevant to nuclear detonation to understand the volatile behavior of uranium in debris from nuclear tests; (2) develop resonance-ionization mass spectrometry (RIMS) for rapid, accurate analysis of uranium and plutonium; (3) determine how uranium-rich compounds are sited, and their associations with nonradiogenic species, in nuclear test debris; and (4) develop an improved version of the Livermore Weapon Activation Code to calculate height of burst and yield based on input from radiochemical diagnostics.

Mission Relevance

This project supports LLNL's national security mission by developing nuclear forensics and attribution capabilities for reducing the threat of the proliferation and use of weapons of mass destruction. This project will also help cultivate the next generation of scientific leaders necessary to ensure the nation's ability to safeguard nuclear weapons and respond to nuclear threats.

F09 Accomplishments and Results

In FY09 we (1) initiated RIMS experiments on uranium-bearing compounds and demonstrated a tenfold improvement in measurement precision for uranium-235 and 238 over conventional methods; (2) used Raman scattering to examine in situ the high-temperature (400°C) oxidation of uranium dioxide—dramatic changes in the Raman spectrum are accompanied by sample breakup, which we relate to the formation of more highly oxidized uranium oxide compounds like U_4O_9; (3) recovered soil samples from a U.S. nuclear test from the 1960s at the Nevada

Test Site and confirmed the presence of unburned nuclear fuel, fission products, and activation products; and (4) demonstrated successful recovery of nanometer-to-micrometer-scale fallout captured on air filters. The successful conclusion of this project demonstrated the feasibility of using RIMS for uranium isotope measurements of nuclear materials, provided new data on the high-temperature oxidation of uranium oxide, and demonstrated the recovery and characterization of nanometer-scale signatures in nuclear fallout from the Nevada Test Site. We will pursue the next steps in enhancing the scientific basis of technical nuclear forensics via an LDRD Strategic Initiative project.

Publications

Isselhardt, B. H., et al., 2009. *Development of resonance ionization mass spectrometry for measuring uranium isotope ratios in nuclear materials.* 18th Intl. Mass Spectrometry Conf., Bremen, Germany, Aug. 30–Sept. 4, 2009. LLNL-ABS-414971.

Isselhardt, B. H., et al., 2009. *Development of resonance ionization mass spectrometry for measuring uranium isotope ratios in nuclear materials.* APSORC ’09, Asia-Pacific Symp. Radiochemistry, Napa, CA, Nov. 29–Dec. 4, 2009. LLNL-ABS-415184.

Knight, K. B., et al., 2009. *Application of resonance ionization mass spectrometry to detection of uranium in natural silicate matrices.* APSORC ’09, Asia-Pacific Symp. Radiochemistry, Napa, CA, Nov. 29–Dec. 4, 2009. LLNL-ABS-415214.

Knight, K. B., et al., 2009. *A world without sample preparation: Developing rapid uranium isotope measurement capabilities by resonance ionization mass spectrometry.* LLNL-POST-413953.

Levine, J., et al., 2009. “Resonance ionization mass spectrometry for precise measurements of isotope ratios.” *Int. J. Mass Spectrom.* **288**, 36. LLNL-JRNL-416961.

EARTH AND SPACE SCIENCES

Laboratory Directed Research and Development

Dense Gas Transport in Complex Environments— Branko Kosovic (07-ERD-020)

Abstract

The potential for intentional or accidental atmospheric releases of hazardous dense gases is increasing with the global risk of terrorism, renewed interest in liquefied natural gas (LNG) as fuel, and carbon dioxide sequestration. Currently there is no general way to accurately predict how dense gases will behave in an urban environment. Models that fail to explicitly resolve the effects of both the buildings and gas density can produce misleading predictions of plume magnitude, location, or direction. We will develop an urban dispersion modeling capability that will include both the appropriate dense-gas physics and the effect of buildings and complex terrain on atmospheric transport and dispersion, including appropriate source terms. We will use field data to validate the model. Dense gases suppress local atmospheric turbulence, whereas buildings and other obstacles generate atmospheric turbulence. Furthermore, heat transfer, affected by phase change, may amplify or reduce turbulence.

A new, validated denser-than-air simulation will establish a new capability for modeling the fate and transport of dense gas in urban and complex terrain, which will enable a more effective response to hazardous releases involving dense gases. There is considerable interest in a dense gas model for hazard assessment, planning, and emergency response. Potential applications include assessing risks associated with the transportation of toxic chemicals, LNG storage, and carbon dioxide sequestration.

Mission Relevance

This project supports the Laboratory's missions in homeland security, environmental management, and energy security, with regards to response to releases of hazardous chemicals, whether intentional or accidental. This capability will enable a more effective response to both terrorist attacks and industrial accidents. For energy, there are specific applications to carbon dioxide sequestration, LNG spills and leaks, terminal safety, and transportation.

FY09 Accomplishments and Results

In FY09 we implemented a dense gas capability into Livermore's FEM3MP (Finite Element Model in 3-Dimensions and Massively Parallelized) code and validated it in complex terrain against data from the Petroleum Environmental Research Forum's Kit Fox dense-gas field experiment. The field site consisted of a dry lakebed containing arrays of rectangular panels to simulate an urban environment. A source-term model controlled the release of carbon dioxide, and measurements were obtained both within and downstream of the array. Simulations using the dense gas physics improved agreement with the data relative to depiction of the gas as neutrally buoyant. Overall, the project resulted in the successful implementation of dense gas physics into an atmospheric simulation model, enabling improved representation of dense gas dispersion in regions of complex terrain, including urban areas. This improved capability will support future programmatic modeling studies of dense gas dispersion, including risk assessment and mitigation strategies in both urban areas and near dense-gas transportation corridors.

Publications

Kosovic, B., and J. D. Mirocha, 2008. *Large-eddy simulation of density currents over complex terrain.* 18th Symp. Boundary Layers and Turbulence, Stockholm, Sweden, June 9–13, 2008. LLNL-ABS-400530.

Kosovic, B., et al., 2007. *Building-resolving simulations of dense gas dispersion.* 7th Symp. Urban Environment, San Diego, CA, Sept. 9–13, 2007. UCRL-PRES-234505.

Cosmochemical Forensics—Lars Borg (07-ERI-005)

Abstract

We propose the use of nuclear forensics to investigate correlated isotopic anomalies associated with short-lived radionuclides, long-lived radionuclides, and oxygen-16 in calcium–aluminum-rich inclusions (CAIs) and planetary materials to carry out four cutting-edge scientific tasks: (1) refine the initial abundance of aluminum-26 in the solar system, (2) determine if aluminum-26 and oxygen-16 originated from a single supernova source, (3) compare the signatures of short-lived radionuclides with oxygen-16 in cometary materials containing normal CAIs, and (4) better define the age of parent-body differentiation. The results will constrain the time scales of formation during the first three million years of solar system history and elucidate astrophysical and cosmochemical models of the evolution of Sun-like stars.

We expect to (1) determine the initial aluminum-26/aluminum-27 ratio in the solar system to better establish chronology for the first five million years of solar system history, (2) connect long-and short-lived chronometers to obtain absolute ages from relative chronometers, and (3) develop absolute chronometry and constrain the timing of the earliest events occurring on parent bodies. These results address fundamental issues in cosmochemistry and will contribute to a better understanding of the earliest history of the solar system and of the sequence of events extending from condensation in a hot, gaseous nebula to

the formation of terrestrial planets. The project also will serve as a mechanism to produce a suite of microanalytical techniques needed for national security applications.

Mission Relevance

The project develops and enhances advanced microanalytical capabilities in support of Lawrence Livermore's national security mission and enhances its mission in basic science. Nonproliferation and homeland security specifically benefit most from advancing forensic capabilities under this project. Furthermore, the techniques developed here for high-accuracy and high-sensitivity analyses on a nanometer scale have broad applicability throughout the Laboratory.

FY09 Accomplishments and Results

Using aluminum-26–magnesium-26 and manganese-53–chromium-53 chronometers, we elucidated the temporal relationship between objects formed in the nebula—such as CAIs and chondrules—and objects formed on planetary surfaces through processes of differentiation and aqueous alteration, such as carbonates, magnetite, and igneous clasts. In summary, our primary goal was to develop a better understanding of the time scale of events leading to the formation of solid bodies in the early solar system, which we accomplished by carrying out new observations of isotope and trace element abundances, coupled to complete petrographic characterization, in a diverse array of primitive meteorites. This successful project enabled determination of the age of early solar system events. Continuation of this research will be supported by NASA.

Publications

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Boyet, M., et al., 2009. "(SM)-S146,147-(ND)-N-142,143 systematics of lunar ferroan anorthosites." *Meteoritics Planet. Sci* **44**, A38. LLNL-PRES-414730.

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Grossman, L., et al., 2008. "Primordial compositions of refractory inclusions." *Geochim. Cosmochim. Acta* **72**, 3001. LLNL-JRNL-401631.

Jacobsen, B., et al., 2008. "Mg isotopic composition of low Al/Mg phases in CAI: The initial solar ^{26}Mn/^{24}Mg?" *Lunar Planet. Sci.* **39**, 2387. LLNL-ABS-403697.

Krot, A. N., et al., 2007. "Oxygen isotopic compositions of the Allende type C CAIs: Evidence for isotopic exchange during nebular melting and asteroidal thermal metamorphism." *Geochim. Cosmochim. Acta* **72**, 2534. LLNL-JRNL-401571.

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Makide, K., et al., 2008. "Magnesium and oxygen isotopic compositions of calcium-aluminum-rich inclusions from CR carbonaceous chondrites." *Lunar Planet. Sci.* **39**, 2407. LLNL-ABS-403701.

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McKeegan, K. D., et al., 2007. "Isotopic compositions of cometary matter returned by Stardust." *Science* **314**, 1724. UCRL-JRNL-225917.

Simon, S. B., et al., 2007. "Formation of spinel-, hibonite-rich inclusions found in CM2 carbonaceous chondrites." *Am. Mineral.* **91**, 1675. UCRL-JRNL-216859.

Symes, S. J., et al., 2008. "The age of the Martian meteorite Northwest Africa 1195 and the differentiation history of the shergottites." *Geochim. Cosmochim. Acta* **72**, 1696. UCRL-JRNL-229742.

Yin, Q.-Z., et al., 2008. "^{26}Al–^{26}Mn and ^{207}Pb–^{206}Pb systematics of Allende CAIs: Reinstated canonical solar initial ^{26}Al/^{27}Al ratio, variable K-values (^{232}Th/^{238}U) and the age of the galaxy." *Lunar Planet. Sci.* **39**, 1525. LLNL-ABS-404118.

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Coordinated Analysis of Geographic Indicators for Nuclear-Forensic Route Attribution—
Hope Ishii (08-ERD-065)

Abstract
We intend to develop a scientific foundation for nuclear-forensic route attribution by exploring which types of signatures are viable over what time scales and why. Transport pathway is key to uncovering smuggling routes and potential distribution sites of illicit material. Environmental and geological particulates and surficial deposits will be analyzed in coordinated studies by x-ray, electron and ion microscopies, and gas chromatography–mass spectrometry to extract geographically specific signatures (i.e., molecular and trace-element chemistry and stable isotope abundances). Accuracy and limitations will be analyzed using real-world materials. Sample recovery from radioactive materials or packaging will be developed as needed with scanning electron microscopy micromanipulation and focused ion-beam machining.

This work will improve our understanding of which, why, and how geographically specific clues identify their environment and can be used as measurable, meaningful signatures of the route of smuggled radioactive and associated materials. We anticipate the first-ever demonstration of isotope signatures for route attribution. The analytical methods and technical capabilities we develop will significantly impact the scientific foundations for more efficient and effective route attribution. This project will leverage LLNL's capabilities and expertise in nuclear forensics, attract young talent into national security work, produce publications, and position LLNL for upcoming work-for-others funding in nonproliferation and nuclear attribution.

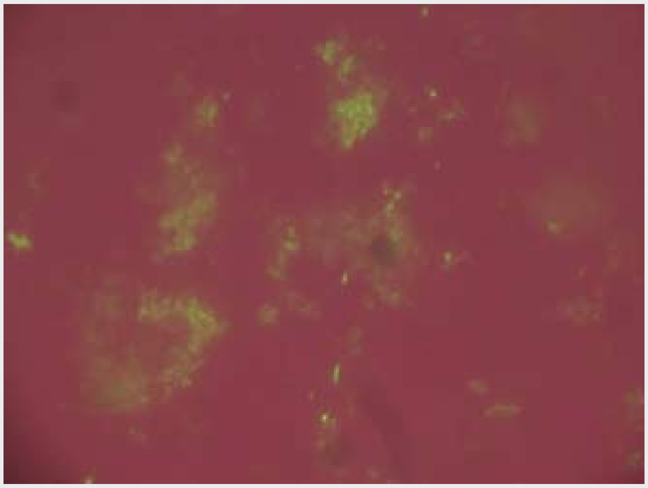
Mission Relevance
This project supports the Laboratory's national security mission by furthering nuclear forensic efforts relevant to nonproliferation and homeland security. The microscale and nanoscale characterization capabilities developed will also support LLNL's mission in bioscience and technology to improve human health by developing new analytical techniques.

FY09 Accomplishments and Results
In FY09 we focused on the feasibility of chemical forensics based on adsorbed and absorbed organics and on the geographic specificity of oxidation layers. Specifically, we completed an organic exposure experiment using common packaging materials and conducted exploratory studies of oxygen isotopes in iron oxidation layers from geographic locations worldwide, revealing geographic trends that could serve as a forensic tool.

Proposed Work for FY10
In FY10 we will (1) study pollen as a chemical forensic substrate—an earlier proof-of-concept study demonstrated its potential—and we plan to address technical challenges of pollen adsorption experiments and explore pollen carrier mechanisms with isotopically labeled compounds, (2) expand the database of geographic samples for oxidation layer studies, (3) perform controlled oxidation experiments with the goal of determining contributions of oxygen from water (globally variable) and from air (not variable) in oxide formation, (4) explore double oxidations with different isotopic compositions, and (5) perform studies of oxidation layers in actual samples acquired from the capture of transported nuclear material.

An Experimental and Theoretical Approach to Visualize Dechlorinating Bacteria in Porous Media—
Walt Mcnab (08-ERD-070)

Abstract
Much of America's groundwater is at risk from contamination by chlorinated solvents. In situ bioremediation may accelerate groundwater cleanup, but it is not known exactly how bioremediation works in the immediate vicinity of solvents trapped in the subsurface. The overall objective of this work is to interrogate the spatial distribution of solvent-degrading microorganisms in porous media. This will be done by visualizing a commercial dechlorination, bioaugmentation culture in a two-dimensional sandbox and in soil cores from an actual contaminated site using various microbiological and molecular biological techniques, and



Dehalococcoides bacteria, along with other species, fluorescing in response to introduction of a vital stain that responds to enzymatic activity.

by developing a new mathematical representation of bioremediation in chlorinated source zones.

If successful, this project will provide the experimental and theoretical means to approach the problem of understanding how bioremediation works in the immediate vicinity of large contaminant source zones. This work will enhance LLNL's capabilities in this area and permit collaborations with other organizations that specialize in the cleanup of solvent-contaminated sites, including sites across the DOE complex.

Mission Relevance

Contamination of groundwater by chlorinated solvents is a problem facing both the Laboratory and the nation as a whole. Developing a novel scientific approach to study this problem relates directly to Livermore's mission in environmental management, and could help accelerate remediation efforts at LLNL and other DOE sites.

FY09 Accomplishments and Results

In FY09 we (1) identified a vital dye that fluoresces at a 520-nm wavelength in response to dehalogenation enzymatic activity, permitting direct imaging of the dechlorinating culture KB-1 without the need for genetic manipulation; (2) initiated experiments to visualize *Dehalococcoides* bacteria in heterogeneous porous media in partnership with researchers at the University of California at Irvine; (3) developed a model for use in interpreting sandbox experiments; and (4) identified and quantified concentrations of *Dehalococoides* in groundwater samples from a field bioaugmentation experiment using a polymerase chain reaction, which enables researchers to produce millions of copies of a specific DNA sequence in a few hours. Identification of a vital stain suitable for imaging, along with a technique based on polymerase chain reaction for identifying *Dehalococcoides* bacteria in groundwater and soil samples, will facilitate understanding of the distribution and activity of these organisms in subsurface environments in response to augmented bioremediation. The techniques developed in this project will be used to support programmatic environmental remediation efforts at LLNL in the upcoming year.

Improving Atmospheric Flow Prediction at Intermediate Scales—Jeffrey Mirocha (09-ERD-038)

Abstract

A significant problem in simulating atmospheric flow in the lowest 2 km of the Earth's atmosphere is how to accurately represent the entire spectrum of flow features—from the large scales of weather to the small scales of turbulence—that influence the near-surface flow. To overcome this problem, we must fill an important knowledge gap involving modeling flow at intermediate scales—that is, those between the large- and small-scale endpoints we understand. In this project, we aim to fill this gap by developing both the physical models and technical expertise required to achieve accurate multiscale flow simulation and prediction capability. Filling this knowledge gap is critical to many important scientific thrusts, including wind energy, climate modeling, and emergency preparedness and response.

If successful this project will overcome several key obstacles to multiscale atmosphere flow simulation and prediction, such as parameterizations for modeling subfilter turbulence at intermediate mesh resolutions, algorithms to represent turbulence interactions across computational meshes of different sizes, and guidance for appropriate computational domain and mesh configurations required for various spatial and temporal scales and flow regimes. The knowledge and tools developed will, by removing these obstacles, yield significant advances in simulating, predicting, and understanding the complex flows that are vital components of many important applications across the atmospheric sciences.

Mission Relevance

By extending the ability to simulate and predict complex atmospheric flows, this work directly benefits efforts in risk and response management, in support of the national security mission, and in wind-resource characterization and dynamic downscaling approaches for addressing regional climate adaptation and mitigation, in support of the environmental management mission.

FY09 Accomplishments and Results

In FY09 we (1) addressed deficiencies in the nesting scheme for the computational grid in the Weather Research and Forecasting model (WRF) by implementing new turbulence stress models and combining them with separate near-wall stress models, (2) quantified equilibration for a few scenarios and ran additional simulations to generalize results, (3) focused on one-way nesting because of encountering numerical instabilities during two-way nesting, and (4) began running multiple-nest simulations over a wind park.

Proposed Work for FY10

In FY10 we will (1) verify algorithms for turbulent flow exchange at mesh interfaces and convergence criteria for multiple nests, (2) extend nesting beyond turbulence-resolving scales to larger scales, (3) investigate some simple approaches to modeling turbulence that span length scales required for many future applications, and (4) use data from previous experiments to validate progress in complex terrain and non-neutral conditions, which will allow us to investigate mesoscale-turbulence interactions involving low-level jet phenomena.

Dynamic Simulation of Processes and Conditions Affecting Cavity Growth During Underground Coal Gasification—Thomas Buscheck (09-ERD-046)

Abstract

The deployment of underground coal gasification (UCG) has been hampered by insufficient capabilities to simulate the physical processes of gas production and environmental mitigation. The objective of this project is to understand processes and conditions affecting UCG by simulating cavity and combustion-zone growth. Leveraging LLNL's multiphysics simulation capabilities and wealth of knowledge and expertise in solving analogous problems, we will achieve a major advance in UCG simulation capabilities for understanding thermal, hydrological, chemical, and mechanical processes; subsurface conditions; and engineering options affecting the cavity and combustion zone of a coal seam during UCG. This work will guide site characterization, parameter calibration, and model validation efforts and enable real-time process control in UCG operation, optimizing it with respect to productivity and environmental impact.

This project will result in a simulation capability with immediate application in power and energy production. This technical advance will also serve as a platform for developing new applications.

Mission Relevance

Our research will support LLNL's mission in energy security by enabling the successful deployment of UCG, which can provide the nation with a clean, sustainable source of energy. Because UCG sites are promising candidates for carbon dioxide sequestration, this project also supports the Laboratory's mission in environmental management.

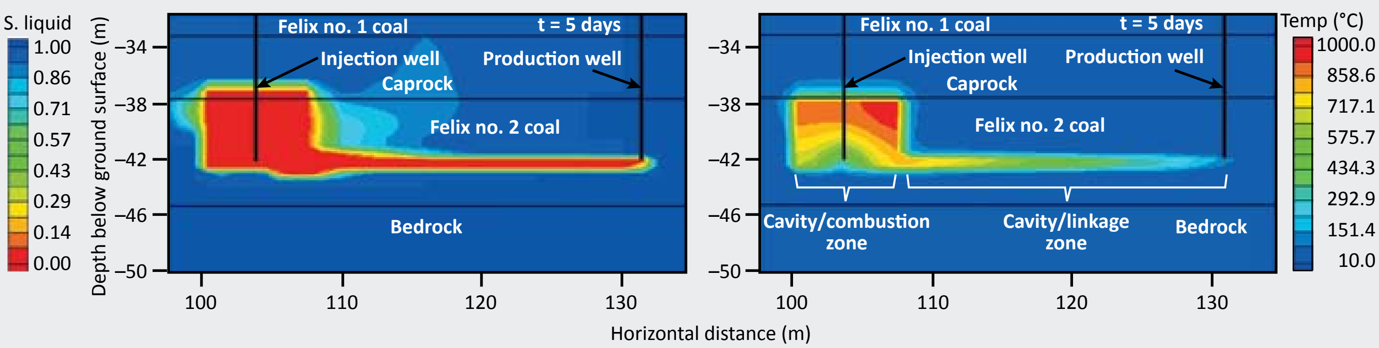
FY09 Accomplishments and Results

In FY09 we (1) customized LLNL's Nonisothermal, Unsaturated Flow and Transport (NUFT) code to address the influence of coal combustion on the heating of host coal and adjoining rock mass, as well as the resulting thermal–hydrological response within the host coal and rock; (2) conducted a parameter sensitivity analysis of the influence of thermal and hydrological properties of the host coal, caprock, and bedrock on cavity temperature and steam production; (3) modified the Livermore Distinct Element Code (LDEC) to simulate stability of the coal mass surrounding an evolving UCG cavity; and (4) performed parameter studies to investigate the relationship between key geological parameters (e.g., in situ stress and cleat spacing) and cavity collapse. Our model, which combines the capabilities of NUFT and the capabilities of LDEC, is a first-of-its-kind tool and will have multiple applications for guiding site characterization, designing pilot tests and geophysical monitoring programs, and developing process control for use in future commercial UCG operations. Next year we will hand off the results from this research and development activity to a new LDRD project that will develop a more fully integrated UCG model.

Publications

Buscheck, T. A., et al., 2009. *Thermal–hydrological sensitivity analysis of underground coal gasification.* 2009 Intl. Pittsburgh Coal Conf., Pittsburgh, PA, Sept. 20–23, 2009. LLNL-CONF-417616.

Morris, J. P., T. A. Buscheck, and Y. Hao, 2009. *Coupled geomechanical simulations of UCG cavity evolution.* 2009 Intl. Pittsburgh Coal Conf., Pittsburgh, PA, Sept. 20–23, 2009. LLNL-CONF-414700.



Computed liquid-phase saturation in the fracture continuum (left) and the temperature (right) are plotted at five days after the start of the Hoe Creek III underground coal gasification pilot test in Wyoming.

Regional Climate Change Prediction for the Twenty-First Century—Curtis Covey (09-ERD-055)

Abstract

With global climate change being a near certainty, it is important to identify the resulting regional impacts—especially on water resources. We propose to create a regional climate change prediction capability for the period 2040 to 2060. Starting with existing simulations of global climate change prepared for the 2007 Intergovernmental Panel on Climate Change, we will conduct global and regionally downscaled simulations to bound climate change in the western U.S., tropical Africa, the Middle East, and other regions. The downscaled simulations will be used to estimate the regional effects of climate change on water resources using surface and groundwater models. We will calculate statistical measures of uncertainty and evaluate our model against existing data.

If successful, this project will create a robust and quantified climate change prediction capability that can be applied to any region in the world. We will also create, as a byproduct of our work, a large and well-documented archive of model-based regional climate change and water resource data for the period 2040 to 2060. Because a number of computational approaches will be tested, the project will identify which approach is best suited for different applications. Furthermore, we will also estimate the limits of regional climate predictability over decadal time scales.

Mission Relevance

The project supports LLNL's missions in energy security and environment management by furthering regional climate predictive strategies and our understanding of the impact of energy production and use on the environment.

FY09 Accomplishments and Results

We used the Community Climate System Model (CCSM) at high resolution to generate boundary conditions for our limited-area, very-high-resolution Weather Research and Forecasting (WRF) model, then used the WRF to create high-resolution output and evaluated its accuracy, focusing on near-surface temperature, rainfall, snowfall, and snowpack accumulation in California's Sierra Nevada. Rainfall was accurately simulated except in "up slope" storm conditions, although we traced and partly corrected the sources of this error. Snowfall and snowmelt were accurately simulated. We also continued evaluating use of LLNL's ParFlow hydrologic model, including both coupling to WRF and incorporating field data from California's Central Valley. This study of the CCSM and WRF hydrology modeling system lays the foundation for predicting U.S. water resources in a globally warming climate. The DOE Office of Science will support follow-on work to that will focus on refining our regional climate and hydrology prediction capability.

Publications

Caldwell, P., et al., 2009. "Evaluation of a WRF dynamical downscaling simulation over California." *Climatic Change* **95**, 499. LLNL-JRNL-403431.

Mapping Patterns of Past Drought in California: Late-Holocene Lake Sediments as Model Diagnostics—Susan Zimmerman (09-ERI-003)

Abstract

We propose to create high-resolution, well-dated paleontological drought records for the last 2,000 years from California lake-sediment core samples. From these, spectral analysis will identify dominant periodicities, and time-slice maps will show spatial patterns, both of which may be linked to forcing mechanisms of climate change. Results will be used to improve the ability of computer models to predict the likelihood of future droughts, which is critical to helping resource managers plan water projects to meet societal demands. To accomplish this, we will radiocarbon date macrofossils such as pollen and twigs from collaborators' core samples for which climate records are under development, to create high-resolution, high-precision radiocarbon and calendar chronologies.

We expect to produce (1) four to six high-resolution records of past droughts in California over at least the last 2,000 years, with high-precision chronologies; (2) spectral analysis of these records; and (3) proof-of-concept time-slice maps at 100-year intervals. The maps will demonstrate the need for many more such high-resolution, well-dated records. The individual records will be an important comparison to annual-resolution tree-ring records over the last 1,000 years and will extend drought reconstructions 1,000 years farther back in time. We expect to better define the paleontological environmental response to the widespread droughts of 900 to 1300 A.D., and describe earlier changes at high resolution.

Mission Relevance

Our research to create drought records for California supports the Laboratory's mission in energy and the environment, with a focus on efforts to address effects of climate change and global warming. We will ultimately provide diagnostic tools in support of Laboratory work to modify the Weather Research and Forecasting Model for regional climate prediction, and which will be of interest for collaborators in this field as well as various federal agencies such as the National Oceanic and Atmospheric Administration and the National Science Foundation.

FY09 Accomplishments and Results

In FY09 we (1) assessed chronologies for seven sites—Summer, Fish, Frog, Zaca, and Mono lakes; Black Lake Bog; and Crooked Meadows; (2) dated wood from tufa geological limestone structures, revealing a detailed history of tufa formation related to extreme dry-to-wet changes; and (3) began dating core samples from the seven sites, finding that those from Fish, Frog, and Zaca lakes exhibit excellent suitability for the project goals—cores from the first two lakes preserve the last 2,000 years in 150 to 200 cm of sediment (about decadal-scale resolution), while a first set of chronology data from the Zaca Lake samples shows the site to be a phenomenal climate archive, with the potential to resolve annual changes.

Proposed Work for FY10

Our FY10 work will focus on (1) sampling and dating cores to be recovered from Crooked Meadows and Mono, Black, Soda, and Zaca lakes; (2) developing calendar-calibrated age models and performing additional dating where required to achieve high-resolution chronologies; (3) carrying out additional, more involved fieldwork for sampling and description for selected sites such as the Mojave lake beds and Tulare Lake; (4) adding additional data to produce robust age models for the Summer Lake and Crooked Meadows sites; and (5) submitting a paper on our results on Mono Lake to a peer-reviewed journal and presenting overall progress on the project at one or more international conferences.

Publications

Stine, S., S. Zimmerman, and S. R. Hemming, 2009. *History of Late Holocene tufa deposition at Mono Lake, California.* American Geophysical Union 2009 Fall Mtg., San Francisco, CA, Dec. 14–18, 2009. LLNL-ABS-419454.

Zimmerman, S., T. Brown, and T. Guilderson, 2009. *Mapping patterns of past drought in California: Late Holocene lake sediments as model diagnostics.* NNSA Laboratory Directed Research and Development 2009 Tri-Lab Symposium, Washington, DC, Aug. 19, 2009. LLNL-ABS-414586.

Stardust Science: Nanoscale Analytical Studies of Materials—John Bradley (09-ERI-004)

Abstract

The National Aeronautics and Space Administration's high-profile Stardust sample-return mission has brought back grains that can provide new insight about the early solar system. We will leverage LLNL's analytical instruments to perform research on such natural astromaterials and on cadmium zinc telluride (CZT), a strategically important man-made semiconductor material with potential application in room-temperature radiation detectors. All of these materials are heterogeneous at the nanometer scale, and we plan to obtain scientific insight about these materials by interrogating them at the nanometer scale using Livermore's unique combination of state-of-the-art instruments.

We seek to achieve a fully integrated analytical capability for analyzing a single expensive nanosample using multiple instruments simultaneously to maximize the science yield. This capability will also be applicable to nuclear forensics samples. We expect to better understand the degree of modification sustained by the comet Wild 2 samples during capture and to gain important new insight about comets, asteroids, other primitive meteoritic materials, and the early solar system. Moreover, our studies of CZT will provide fundamental scientific insight at the nanoscale about the growth of defects in semiconductors, thus laying the foundation for high-performance, defect-free CZT for room-temperature radiation detection devices.

Mission Relevance

This project supports the Laboratory's national security mission by gaining insight into an important material for radiation detection. Other aspects of the project support LLNL's mission in breakthrough science by addressing fundamental planetary science questions and the properties of these and other materials at atomic or near-atomic level. The proposed research will also attract top young scientists to the Laboratory.

FY09 Accomplishments and Results

In FY09 we (1) identified the highest temperature mineral yet identified in a comet, the mineral osbornite (titanium vanadium nitride), which forms at around 2000 K, showing that materials from the hottest region of the early inner solar system were transported to the outermost cold regions of the solar accretion disk; (2) made the first-ever age dating of a comet by measuring the aluminum-26 and magnesium-26 isotope systematics of an approximately 5-µm refractory particle, nicknamed Coki, that was returned from comet Wild 2; and (3) used the super scanning transmission electron microscope to interrogate CZT crystals—a potential room-temperature gamma-ray detector material—and extraterrestrial materials.

Proposed Work for FY10

In FY09 we will (1) measure additional Stardust sample grains to verify our initial age-determination measurement; (2) employ the Laboratory's fully commissioned super scanning transmission electron microscope to interrogate Stardust samples at close to the atomic scale, with the goal of understanding their petrogenetic relationship to other classes of materials (e.g., meteorites from the asteroid belt); (3) examine, using nanometer-scale secondary-ion mass spectroscopy, nucleosynthetic signatures of the earliest water-based reactions that occurred in the solar nebula; and (4) broaden our space science activities to include instrument design concepts for future missions.

Publications

Bradley, J. P., and Z. R. Dai, 2009. "Analytical SuperSTEM in extraterrestrial materials research." *Met. Planet. Sci.* **39**, 1. LLNL-JRNL-416911.

Chi, M., et al., 2009. "The origin of refractory minerals in comet 81P/Wild 2." *Geochim. Cosmochim. Acta* **73**, 7150. LLNL-JRNL-410054.

Matzel, J., et al., 2009. "Mg isotope measurements of a Stardust CAI: No evidence of 26Al." *Met. Planet. Sci.* **44**, A136. LLNL-PRES-414494.

Natural Perchlorate in Groundwater: Source, Formation Mechanisms, and Fate—Darren Hillegonds (09-LW-104)

Abstract

Low-level exposure to perchlorate is known to be widespread, but the health effects of this exposure are poorly understood. We will measure perchlorate isotope systematics in groundwater having no known anthropogenic perchlorate sources. We will do this by exploiting the ubiquitous natural presence of the rare chlorine-36 isotope to determine the source, formation mechanisms, and fate of groundwater perchlorate. We will demonstrate the ability to measure chlorine-36, along with chlorine-35 and chlorine-37, in very small perchlorate samples, and then measure perchlorate isotope systematic effects in groundwater. Samples will also be dated and assessed for recharge conditions, further improving our ability to identify and characterize the source and environmental disposition of groundwater perchlorate. This project will leverage LLNL's unparalleled technical capabilities in accelerator mass spectrometry and noble gas mass spectrometry.

If successful, this project will provide clear and definitive proof of the source of naturally occurring perchlorate in groundwater and provide a method for basic scientific investigations to understand the risks associated with long-term, low-level perchlorate exposure. In doing so, we will provide regulatory agencies and cleanup efforts with critically needed scientific information with which to make decisions about how to manage perchlorate contamination in the U.S. water supply.

Mission Relevance

This project supports LLNL's environmental management mission by answering important basic questions about the source of perchlorate contamination in pristine wells, by elucidating historic perchlorate exposure (which helps determine scientifically defensible regulations), and by understanding the storage and release of perchlorate during expected changes in the nation's water supply caused by climate change.

FY09 Accomplishments and Results

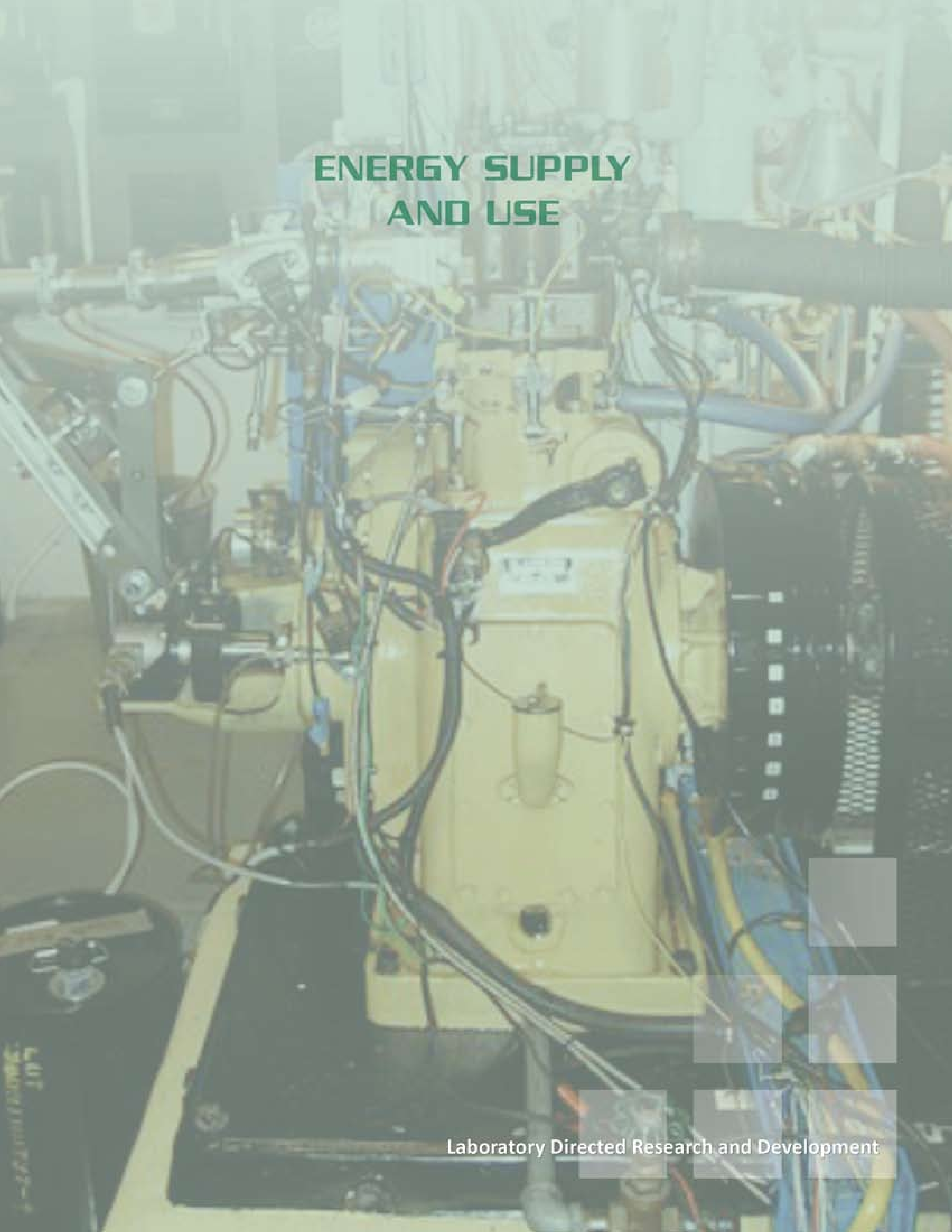
During FY09 we (1) measured the chlorine-36/chlorine ratio in artificially produced perchlorate salts, including replicate measurements to establish overall variability in standard atomic mass spectrometry preparation methods for perchlorate samples—results suggest no modification of our preparation methods will be needed, and that variability in stable chlorine isotope ratios (i.e., chlorine-35/chlorine-37) is low (~1%) and amenable to isotope dilution methodology for minimization of sample requirements; (2) tested an isotope dilution method, allowing us to establish a sample size minimum of 10 µg of chlorine;

(3) developed and tested a method for extraction of perchlorate from groundwater; and (4) developed sample preparation methods for stable isotope analysis.

Proposed Work for FY10

In FY10 we will concentrate on acquisition of water samples and analysis of perchlorate isotope ratios, principally chlorine isotopes measured via accelerator mass spectrometry and infrared mass spectrometry. Following testing and validation, we will acquire appropriately sized or concentrated samples from previously identified wells thought to be contaminated with naturally produced perchlorate. We anticipate that the presence of naturally produced perchlorate will be easily identifiable via an excess of chlorine-36 over what we have measured for synthetically produced perchlorate salts and up to the chlorine-36/chlorine ratio of approximately 2×10^{12} found in surface water.

ENERGY SUPPLY AND USE



Laboratory Directed Research and Development

Fossil-Fuel Emission Verification Capability— Thomas Guilderson (07-ERD-064)

Abstract

The capability to quantify and verify carbon emissions to ensure adherence to emission limits is vital to California as well as national and global environmental management and energy security efforts. Expertise in carbon isotope analysis, atmospheric modeling, and computational physics make Lawrence Livermore uniquely qualified to supply independent verification of emissions of carbon dioxide (CO_2) resulting from burning of fossil fuels. This project will provide the basis for a measurement program that will be intimately coupled with advanced atmospheric transport and inversion models to provide a transparent and independent capability for verification of fossil-fuel CO_2 emissions in California. We propose to solve the inversion problem and numerically estimate the emission magnitude and distribution of chemical species given measurements of chemical concentrations.

This project will create a simulation-based framework for locating and tracking fossil-fuel emissions for California and will document the need for an independent emissions estimate using conventional CO_2 concentrations and carbon isotope ($^{14}CO_2$) analyses. These results will also further our understanding of other inert trace greenhouse gases in the atmosphere. California is a challenging test bed for this potential tool, but federal agencies are looking at California as a model for a possible future national program.

Mission Relevance

This project supports LLNL's missions in environmental management and energy security by promoting advancements in carbon and climate research.

FY09 Accomplishments and Results

In FY09 we (1) continued work on implementing a filter protocol that allows for a more streamlined process to obtain the ensemble average estimate and allows for incorporation of observations to additionally constrain the transport model, (2) formally established a collaboration with the Earth System Research Laboratory at the National Oceanic and Atmospheric Administration that included porting a "carbon tracker" to the Livermore Computing Center for performance analysis and potential ensemble comparison against Livermore's IMPACT (massively parallel atmospheric chemical transport) code and the community WRF (Weather Research and Forecasting) model, and (3) hired a new researcher to supplement the research team on this project.

Proposed Work for FY10

Given the importance of uncertainty in model parameterizations to the retrieved error, it is clear that the model parameters and parameterizations must be retrieved simultaneously with the emission amplitudes. To this end, we will develop a second-generation research code for retrieving fossil-fuel emissions from carbon-14 observations (based on either an ensemble Kalman filter or an advanced stochastic sampling algorithm). We will then evaluate this new code using $^{14}CO_2$ and other greenhouse gas and emission "fingerprinting" using available experimental data.

Publications

Aines, R., W. L. Bourcier, and M. R. Johnson, 2006. "Separation of carbon dioxide from flue gas using ion pumping." *Proc. 8th Intl. Conf. Greenhouse Gas Control Technologies.* UCRL-CONF-220812.

Cameron-Smith, P., et al., 2009. *Fossil fuel emission verification modeling at LLNL.* LLNL-TR-415915.

Delle Monache, L., et al., 2008. "Toward regional fossil fuel CO_2 emission verification using WRF-CHEM." *EOS Trans. AGU* **89**(53), A53H-03. LLNL-ABS-406850.

Direct Simulation of Dynamic Fracturing During Carbon Storage and Prediction of Potential Storage Failures— Joseph Morris (08-ERD-039)

Abstract

Large-scale carbon dioxide (CO_2) storage projects are required to reduce greenhouse gas emissions. This project seeks to develop and apply a simulation capability for predicting the stability of geologic carbon storage. Integrity of the caprock overlying storage reservoirs is critical to safe and effective long-term subsurface CO_2 storage. We will develop and apply a capability for simulating dynamic fracture and reactivation of existing fractures and faults in caprock, leveraging existing LLNL codes. We intend to modify LDEC (a finite-distinct element code with dynamic fracture and fully coupled fluid-flow capabilities) to directly simulate potential damage within caprock. A reservoir-scale fracture network simulator (FRAC–HMC codes) will evaluate the large-scale consequences of these dynamic events.

To date, the geomechanical deformation of caprock has not been addressed with any fidelity, and almost no work has proceeded on fault and fracture reactivation. If successful, the project will deliver a versatile tool for simulating permeability change at the field scale in response to dynamic fracture activation and from changes in pore fluid pressure. We will perform a

parameter study investigating the response of caprock to typical CO_2 storage scenarios. The proposed work will lead to improved understanding of the geomechanical risk factors that degrade caprock integrity and lead to release of sequestered CO_2. The tools developed can also be used for other energy-related activities such as optimization of gas recovery from shale using hydrofracturing techniques.

Mission Relevance

This research supports Laboratory missions in energy security and long-term energy needs and will contribute to DOE's missions in energy security and carbon management. This work will make a significant contribution to our understanding the geomechanical sources of risk from CO_2 storage.

FY09 Accomplishments and Results

We made significant progress towards the goal of capturing the reactivation of faults and coupled fluid–rock mechanics, including the further development of a coupled finite-volume and distinct, finite-element code to support the scalable, parallelized solution of large flow network problems. This new tightly coupled feature, which can represent the reservoir-scale fracture networks that are the focus of this study, has supplanted the need for the loosely coupled FRAC–HMC approach initially envisioned.

Proposed Work for FY10

In FY10 we will extend the LDEC capability to include prediction of CO_2 flow within the evolving fracture network. Previously we focused on the effect of displaced water upon the evolving fractures and fracture networks. Although effects of the displaced water are a key component of caprock integrity prediction, this capability is also necessary to consider the flow of the injected CO_2. Leveraging the parallelized simulation capabilities we developed, we will explore specific problems at relevant CO_2 sequestration sites to both validate the code capabilities and provide enhanced characterization of the sites. The code capabilities will also be used to provide scenario analysis for determining reservoir response under various CO_2 injection conditions.

Publications

Johnson, S. M., and J. P. Morris, 2009. *Hydraulic fracturing mechanisms in carbon sequestration applications.* 43rd U.S. Rock Mechanics Symp. and 4th U.S.–Canada Rock Mechanics Symp., Asheville, NC, June 28–July 1, 2009. LLNL-PRES-414160.

Morris, J. P., and S. M. Johnson, 2009. *Coupled hydromechanical and reactive transport processes with application to carbon sequestration.* 43rd U.S. Rock Mechanics Symp. and 4th U.S.–Canada Rock Mechanics Symp., Asheville, NC, June 28–July 1, 2009. LLNL-CONF-411888.

Morris, J. P., and S. M. Johnson, 2009. *Permeability evolution in a fractured rock mass in response to fluid injection.* Intl. Conf. Rock Joints and Jointed Rock Masses, Tucson, AZ, Jan. 4–10, 2009. LLNL-PRES-409533.

A Hydrogen–Oxygen–Argon Internal Combustion Engine System: The Mechanical Equivalent of a Fuel Cell—

Salvador Aceves (08-ERD-042)

Abstract

We propose to demonstrate the concept for a hydrogen engine that can potentially deliver the highest efficiency of any internal combustion engine ever built. The engine will enable practical vehicles that could help in a transition from oil-based to carbonless transportation. Our concept consists of mixing hydrogen and oxygen with the noble gas argon in a combustion chamber. Argon has a high specific-heat ratio (1.67, compared to <1.4 for air), which can considerably improve engine efficiency—theoretically to approximately 80% and in practice to approximately 50% after heat transfer and friction losses. Our goal will be accomplished by conducting fundamental research on basic issues such as ignition, flame propagation, and detonation that control engine efficiency at the operating conditions of this engine.

Demonstrating the most efficient engine in history demands an improved understanding of combustion and engine operation in a new operating regime. Because of its unusual composition and high specific-heat ratio, our proposed engine will operate at conditions that have not been adequately explored by simulation, experiment, or theory. In this project, we will conduct basic research to characterize the relevant processes to deliver optimum efficiency. On the road to characterizing this engine we will explore and document the combustion science of hydrogen, oxygen, and argon at high pressures.

Mission Relevance

This project will develop a new capability in the numerical analysis of fluid flow in ignition and combustion, which will be applicable to the analysis of liquid explosives, in support of the Laboratory's national security mission. Our proposed high-efficiency engine will help in the development of efficient and inexpensive hydrogen-fueled vehicles, and accelerate the transition to hydrogen in support of LLNL's missions in energy security and environmental management.

FY09 Accomplishments and Results

In FY09 we (1) developed and validated a detailed chemical kinetic model for high pressure hydrogen–oxygen–argon combustion, (2) incorporated this chemical kinetic model into Los Alamos National Laboratory's KIVA fluid mechanics model and ran it with a well-defined engine mesh, (3) exercised and refined our systems model and identified over-expanded engines as most appropriate for this application, and (4) conducted series of experiments at various engine speeds, compression ratios, and equivalence ratios, developing a preliminary engine performance map.

Proposed Work for FY10

In FY10 we will demonstrate the efficiency of our approach for hydrogen engines. Specifically, we will (1) operate the engine at optimum regions for maximum efficiency without engine knock; (2) modify the engine (e.g., increase the flame speed) to allow higher efficiency operation; (3) exercise the KIVA3V engine model, using our experimental data to validate it for this application; (4) use KIVA3V to lead the experiments to achieve higher engine efficiency; and (5) validate greater than 50% engine efficiency through optimal selection of operating parameters.

Data acquisition computer

Hydrogen gas line

Gas bottles and manifolds

CFR engine

A variety of equipment is used in our ongoing hydrogen–oxygen–argon experiment to develop a high-efficiency internal combustion engine.

Toward More Intrinsically Secure Nuclear Fuel Cycles—

Keith Bradley (08-ERD-056)

Abstract

The rapid growth in nuclear fission energy production worldwide poses dramatic risks for the proliferation of nuclear weapons materials. The objective of this project is to assess and enhance the utility of partitioned spent nuclear fuel that could arise in numerous fuel recycle schemes currently being considered domestically and abroad. We will continue to advance our capability and process-based understanding. Our approach will include determining the dynamic and nuclear properties of submixtures of partitioned spent nuclear fuel, assessing the attractiveness of various mixtures for use in nuclear explosive devices, and developing the means to reduce their potential utility as a nuclear explosive.

We expect to produce a methodology for assessing the attractiveness of formerly unaddressed nuclear materials and identify one or more concepts of engineered fuel systems or fuel cycles that need additional research and development. This will provide tools to enhance the nation's ability to counter proliferation of nuclear weapons materials while enabling advances in nuclear power generation.

Mission Relevance

This project supports LLNL's national security mission by improving the proliferation resistance of nuclear fuel cycles.

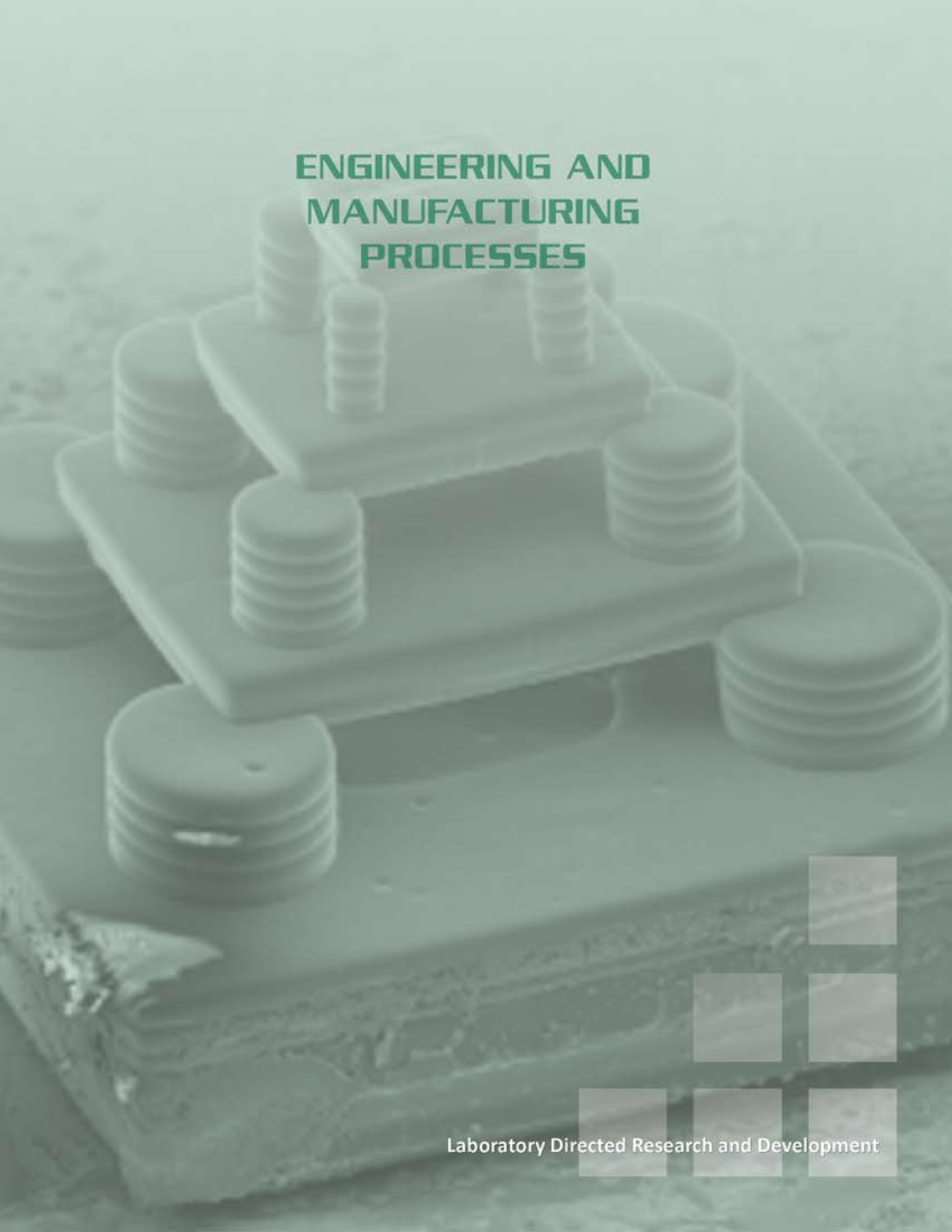
FY09 Accomplishments and Results

In FY09 we completed the first phase of the project, which included demonstrating a dynamic assessment capability for material attractiveness of nuclear compositions appearing in various stages throughout spent fuel reprocessing schemes, as well as exploration of the efficacy of breedable neutron poisons that would accumulate in spent fuel as it cools. We identified at least six candidate seedants and performed calculations to quantify degradation in performance as a function of poison concentration. We also embarked on the second phase of the project, which focuses on identifying and exploring candidates for complicating and/or delaying the partitioning of plutonium in used light-water reactor fuel.

Proposed Work for FY10

A natural progression of our work has been to identify avenues for impeding extraction of weapons materials from spent fuel. Last year, we analyzed several approaches and eventually narrowed them down to a concept that exploits the novel properties of nanosized systems that would render the separation of fissile components more difficult. Conventional reprocessing usually relies on solvents interacting with the spent fuel. Our concept is to develop a nanofuel with coatings that are chemically resistant. The enhanced toughness and strength of nanosystems is well established, and we believe such a fuel would be highly difficult to mechanically and chemically defeat. As a proof-of-principle, in FY10 we will demonstrate a key property of a surrogate nanosystem—the resistance to mechanical attack.

ENGINEERING AND MANUFACTURING PROCESSES



Laboratory Directed Research and Development

Transport Behavior and Conversion Efficiency in Pillar-Structured Neutron Detectors—Rebecca Nikolić (06-ERD-067)

Abstract

A radiation detection device that can be easily fielded and that offers high detection efficiency is vital to national security efforts. In this project, we will demonstrate a technology that could lead to a device with over 70% thermal neutron-detection efficiency. By applying microtechnology methods to neutron detection, we expect to make revolutionary improvements in device efficiency and field usability. We will take advantage of recent advancements in material science, charged carrier transport, and neutron-to-alpha conversion dynamics to fabricate semiconductor pillars in a three-dimensional matrix in which the neutron-to-alpha conversion material has adequate density to capture the full neutron flux.

With this project, we intend to develop and demonstrate a proof-of-principle device, and we will devise a roadmap for scaling the device to optimal efficiency. This is significant because current technology suffers from poor efficiency and adaptability to field use, high voltage, sensitivity to microphonics, a large device footprint, and high pressure, resulting in significant complications in air transport and deployments. The advances we propose in microfabrication and nanofabrication methods are applicable to many other fields, including biochemical detection, communications, and computations.

Mission Relevance

Our project supports the Laboratory's national security mission by advancing technology for the detection of special nuclear materials and radiological dispersal devices. If our demonstration device meets the requirements for high efficiency and demonstrates suitability for field use, it would pave the way to manufacturing field-ready devices in partnership with an industrial collaborator.

FY09 Accomplishments and Results

For FY09 we (1) determined the fundamental scalability limitations of the conformal coating of boron chemical vapor deposition, (2) studied the scalability limitations of the pillar detector, (3) performed alpha and neutron measurements for the detector, (4) benchmarked simulated efficiencies with experimental data of varying pillar height, and (5) updated the physics-based pillar detector model to account for losses. In summary, this project has delivered a novel design for high-efficiency thermal neutron detectors.

Publications

Conway, A. M., R. J. Nikolić, and T. F. Wang, 2007. *Numerical simulations of carrier transport in a pillar-structured solid-state thermal neutron detector.* Intl. Semiconductor Device Research Symp. 2007, College Park, MD, Dec. 12–14, 2007. UCRL-CONF-235094.

Conway, A. M., et al., 2008. "Numerical simulations of pillar structured thermal neutron detector efficiency and gamma discrimination." *IEEE Trans. Nucl. Sci.* **56**, 2802. LLNL-JRNL-405025.

Conway, A. M., et al., 2009. *Si-based thermal neutron detectors.* 2009 CMOS Emerging Technologies Workshop, Vancouver, Canada, Sept. 23–25, 2009. LLNL-PRES-410572.

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Deo, N., et al., 2007. *Chemical vapor deposition of boron.* Materials Research Society Spring Mtg., San Francisco, CA, Apr. 9–13, 2007. UCRL-PRES-229731.

Deo, N., et al., 2008. "Conformal filling of silicon micro-pillar platform with boron-10." *J. Vacuum Sci. Tech.* **B26**, 1309. LLNL-JRNL-401189.

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Standing-Wave Probes for Micrometer Scale Metrology— Richard Seugling (07-ERD-042)

Abstract

The objective of this project is to develop a low-force, high-aspect-ratio contact probe for the nondestructive characterization of components and assemblies developed for fusion-class laser targets. The key concept for the standing-wave probe is correlation between the dynamic response of an oscillating, slender cantilever rod and its interaction with a material surface. The goal of this project is to provide information about surface topography and localized material properties, specifically in low-density foams. A principal component is a detailed analysis of the fundamental contributions to the uncertainty of the measurement process, including the surface science of probe–sample interaction, the dynamic response of the probe, and limitations of scale.

The expected results of this project include (1) a functional probe system capable of determining surface location, material properties, and possible surface modification; (2) a fundamental understanding of probe–surface interactions and the resulting uncertainty related to the measurement based on analytical models and experimental results; (3) an assessment of the fundamental limitations of this technology as scale decreases; and (4) an evaluation of expanding probe sensitivity to multiple dimensions. It is the goal of this work to develop a fundamental understanding of how surface–probe interactions affect the dynamic response of the probe system and how these variations in dynamic response can be attributed to parameters such as surface location, hardness, and elastic modulus.

Mission Relevance

Two specific areas of relevance for this work are stockpile science and technology and high-energy-density science and technology as they relate to characterization of high-power laser target parts and assemblies. Immediate applications include dimensional characterization of target geometry with micrometer features, with future applications in dimensional as well as material characterization of low-density materials such as aerogels and metallic foams.

FY09 Accomplishments and Results

Using an enhanced-performance probe system, a measurement system was built at the University of North Carolina at Charlotte by InsituTec as a development platform for qualifying performance of the probe system for measuring features and materials of interest to this project. Noncontact measurements of foam features were performed (i.e., the probe traces the surface without directly contacting the material). A prototype two-dimensional probe was created that will expand the one-dimensional system with nanometer-level sensitivity, and a record of invention was filed. As a result of this project, we gained a better understanding of the fundamental physics governing the measurement uncertainty of a standing-wave fiber probe and used this information to increase sensitivity and operate the probe in both contact and noncontact modes. In addition, a scaled one-dimensional and an expanded two-dimensional probe have been modeled and designed.

Publications

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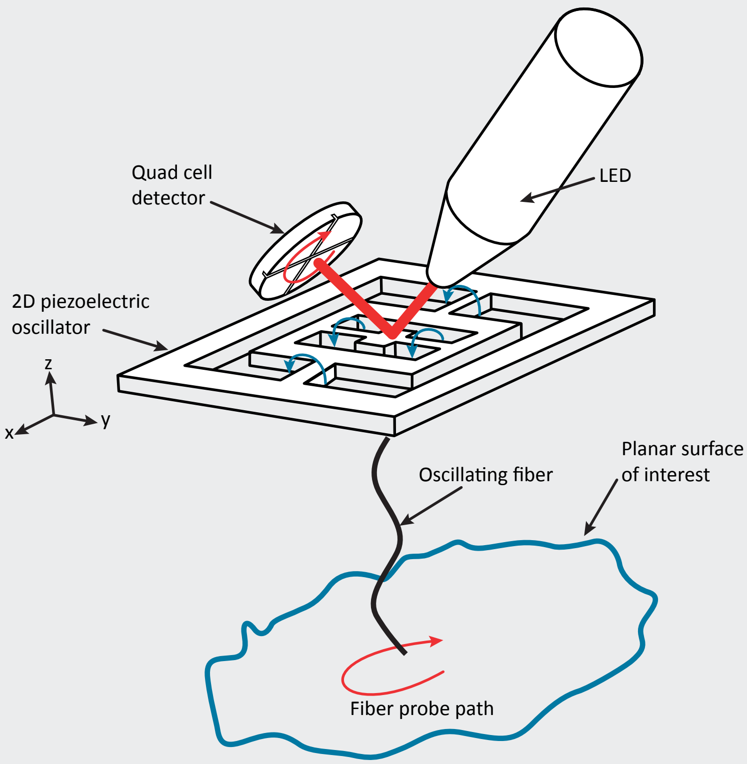


Design of a two-dimensional standing-wave probe for dimensional metrology applications. The system incorporates a two-dimensional oscillator, fiber probe, and optical lever as a feedback mechanism.

Ultrahigh-Velocity Railgun—Jerome Solberg (07-ERD-055)

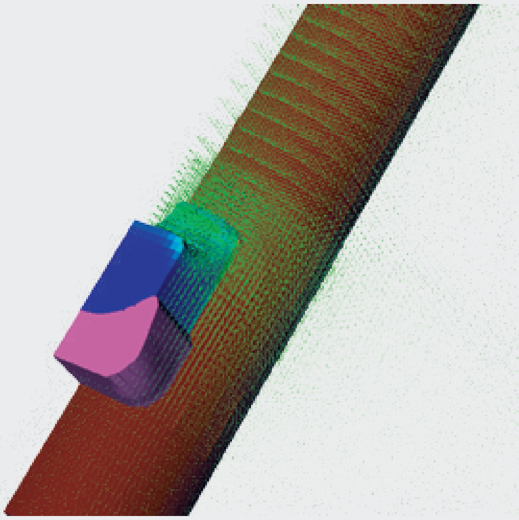
Abstract

Previous efforts to develop ultrahigh-velocity railguns for shock physics experiments were limited by the lack of appropriate simulation tools for the three-dimensional nature of plasma in the armature. However, the availability of a new, three-dimensional magnetohydrodynamic code, along with railgun components available at LLNL, allows us to gain a detailed understanding of armature plasma behavior. We propose a combination of simulations and experiments aimed at creating a class of ultrahigh-velocity railguns utilizing a hybrid armature of solid and plasma brushes. Such a railgun would provide a means for equation-of-state research at pressures unattainable by gas guns.

If successful, this project would provide an experimentally and computationally validated railgun simulation capability to enable designs capable of achieving velocities up to 15 km/s, far surpassing that possible with current gas guns, and allowing for pressures exceeding 20 Mbar. Such a device would be of great use in equation-of-state research, and the basic simulation technology has wide application in many areas of pulsed power.

Mission Relevance

This project supports future applications in support of LLNL's stockpile stewardship mission by designing a device capable of reaching, in a controlled fashion, physical states not easily attainable by any other technology. In addition, the simulation and experimental capabilities developed in this research will be transferable to a number of other national security efforts involving explosive pulsed power and high-energy physics, such as magnetic flux compression.



A hybrid armature railgun modeled in quarter-symmetry with the code ALE3D, whose treatment of mixed-element joule heating was enhanced for this project.

FY09 Accomplishments and Results

We continued our simulation efforts, including more refined two- and three-dimensional models of the fixed hybrid armature experiment and making changes to the treatment of mixed-element joule heating in the ALE3D (arbitrary Lagrange–Eulerian three-dimensional) code. We successfully modeled plasma and solid-armature railguns to a level sufficient to allow us to propose an experimental campaign. We then designed and fielded a railgun experiment utilizing available infrastructure in partnership with a Department of Defense (DoD) railgun contractor, with the primary hardware—rails, insulators, and armatures—designed and manufactured by LLNL. The experiment yielded promising results. This project has enabled a capability for modeling and simulating, in three dimensions, complex solid–fluid–plasma, including those in railguns, and has led to novel ultrahigh-velocity railgun designs, which showed promise in initial tests. The code advancements we made have already been adopted by LLNL for a number of efforts, and the DoD has expressed interest in the materials and diagnostic technologies created in this project.

Publications

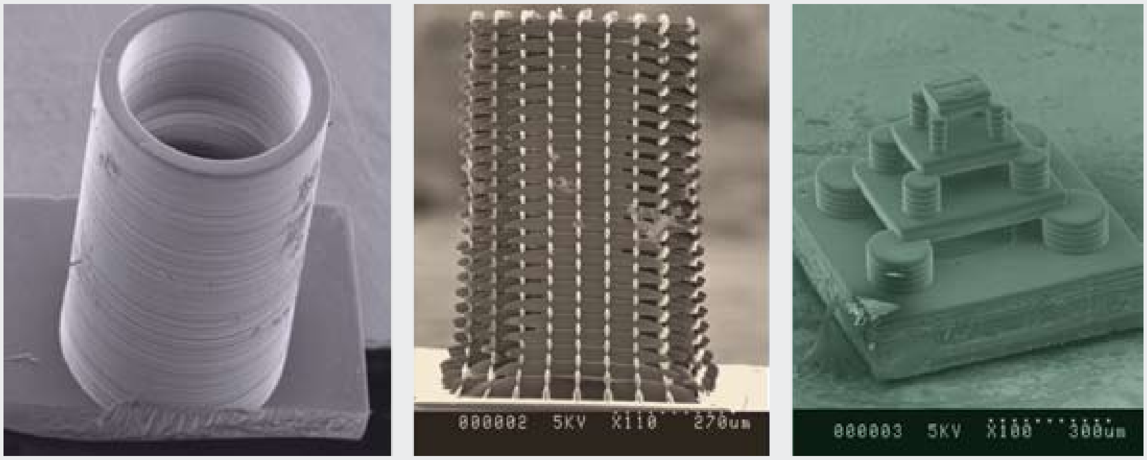
Solberg, J. M., et al., 2008. *Fixed hybrid armature railgun experiments.* DoD Innovative Science and Technology EM Railgun Workshop, Albuquerque, NM, Sept. 23–25, 2008. LLNL-ABS-405307.

Solberg, J. M., et al., 2008. *Overview of electromagnetic launch-related activities at Lawrence Livermore National Laboratory.* 14th ElectroMagnetic Launch Conference, Victoria, Canada, June 10–13, 2008. LLNL-ABS-402745.

High-Resolution Projection Microstereolithography for Advanced Target Fabrication—Christopher Spadaccini (08-ERD-053)

Abstract

Target fabrication for future fusion-class lasers has been a factor limiting the scope of potential experiments. Livermore efforts have focused on developing new fabrication techniques that can generate mesoscale to microscale targets with microscale to nanoscale precision. Although much progress has been made, several key target features have been elusive, including double-shell spherical geometries with low surface roughness, graded-density materials, exotic three-dimensional (3D) geometries with compound curvatures, wide variety of materials, and rapid, low-cost manufacturing. Our objective is to advance the state-of-the-art



Scanning electron microscope images of fusion target components fabricated with projection microstereolithography: a cylinder, lattice structure, and three-dimensional component with overhanging features (left to right).

in target fabrication using projection microstereolithography, and then extend this technique to nanometer-scale resolution, multi-layer structures, and graded-density materials.

We expect this project will result in a new high-resolution, 3D fabrication technique that will advance laser target fabrication as well as microfabrication technology. Specifically, we expect to develop (1) feature resolution on the scale of tens of nanometers; (2) multilayered spherical structures with low surface roughness; (3) an ability to directly transcribe fine features on the internal surfaces of spherical shells; (4) graded-density materials ranging from full density to less than 5% in tens of micrometers; (5) an empirically validated, model-based design tool; (6) high-visibility publications; and (7) new devices and structures.

Mission Relevance

This project will provide a new microfabrication and nanofabrication capability to benefit future fusion-class laser systems in support of the Laboratory's stockpile stewardship and energy missions. The ability to meet specific target fabrication metrics in materials and geometry is critical for obtaining useful data for physics model validations as well as inertial-confinement fusion experiments. In addition, our project will provide a new microfabrication and nanofabrication technology that will be a key enabler for 3D microsystems.

FY09 Accomplishments and Results

In FY09 we (1) fabricated many 3D components relevant to fusion targets; (2) fabricated and demonstrated a working plasmonic superlens, then began integrating it with the overall system; (3) validated our optical–chemical model; (4) demonstrated microfluidics with projection microstereolithography, fabricating a microfluidic channel and using it to deliver a liquid monomer slurry with silica particles; and (5) developed a concept for using multiple light beams to create controlled 3D diffraction patterns.

Proposed Work for FY10

For FY10 we propose to (1) complete the model-based design tool by incorporating our optical–chemical–fluidic interaction models, (2) fabricate components with multiple materials, (3) produce a selected set of components with nanoscale features, and (4) establish a holographic lithography capability by interfering multiple light beams.

Publications

Spadaccini, C. M., et al., 2009. *High-resolution projection microstereolithography (PuSL) for 3-D fabrication.* National Nanomanufacturing Summit, Boston, MA, May 29, 2009. LLNL-PRES-413420.

Enabling Transparent Ceramics Optics and Advanced Armor with Nanostructured Materials Tailored in Three Dimensions—Klint Rose (09-ERD-029)

Abstract

Our objective is to develop three new techniques using electrophoretic deposition to fabricate novel nanostructured materials. Functionally graded materials fabricated with gradients in composition, microstructure, or density produce

enhanced bulk properties, but current techniques are limited to gradients of composition along a single axis. Using our new techniques, we plan to demonstrate new nanostructured materials including transparent ceramic optics with three-dimensional tailored doping profiles, noncubic transparent ceramics fabricated from aligned nanorods, and ceramic armor with complex geometry and graded material composition. To achieve this, we will develop the necessary particle chemistries, instrumentation, and protocols optimized through experiments and modeling.

Overall, we expect to develop a new nanofabrication system with three-dimensional composition control, controlled orientation of precursor material, and deposition geometries with nonplanar shapes. Success in reaching these milestones will (1) dramatically expand the design space of ceramic optics and immediately impact high-average-power laser design, (2) potentially create a paradigm shift in the field of optical materials by producing transparent ceramics from noncubic materials, (3) enable ceramic armor with optimal performance, (4) provide an empirically validated deposition model for future designs and applications, and (5) result in high-impact publications on the fabrication technique as well as the new materials and structures from each application.

Mission Relevance

This project will provide a new nanofabrication capability that supports the Laboratory's national and energy security missions. This new technology enables novel composites and structures using readily available precursor materials. The work will enhance ongoing Laboratory efforts in ceramic optics and armor, provide future capability in fabricating inertial-fusion energy targets, and enable superlattice substrates from novel materials for radiation detection and other national security applications.

FY09 Accomplishments and Results

In FY09 we (1) fabricated and tested a new deposition chamber, enabling automated injection and removal of particle suspensions and automated control of the electric field for deposition; (2) synthesized fluorapatite and hydroxyapatite nanowires; (3) began setting up our dynamic electrode system with a high-luminosity computer-controlled light source; and (4) integrated particle–particle interactions into the Stokesian dynamics model, which already included electrophoretic, dielectrophoretic, hydrodynamic, and Brownian motion effects.

Proposed Work for FY10

In FY10 we will continue with previously proposed work that was not addressed because of funding restrictions. We will focus on expanding the capabilities of an existing electrophoretic deposition system, begin synthesizing particle suspensions, and confirm transparent sintering of demonstration structures. Specifically, we will (1) confirm transparent sintering of homogeneous particle depositions, (2) synthesize and characterize yttrium–aluminum–garnet particle-suspension nanorods of noncubic material, (3) implement z-axis control and demonstrate a transparent sintered part with a depth-wise composition gradient, (4) implement fixed-mask *x*–*y* axis control and demonstrate a transparent sintered part with a planar composition gradient, and (5) begin testing of dynamic *x*–*y* control.

Maskless, Low-Cost, High-Performance Polymer Waveguides—Klint Rose (09-ERD-057)

Abstract

Our proposed study will explore a new maskless material fabrication approach being developed at the University of Illinois that has multiple technological applications in composites, microfluidics, and photonics. This technique, direct ink writing, will enable new capabilities in the synthesis of complex structures from a variety of materials. As an initial proof-of-concept demonstration, we will use direct ink writing to fabricate a new generation of high-performance polymer optical waveguides with high optical transmission. We will collaborate directly with the development group at the University of Illinois to develop and optimize the fabrication technique for our desired materials, surface roughness, and geometry specifications.

Throughout this study we will work with our collaborators at the University of Illinois to develop the necessary protocols to fabricate polymeric waveguides with the desired surface roughness and geometry to achieve optical transmission losses in the waveguide below 0.1 dB/cm. These losses are strongly correlated with the material, surface roughness, and geometry of the waveguide. By optimizing direct ink writing fabrication for a selected set of polymers, we expect to achieve this low-loss level. We also expect to demonstrate this performance with multilayer waveguides patterned into compact three-dimensional structures. This optimization process will enable future applications requiring complex three-dimensional structures and materials not compatible with standard microfabrication techniques.

Mission Relevance

The broad range of structures and filament cross-sections achievable with direct ink writing and the diverse materials compatible with the process enable many applications of interest to LLNL in support of several missions, including national and homeland security as well as energy security. Examples of potential applications include self-healing materials, inertial fusion energy targets, three-dimensional microfluidics, and photonic crystals. Direct ink writing may be ideal for fabricating low-cost polymer waveguides with low optical losses, which are also of interest to numerous LLNL photon science efforts in defense, energy, and basic science.

FY09 Accomplishments and Results

In FY09, we (1) characterized the rheology of three polymer materials (polyvinyl methacrylate, polystyrene, and a standard two-part epoxy), (2) used the rheology data to select fabrication parameters for each material and successfully fabricated waveguides from each, (3) analyzed all waveguides using atomic force microscopy scans to determine surface roughness and optical measurements to determine losses, and (4) determined, for each material, the ideal process parameters (e.g., temperature, write speed, and ultraviolet exposure) to limit optical losses to 0.3 dB/cm or less.

Proposed Work for FY10

In FY10 we will (1) continue to fabricate and test waveguides to determine the ideal writing conditions to achieve minimal optical losses, (2) select the optimal materials for this application and fabricate more complex waveguide structures that include bends and three-dimensional structures, and (3) continue to measure, for each waveguide, the optical losses to determine optimal material and fabrication conditions.

Laser-Based Comminution of Debris Samples for Post-Detonation Forensics—Raymond Mariella (09-FS-002)

Abstract

In the event of a nuclear detonation by a terrorist in an urban area, speed is critical in analyzing the explosion debris to determine key forensic signatures that identify the source of the nuclear material used in the blast. Current state-of-the-art sample processing utilizes a hydraulic press to crush debris samples into millimeter-scale particles before dissolution in acid. However, dissolving large particles is time-consuming, thus delaying the radiochemical signature-identification process. A way to greatly speed up this process would be to break down the particles to micrometer scale for rapid dissolution. We will study the feasibility of using laser ablation in preparing debris from a nuclear explosion for forensic analysis. Laser ablation has the potential to enable the “day-one” forensics of such debris without sacrificing accuracy or sensitivity. Our goal is to understand the physical processes that affect ablated particles so that we can design a pulsed-laser-based processing system capable of entirely and quantitatively processing approximately 15-g solid debris or core samples into submicrometer particles within 2 h.

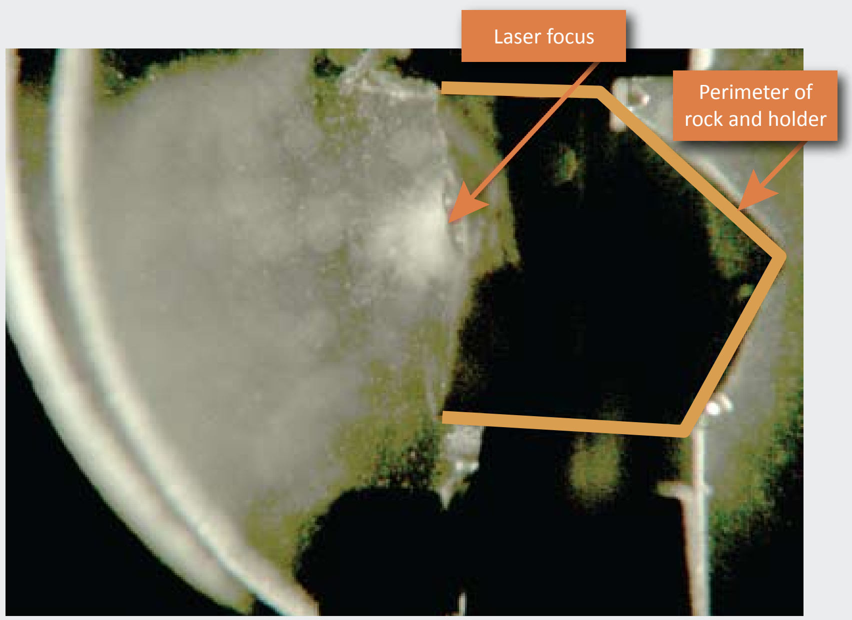
In addition to the feasibility of laser ablation for debris sample preparation, we will also determine optimum sample particle size in terms of tradeoffs in equipment costs, reliability, training requirements, and processing time.

Mission Relevance

This project supports the Laboratory’s homeland security mission by helping to enable rapid day-one forensic identification of the source of nuclear materials used in a nuclear incident in an urban area.

FY09 Accomplishments and Results

In FY09 we successfully ablated micrometer-scale particles from concrete debris using 15-ns, 351-nm laser pulses with a fluence of roughly 0.5 J/cm^2. More than 90% of the ablated particles were 1.1-µm diameter or smaller when using this fluence. In another study, we ablated particles with a laser fluence that exceeded 1 J/cm^2. The higher power was not necessary for the ablation of particles, however, and led to far less overall control of the process, including the ejection of particles as large as 0.1 mm in diameter. Because our goal was both to generate



Material ablated from a submerged quartzite rock sample by a 0.7-J ultraviolet laser pulse. Microparticles form via ablation, but larger chunks are ripped from the surface by bubble collapse, cavitation, or water jets.

micrometer-scale and smaller particles and to control the process as much as possible, further work will investigate ablation with fluences less than 1 J/cm^2. With this project, we were able to demonstrate that laser pulses generated by numerous commercial pulsed-laser systems could comminute rock or concrete debris into micrometer-scale particles at rates sufficient to process 15-g samples in less than 1 h.

Latent Heat Reservoirs for Thermal Management of Laser Diode Pumps—Robert Deri (09-FS-004)

Abstract

Higher-power laser diodes are important for pumping advanced optical sources such as laser-driven gamma sources and accelerators that enable scientific exploration. Laser diode power is currently constrained by heat dissipation that prevents the output power to scale with existing laser drivers and creates reliability limits. We propose to investigate a novel, high-risk, high-payoff concept that has the potential to significantly improve quasi-continuous wave thermal management. We will study the feasibility of a thermal management approach based on latent heat reservoirs, and will use heat-transfer simulations to ascertain if the concept is viable.

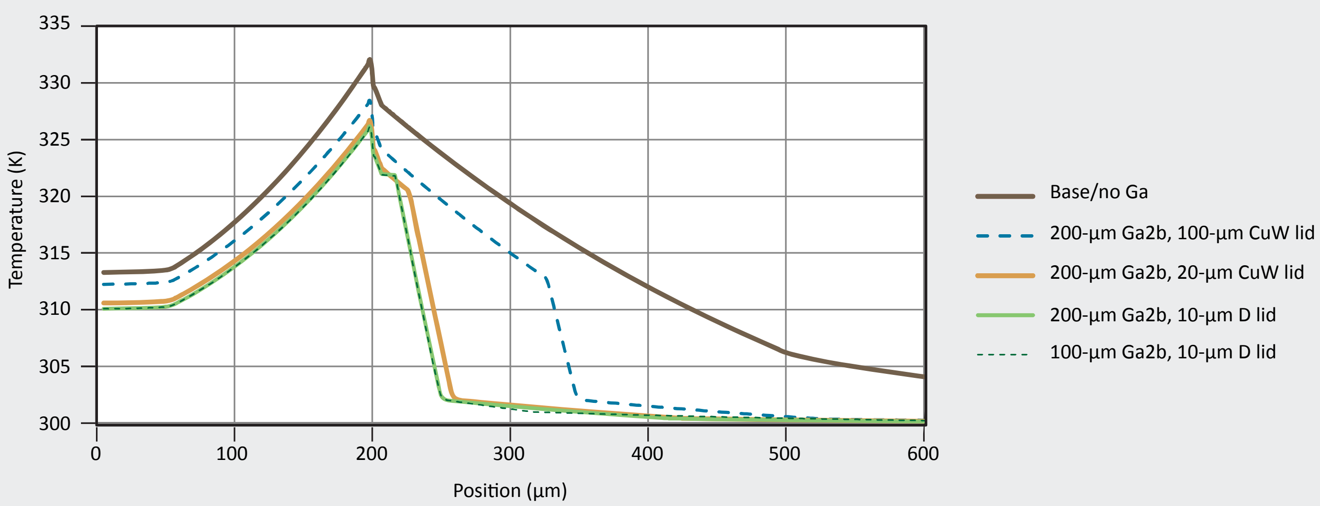
We expect to determine the maximum electrical drive current and maximum increase in laser diode junction temperature that can be achieved using a novel thermal management approach. This project will determine the essential feasibility of the approach via simulation. If our simulations show promise, subsequent experimental work will be required to demonstrate that our approach can be achieved in practice. If our approach is ultimately successful, it will enable operation of laser diodes at significantly higher optical outputs. This will enable more capable pulsed optical solid-state lasers with higher brightness.

Mission Relevance

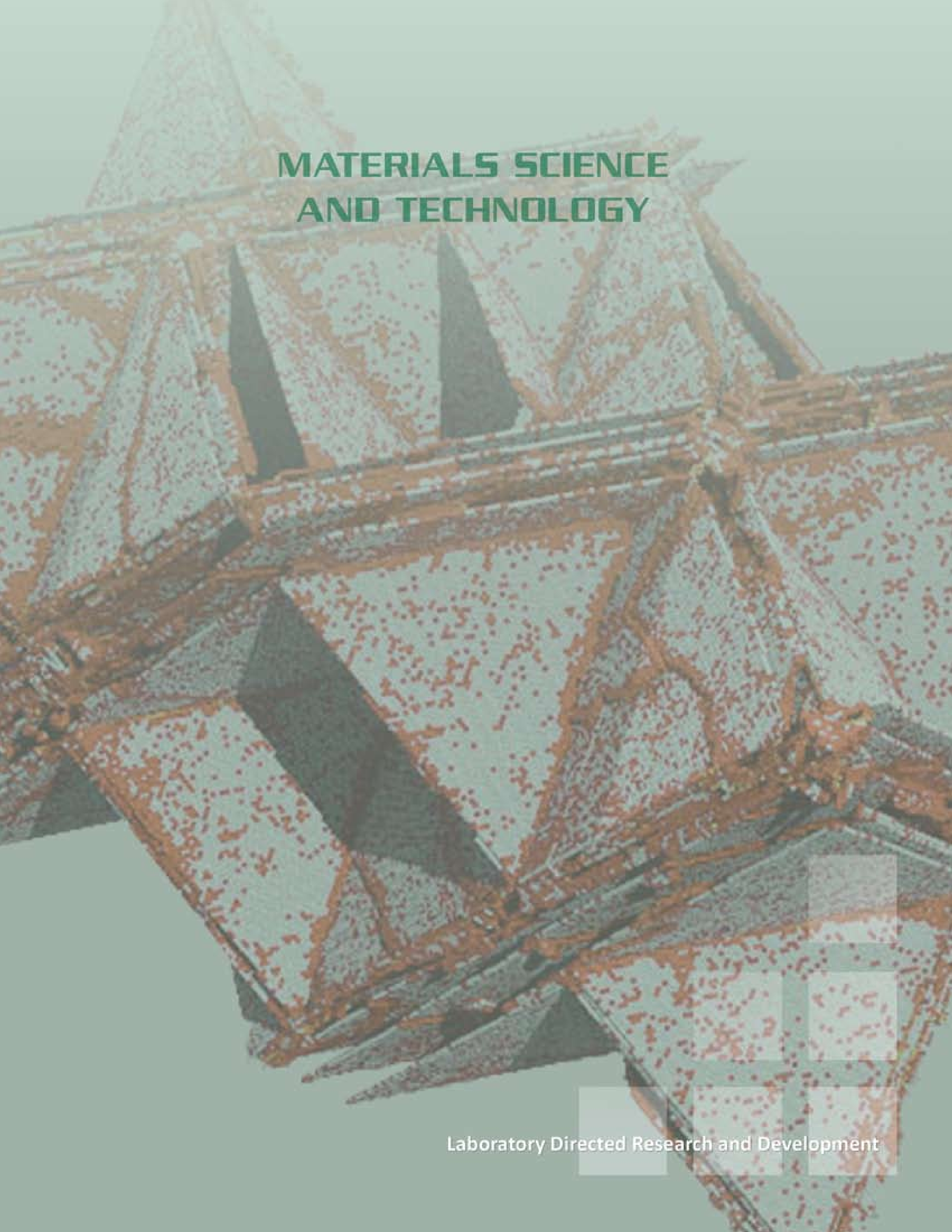
This work supports LLNL's mission in energy security by focusing on greater performance from laser pump diodes, which will enable realization of power plants with lower cost-to-performance ratios. This project is also relevant to the Laboratory's strategic mission thrust of advanced laser systems, and could enable optical sources with higher brightness for use in a variety of application-specific systems that support Laboratory missions in nonproliferation and frontier science.

FY09 Accomplishments and Results

In FY09 we (1) developed two methodologies for simulating time-dependent latent heat reservoirs—one based on commercial software and one on an internally written software package—and validated the methods against simple analytical models, (2) optimized latent heat structures to minimize junction temperature increases by exploring both planar and more complex geometries, and (3) showed that, using a gallium reservoir, the junction temperature rise of a 10-mm^2 device operating at 500 W can be reduced by 5°C using a planar structure, and up to 9°C using a more complex one. The successful conclusion of this project demonstrated that latent heat reservoirs can improve thermal management of laser diode pumps. The results are being used to evaluate whether this concept should be prototyped at this time and to support a patent application in preparation.



Simulated temperature profiles after a 1-ms, 250-W heat pulse for planar structures with and without a gallium reservoir. The reservoir clearly reduces the peak temperature.



MATERIALS SCIENCE AND TECHNOLOGY

Laboratory Directed Research and Development

Transformational Materials Initiative—Robert Maxwell (06-SI-005)

Abstract

The goal of this project is to provide the underlying science and technology for converting America's nuclear weapons complex to one that is smaller, safer, and more agile. We will create new materials, processes, and diagnostics to facilitate the nuclear weapons complex transformation by (1) reducing the cost and time required to produce and maintain the stockpile, (2) enhancing weapon safety, (3) ensuring future stockpile longevity, and (4) optimizing stockpile performance. Our multidisciplinary team combines capabilities in materials synthesis, characterization, theory, and modeling to deliver cutting-edge advances in high explosives, multifunctional materials, metals, and sensing.

The project will create basic scientific and technical capabilities that, if successful, will help transform the nuclear weapons complex. Success will make it more efficient and effective by achieving fundamental scientific advances in synthesis chemistry, metallurgy, dynamic experiments, molecular design, and sensor design, fabrication, and performance.

Mission Relevance

This project will achieve enhanced reliability, improved safety, easier manufacturing, and reduced surveillance requirements for the nuclear weapons complex and help ensure the continued success of the Stockpile Stewardship Program.

FY09 Accomplishments and Results

In FY09 we synthesized, constructed, or fabricated prototype materials and components in all four categories of the project—high explosives, metals, multifunctional materials, and sensors—and tested the properties of these materials and devices. The successful conclusion of this project has provided key advanced material and sensor concepts and prototypes to the weapons program that could save the weapons complex tens to hundreds of millions of dollars in future cost-avoidance scenarios. Follow-on support has been secured from the Laboratory and from work-for-others sponsors.

Publications

Baumann, T., et al., 2009. "Synthesis and characterization of novel PDMS–POSS nanocomposites using multiscale crosslinking elements." *J. Poly. Sci. A* **47**, 2589. LLNL-JRNL-404145.

Glascoe, E., et al., in press. "Picosecond time-resolved and steady-state infrared studies of photoinduced decomposition of TATB at ambient and elevated pressures." *J. Phys. Chem. A.* LLNL-JRNL-407819.

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Letant, S. E., 2009. "Polyhedral Oligomeric Silsesquioxane (POSS)-stabilized Pd nanoparticles: Factors governing crystallite morphology and secondary aggregate structure" *J. Phys. Chem. C.* **113**, 19424. LLNL-JRNL-404273.

Lewicki, J. P., et al., 2009. "Effect of meta-carborane on segmental dynamics in a bimodal poly dimethyl siloxane network." *Macromolecules* **41**, 9179. LLNL-JRNL-404634.

Maiti, A., et al., 2008. "Constitutive modeling of radiation effects on the permanent set in a silicone elastomer." *Poly. Deg. Stab.* **93**, 2226. LLNL-JRNL-402192.

Maiti A., et al., 2009. "Kinetics of hydrogen uptake by scavenger molecules: Insights from molecular modeling." *Chem. Phys. Lett.* **475**, 223. LLNL-JRNL-411589.

Marian, J., et al., 2009. "Compaction behavior and mechanical properties of uniaxially pressed Bi–W composites." *Metall. Mater. Trans. A* **40**, 9. LLNL-JRNL-412903.

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Wu, C. J., et al., 2009. "Catalytic behavior of dense hot water." *Nature Chem.* **1**, 57. LLNL-JRNL-404557.

Kinetics of Phase Evolution: Coupling Microstructure with Deformation—James Belak (07-ERD-007)

Abstract

Confidence in predictions of material behavior at extreme conditions is limited by our lack of knowledge of microstructures and their rate of formation following first-order solidification and solid–solid phase transitions. We propose to reliably predict microstructure by extending our highly successful molecular dynamics techniques for nucleation to hydrodynamic length and time scales. Phase and microstructure calculated by molecular dynamics will serve as initial conditions for our continuum microstructure evolution model, whose dynamics will be validated with molecular dynamics and recovery experiments. This new phase-field capability will employ a real-space representation of the time-dependent Ginzburg–Landau equations in a scalable simulation code amenable to LLNL's world-class computing.

We expect to obtain the first reliable prediction of material microstructure following first-order phase transition at extreme conditions, as observable on emerging x-ray platforms such as the Linac Coherent Light Source. Our results are directly tied to molecular dynamics simulations using potentials applicable to metals and alloys of interest, and extend the molecular dynamics to hydrodynamic scales. We will create the first phase-field modeling capability scalable to LLNL's high-performance computers. By using this material microstructure prediction to calculate material behavior, we will increase confidence in calculations at extreme conditions, for which experimental data are either obtained indirectly or entirely lacking. We will position the Laboratory for emerging opportunities in nuclear energy, radiation detection, and advanced scientific computing.

Mission Relevance

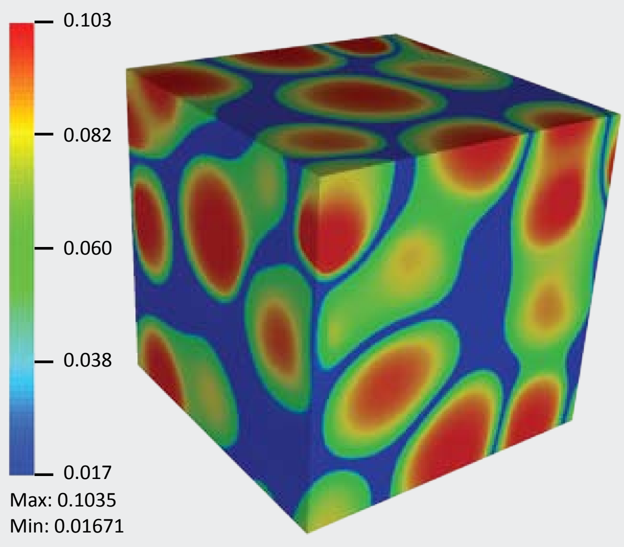
Upon completion, this new capability will be available to provide a realistic prediction of microstructure for relevant alloys under extreme conditions and to directly simulate, for the first time, experiments of first-order phase transformations under highly dynamic conditions such as those observed with the dynamic transmission electron microscope and the Joint Actinide Shock Physics Experimental Research facility. Our new capability will both increase confidence in stockpile calculations, in support of the national security mission, and have applications in the DOE Nuclear Fuel Initiative, in support of the energy security mission.

FY09 Accomplishments and Results

During FY09, we (1) added a numerical solution for elastic energy to the LLNL phase-field code AMPE by developing new multiphysics numerical algorithms to solve for elastic energy concurrently with transformation kinetics, making it possible to properly represent the physics of phase transformations involving large volume or shear strain; (2) analyzed phase transformations in plutonium–gallium systems and used experimental microscopy on gallium coring to validate simulations with the modified code; (3) extended the free-energy representation to include multiphase actinide nuclear fuels and large temperature gradients; and (4) added a model for helium bubble formation to the code and used it to simulate segregation to grain boundaries. The successful conclusion of this project has established phase-field simulation based on AMPE as a core capability at LLNL. DOE's Office of Basic Energy Sciences has begun supporting use of the enhanced AMPE code to analyze the stability of microstructures under extreme conditions, and the code is also being used to analyze transitions of interest—including twinning—and to analyze phase stability and species redistribution in nuclear fuels.

Publications

Belak, J., P. Turchi, and M. Dorr, 2008. *Phase-field modeling of irradiated metallic fuels.* Radiation Stability of Microstructures Workshop, Santa Fe, NM, Sept. 1–4, 2008. LLNL-ABS-406523.



Phase-field simulation of microstructure formation and gallium alloy redistribution following transformation from the high-temperature body-centered-cubic (bcc) phase to the room-temperature face-centered-cubic (fcc) phase in plutonium–gallium alloys. (The unit is the ratio of bcc to fcc.)

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Developing a First-Principles Computational Toolkit for Predicting the Structural, Electronic, and Transport Properties of Semiconductor Radiation-Detection Materials—Vincenzo Lordi (07-ERD-013)

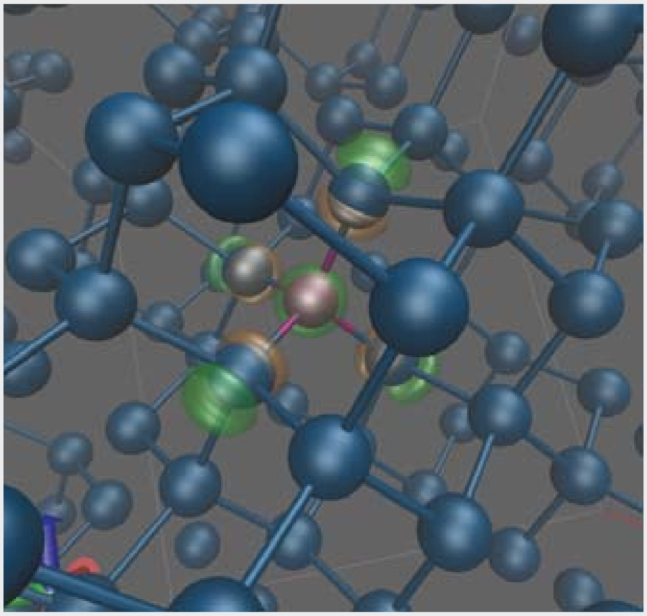
Abstract

The nature of carrier dynamics and lifetimes in semiconductors used for gamma-ray detection is essentially unknown. The objective of this project is to use first-principles computer simulations to guide and accelerate the development of new semiconductor materials for gamma-radiation detectors. We will develop a computational "toolkit" for predicting the structural, electronic, and transport properties of candidate semiconductor detector materials. For a given candidate material, we will evaluate formation energies of defects and predict how carrier mobilities and lifetimes are determined by these defects. The fundamental understanding of the sensitivity of transport properties to material structure will help identify promising semiconductor materials and optimize existing materials.

This project will provide initial information on the nature of electron and hole states in gamma-ray-detecting semiconductor materials and how they interact with materials defects. This information cannot be obtained from experiments. For example, while large structural defects can be imaged by transmission electron microscopy, single dopant impurities and small structural defects cannot. We anticipate that the results of this project's first-principles studies will have a large impact not only on radiation detectors, but also on the larger semiconductor physics community.

Mission Relevance

By furthering the development of gamma-radiation detectors, this project supports LLNL's national security mission in the area of nonproliferation, and detecting weapons of mass destruction in support of the homeland security mission.



A boron atom in a silicon crystal affects the flow of electrons by distorting the structure.

FY09 Accomplishments and Results

We (1) completed the prediction of carrier trapping lifetimes, calculating lifetimes associated with all native and impurity defects in aluminum antimonide and finding that carrier time is significantly degraded only by very deep defects and not by trapping from dominant point defects; (2) completed a first-principles analysis of the concentration-dependent mobility of indium-compensated cadmium telluride; (3) constructed a validated alloy model for cadmium zinc telluride; (4) analyzed defects in gallium telluride and gallium selenide and predicted two possible methods of fabricating a high-resistivity material; and (5) benchmarked and applied quantum Monte Carlo for the accurate prediction of band gaps and defect energy levels. This project has led to the development of new predictive computational methods—including "computational combinatorial chemistry"—for rapidly screening semiconductors for detrimental and beneficial defects and impurities, enabling the design of materials with optimal transport properties for a given application, particularly radiation detection. A noteworthy success was an order-of-magnitude improvement in the performance of aluminum antimonide detectors based on our predictions. Based on work completed in this project, the NNSA Office of Nonproliferation Research and Development will support continued research efforts in the application of predictive first-principles modeling of defects and transport in semiconductors to help optimize new materials for room-temperature gamma radiation detectors.

Publications

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Deformation of Low-Symmetry and Multiphase Materials—Nathan Barton (07-ERD-024)

Abstract

Materials composed of low-symmetry crystals or of multiple solid phases exhibit heterogeneous deformation at the microstructural scale, presenting significant challenges to efforts to construct macroscale constitutive models. We are developing an approach that allows for the explicit incorporation of microstructure and deformational heterogeneity in a framework appropriate to use in analysis of engineering-scale components. In multiphase and low-symmetry materials, microstructure influences yield stress, ductility, high-cycle and low-cycle fatigue, creep, and fracture toughness. Given advances in computing resources, constitutive models, and software infrastructure, we are in a unique position to significantly advance the constitutive modeling of complex materials.

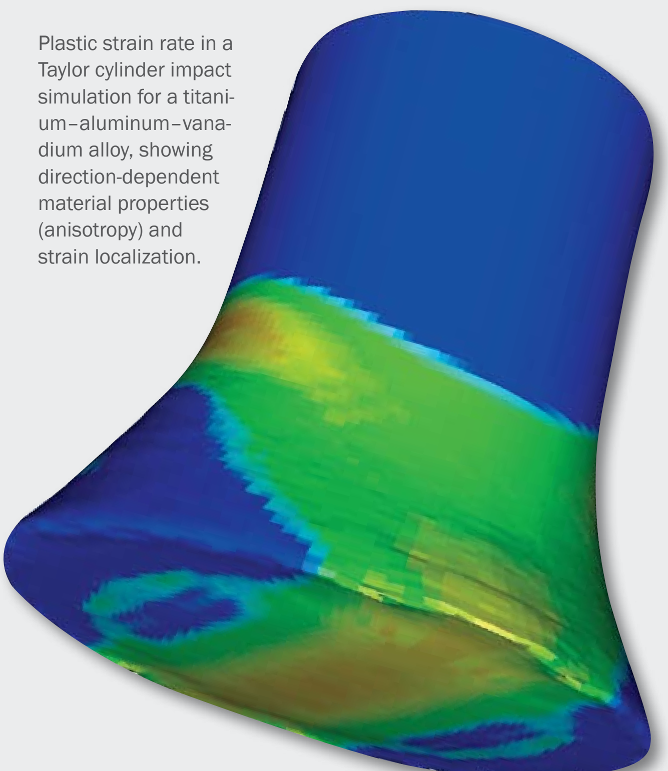
We are targeting applications involving fully developed plastic flow in which the microstructure is known. Explicit inclusion of the microstructure allows for the effective treatment of deformational heterogeneities at the microstructural scale, and we will build on emerging technologies to effectively combine microscale plasticity simulations with macroscale models. The goal is to homogenize the microscale response to obtain effective macroscale models for materials whose macroscopic behavior is difficult to capture using conventional approaches. In addition to multiphase alloys, the approach is applicable to low-symmetry crystalline materials. New capabilities will allow for effective assessment of the impact of microstructure on the performance of engineering-scale components.

Mission Relevance

In the search for robust and cost-effective systems, there is a need for tools that predict material behavior both during processing and while in service. Such behavior is central to the success of many research and development programs at the Laboratory that rely on multiphase alloys and low-symmetry crystalline materials, particularly those that support both stockpile stewardship and homeland security. Prediction of the behavior of these materials is also critical to the Responsive Infrastructure Initiative at NNSA and industrial production of a vast range of consumer goods. Finally, it contributes to the Laboratory's mission in advancing basic materials and computational science.

FY09 Accomplishments and Results

In FY09, we increased model fidelity through more detailed evolution of the material state. Specifically, we developed a method for evolving the probability density distribution of crystal lattice orientation based on discrete harmonics, with flexible control of both initial state accuracy and state evolution accuracy. Accuracy was assessed by comparison to direct simulations using discrete orientations. We determined that evolution is governed by a partial differential equation over a non-Euclidean space, with nonlocal terms from twinning. Collaborators at Los Alamos National Laboratory developed the ViscoPlastic Self-Consistent Scheme, a polycrystal-level model that was calibrated to a variety of materials of interest. Using this model, they successfully calibrated a slip and twinning model of alpha uranium based on data from deformation experiments. Ongoing use and development of our advanced material models will be funded by the Department of Defense, and the modeling capabilities will be used in programmatically relevant simulations.



Plastic strain rate in a Taylor cylinder impact simulation for a titanium–aluminum–vanadium alloy, showing direction-dependent material properties (anisotropy) and strain localization.

Publications

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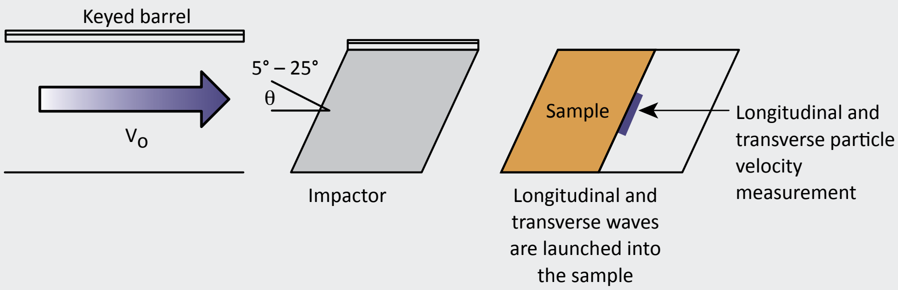
Plasticity at High Pressures and Strain Rates Using Oblique-Impact Isentropic-Compression Experiments— Jeffrey Florando (07-ERD-034)

Abstract

Various aspects of the Laboratory's national security mission depend on accurate computer code simulations of high-strain-rate plastic flow (i.e., nonreversible deformation) under conditions of high hydrostatic pressures. While progress has been made in recent years, especially at extreme pressure or strain



Schematic representation of the oblique-impact compression experiment using windowed interferometry.

rate, uncertainty still exists in understanding the strength of materials under conditions of both high strain rate (10^4–10^6 s^{-1}) and high pressure (1–100 GPa). We intend to use a new, oblique-impact isentropic-compression experiment to study strength properties in these combined pressure and strain-rate regimes. When completed, this work will increase the Laboratory's ability to develop predictive strength models for use in computer code simulations

If successful, we expect to use the oblique-impact isentropic-compression experiment to study the strength of materials under conditions of combined high pressure and strain rate. An understanding of the underlying deformation mechanisms at work under these conditions will lead to development of more accurate strength models. An initial feasibility study using computer code simulations has shown that the transverse wave, which is generated by the oblique impact and trails the longitudinal wave, can be used to assess the strength of the material under pressure. In addition, these experiments could potentially be modified to be fielded at gas-gun or fusion-class laser facilities.

Mission Relevance

The ability to accurately predict the strength of materials under high pressure and dynamic loading conditions (high strain rate) is a main component of the assessment and certification portion of LLNL's Stockpile Stewardship Program. This project supports the stockpile stewardship mission by providing previously unobtainable experimental data on materials strength under those conditions.

FY09 Accomplishments and Results

This year we (1) performed experiments on vanadium, (2) used the data to refine strength models, and (3) performed experiments at higher velocities and pressures on a large gun with iron targets, and published our results. We were not able to explore designs to achieve pressures greater than 50 GPa because of funding reductions. However, the successful completion of this project established an experimental technique to explore the strength of materials subjected to both pressure and shear loading, which is now being applied to study programmatic materials.

Publications

Florando, J. N., et al., 2009. *High rate plasticity under pressure using a windowed pressure-shear impact experiment.* TMS 2009 Ann. Mtg. and Exhibition, San Francisco, CA, Feb. 15–19, 2009. LLNL-ABS-41096.

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Investigation of Double-C Curve Behavior in the Plutonium–Gallium Time–Temperature–Transformation Diagram—Kerri Jayne Blobaum (07-ERD-047)

Abstract

Over 30 years ago, time–temperature–transformation diagrams for plutonium–gallium alloys were published showing two temperatures that maximized the delta-to-alpha-prime phase-transformation rate. The mystery of this "double-C curve" kinetic behavior in transformation of these alloys has remained unsolved ever since. We intend to study and explain this unusual behavior, which is important because it will help to correlate 5f electronic structure with observed structural phase transformations and help with understanding the delta-to-alpha-prime transformation under pressure. We will use differential scanning calorimetry, optical microscopy, and x-ray diffraction to confirm the purported double-C curve behavior and determine the mechanisms responsible for observed kinetics.

We expect to confirm or disprove that the delta-to-alpha-prime transformation in a plutonium–gallium alloy has double-C curve kinetics. We will provide a comparison of the microstructures and morphologies of the alpha-prime products formed in

the upper- and lower-C curves. This work will lead to a model and explanation of the mechanisms responsible for this unusual kinetic behavior. Because many plutonium–gallium research alloys have gallium concentrated in the centers of the grains, we will determine if this inhomogeneity contributes to the double-C curve behavior. This project will lay the foundation for studying the delta-to-alpha-prime phase transformation under pressure.

Mission Relevance

This work directly supports the stockpile stewardship mission by forming a basis for modeling plutonium–gallium phase transformations under dynamic conditions and by enhancing the Laboratory's small-scale plutonium metallurgy capabilities.

FY09 Accomplishments and Results

Building on previous microstructural characterization, we performed differential scanning calorimetry measurements to determine the nucleation mechanism of the conditioning effect that seems to explain the double-C curve kinetics in plutonium–gallium alloys. The conditioning effect and its repercussions are directly related to the aging of plutonium alloys and represent a source of new information about phase stability as a function of thermal history. Using the Advanced Photon Source, we performed in situ time- and temperature-dependent x-ray diffraction measurements, revealing distinct differences in the transformation mechanisms of the upper- and lower-C curves. In summary, this project demonstrated that the delta-to-alpha-prime phase transformation in a plutonium–gallium alloy exhibits its double-C curve kinetics enabled by an unexpected room-temperature conditioning treatment. Programmatic funding is supporting additional work in this area to determine how these kinetics are affected by aging.

Publications

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Controlling the Structure of a Quantum Solid: Hydrogen—George Gilmer (07-ERD-049)

Abstract

The success of fusion-class lasers is dependent upon our ability to create solid films of hydrogen isotopes, which are quantum solids, with high homogeneity and low surface roughness. Recent studies on nucleation and growth of crystalline films have shown chemically patterned substrates can be used to direct orientation, morphology, polymorphs, and size of nucleating crystals. The purpose of this project is to explore approaches to control the nucleation, growth, and defect population of hydrogen isotope crystals. We will develop templates that will provide preferential nucleation sites and set the orientation of the crystalline material. This project will combine atomistic simulations with experiments to better control crystal structure.

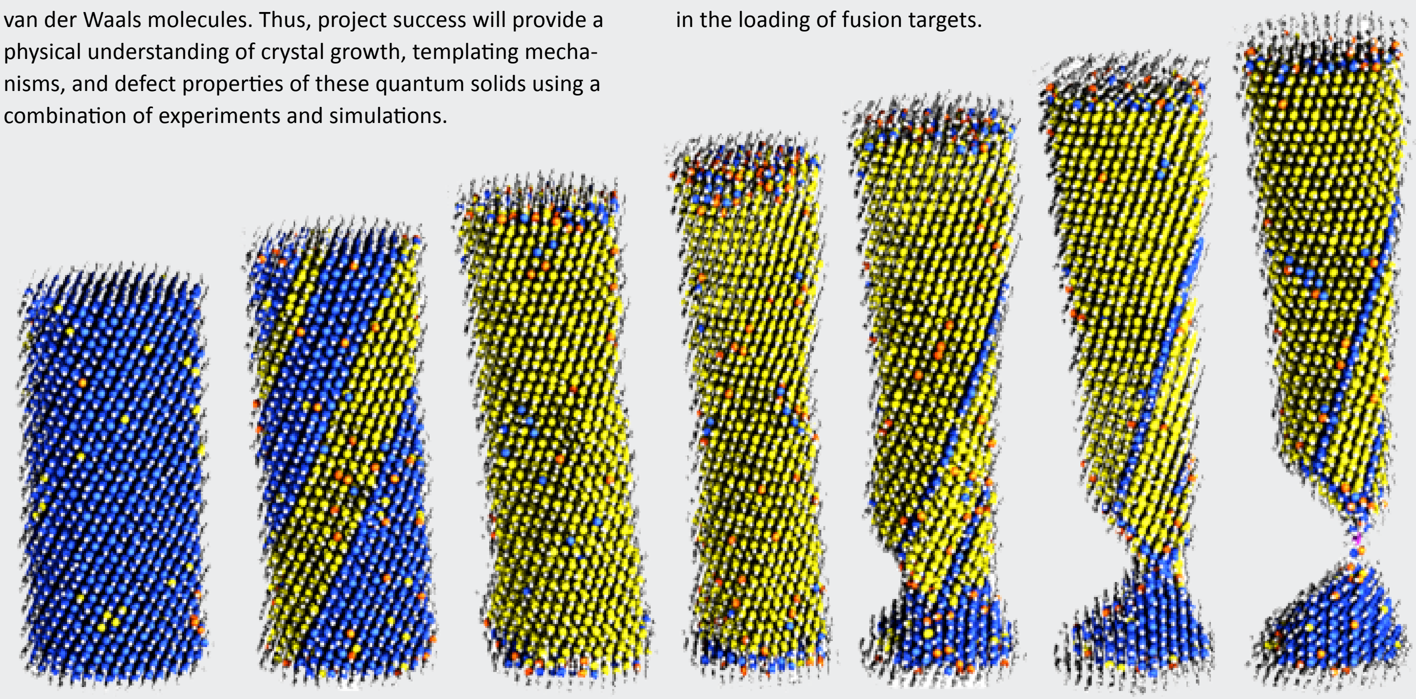
Hydrogen isotopes provide a challenging but rich system for better understanding of templating mechanisms and crystalline-to-amorphous transitions. For example, the lattice-constant difference between isotopes provides a method to test how templating mechanisms are affected by film stress. Similarly, low-binding energy and different molecular diameters of the isotopes suggest it may be possible to insert defects or make solids amorphous using particle radiation. The isotopes can be accurately modeled as computationally simple, point-interacting van der Waals molecules. Thus, project success will provide a physical understanding of crystal growth, templating mechanisms, and defect properties of these quantum solids using a combination of experiments and simulations.

Mission Relevance

This project will couple computational material science to nanoscale research, which supports the Laboratory mission in national security. Scientific findings will aid in developing strategies for ignition targets at future large fusion-class lasers.

FY09 Accomplishments and Results

In FY09 we (1) assembled the Raman spectroscopy components for the cryo stage previously constructed for flat substrates; (2) performed simulations of hydrogen isotope surfaces and measured surface diffusion rates and other properties, including the thickness of quasi-liquid layers that form near the triple-point temperatures; (3) conducted simulations of epitaxial deposition on gold and nickel ([111] and [001]), finding significant differences in the quality of the epitaxial layers; (4) developed a large-scale, efficient atomistic simulation technique for quantum dynamics, including the evaluation of error limits; and (5) designed simulations to determine the stress developed during solidification of alloys of hydrogen isotopes. Our project produced accurate models of the crystallization of hydrogen isotopes and alloys and their properties, including the response of crystalline hydrogen to stress, delamination of epitaxial films, grain boundary grooving, segregation during the vapor deposition of alloys, and the saturation limit of helium in crystalline deuterium. These simulations have found applications in the loading of fusion targets.



Extended by the application of tensile strength, a pillar of dideuterium transitions from a hexagonal closely packed lattice to a face-centered cubic lattice.

Publications
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Nanomaterials for Fusion Application Targets—

Alex Hamza (08-SI-004)

Abstract

The assembly of functional nanomaterials requires atomic-level control of the processes involved. Complex targets for the study of mix in burning hydrogen plasmas, nuclear physics in high-neutron-brightness environments, and fast-ignition inertial-confinement fusion require precisely placing nanoporous materials and small quantities of dopants inside a target capsule. In this project, innovative techniques will be developed for fabrication of these complex targets. Specifically, we will use a "chemistry in a capsule" approach to grow nanoporous materials inside a spherical target. We will develop methods for doping metal foams using both atomic layer deposition and ion implantation. Finally, we will investigate the structural evolution and mechanical properties of thick metal films.

An important long-term benefit of this effort will be the capability for design and assembly of tailored nanomaterials and nanostructures. More specifically, we will create the capability for assembly and manipulation of nanostructured materials in confined geometries with tailored composition and function. Because of the unique reactive, absorptive, mechanical, and optical properties of nanostructured materials, this capability will be broadly applicable in catalysis, hydrogen storage, advanced nuclear materials, corrosion-resistant coatings, and photonics.

Mission Relevance

This project supports LLNL's missions in national and energy security by developing the science and technology to fabricate complex targets for experiments to (1) understand boost physics, (2) investigate the dynamics of nuclear excited states, (3) pursue inertial-confinement fusion fast ignition, and (4) create new materials for catalysis, hydrogen storage, and self-healing nuclear reactor materials.

FY09 Accomplishments and Results

We have made significant progress in all areas of our proposed research. Specifically we (1) demonstrated filling, synthesizing, and doping of thin films of low-density carbon aerogels inside a capsule; (2) studied wetting of low-density carbon aerogels by liquid hydrogen and demonstrated that they can survive repeated wetting and freezing cycles via in situ x-rays; (3) developed mechanically robust carbon nanotube foams and demonstrated that doping of aerogels by atomic layer deposition can be controlled by surface functionalization; (4) measured the three-dimensional morphology of target components with nanometer precision using our unique "nanofinger;" (5) established a film stress–morphology correlation; and (6) developed a virtual sputter chamber, including atomic scale modeling of growth.

Proposed Work for FY10

In FY10 we will (1) continue to cast thin films of aerogels in target capsules and enhance liner uniformity by improving the aerogel process with lower vapor-pressure solvents, new chemistries and curing methods, and better injection control and by improving surface engineering with controlled wetting and adhesion; (2) continue to study the wetting of aerogels by liquid hydrogen, both inside and outside of a capsule, and check the validity of nondestructive in situ x-ray techniques by other methods; (3) continue to develop novel atomic-layer deposition precursor chemistries for high-atomic-number doping and area-selective atomic-layer deposition processes for aerogels and diamond both inside and outside of a capsule; and (4) demonstrate the assembly of a cryogenic fast-ignition target and deliver the virtual sputter chamber.

Publications

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Zepeda-Ruiz, L. A., et al., 2009. "Understanding the relation between stress and surface roughness in sputtered films: Kinetic Monte Carol simulations and experimental measurements." *Appl. Phys. Lett.* **95**, 151910. LLNL-JRNL-417093.

Dynamics of Material Motion and Transformation Following Localized Laser-Energy Deposition in Transparent Dielectrics—Stavros Demos (08-ERD-001)

Abstract

The objective of this project is to study the dynamic response of optical materials during laser-induced damage. The fundamental processes involved include solid-state material response to localized high temperature and pressure, energy transport through complex material phases, and material transport and lattice deformation. Using novel portable diagnostic instrumentation that can be deployed in host high-energy and high-power laser facilities, we will study the evolution of different types of damage events through their timeline. Time-resolved micro-shadowgraphy and microspectroscopy will be used in combination with different pump- and probe-laser sources to explore a wide range of relevant excitation conditions with adequate spatial and temporal resolution.

Our research will significantly enhance fundamental understanding of the processes involved during laser-induced damage in optical materials under operational conditions similar to those found in inertial-confinement fusion lasers. Specifically, we will investigate the timeline of events leading to the formation of bulk and surface damage sites, the kinetics of the ejecta, and the processes involved during damage growth. This work also will extend our current knowledge regarding the interaction of high-power laser light with large-bandgap dielectric materials and solid-state material response to confined energy deposition.

Mission Relevance

This project supports LLNL's national security mission by providing basic measurements to help quantify and predict the damage performance of optical materials for large-aperture laser systems and to devise solutions to cope with adverse effects. Furthermore, this project will help develop advanced material-processing methods and a new generation of materials with enhanced performance characteristics in support of the Laboratory's mission in breakthrough science and technology.

FY09 Accomplishments and Results

During FY09 we (1) acquired time-resolved images using a variety of imaging configurations through the entire timeline of dynamic events during damage initiation and crater formation for surface damage, as well as for crater expansion in surface damage growth in both fused silica and potassium dihydrogen phosphate; (2) measured the kinetics of the ejecta during surface damage initiation and growth; and (3) used existing modeling tools to explain experimental results. The results provided remarkably detailed information on the sequence of events—material modifications, pressure and shock wave propagation, and material ejection—that are responsible for crater formation and growth, furthering our understanding of the physics that leads to the appearance of damage sites under different excitation conditions.

Proposed Work for FY10

We will determine how the previously observed behavior depends on the material properties, including mechanical, thermodynamic, and crystalline structure. Specifically, we will (1) examine response during the damage timeline, including size and speed of ejecta and corresponding ejection times, properties of the shock front, and expansion speed of the absorbing front in various materials that could help establish the key relationships; (2) perform time-resolved Raman scattering measurements to probe the state of ejected material at various times; and (3) examine, using the same measurement techniques, the state of the absorbing front during the energy-deposition phase.

Publications

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Negres, R. A., et al., 2008. "Laser damage performance of $KD_{2-x}H_xPO_4$ crystals following x-ray irradiation." *Optic. Express* **16**, 16326. LLNL-JRNL-400735.

Tailored Ceramics for Lasers—Thomas Soules (08-ERD-006)

Abstract

Transparent ceramics have the demonstrated potential to enable solid-state heat-capacity lasers with world-record power for national security applications. Amplifier slabs made from such ceramics have been shown to perform flawlessly and robustly. The goal of this project is to develop methods for tailoring transparent ceramics for improved laser performance. This tailoring could include grading activator concentrations, introducing more

than one activator ion in different regions of a sample, modifying shapes, and using new materials. We will accomplish grading by introducing activators into the green structure before sintering. Methods for grading suspensions of different activator concentrations will be based on multilayer approaches. In all cases, tailored preforms will be fabricated and sintered. In addition, transparent ceramics based on new materials will be developed. This project will leverage state-of-the-art ceramic fabrication equipment at LLNL as well as the achievements of a previous LDRD project that demonstrated the ability to make small samples of transparent yttrium–aluminum–garnet (YAG) ceramics.

Because tailored transparent ceramic laser components have not been previously fabricated, this project, if successful, will not only provide methods for improving laser performance but will also generate significant intellectual property. We expect to develop techniques for achieving graded dopant concentrations across an aperture. This could remove preferential absorption near the edge during edge pumping or provide specified gain profiles. We will investigate guiding pump light to optically active regions and conducting heat away from the optically active region in a single composite ceramic. Another tailored ceramic design incorporates amplified spontaneous emission suppression integrally, enabling much larger aperture slabs of high-gain materials. In addition, new ceramic laser materials will be developed.

Mission Relevance

This project will develop new ways to enhance laser performance by taking advantage of the unique design flexibility afforded by ceramics and to possibly enable new, more compact and more efficient laser geometries for applications in stockpile stewardship and fusion energy, in support of the Laboratory's national and energy security missions.

FY09 Accomplishments and Results

In FY09 we (1) commissioned the large vacuum furnace for sintering transparent ceramic parts and completed the ceramic parts casting lab; (2) developed a new gel-casting process for making parts of arbitrary shape and size and filed a patent application for the process; (3) fabricated several transparent ceramic parts; (4) identified issues with starting material, phase impurities, and large parts as well as developed a method to classify particle size; (5) made composite parts by gel casting and filed a patent for this process; and (6) characterized and modeled neodymium diffusion in YAG ceramics.

Proposed Work for FY10

Now that we have established a process for making gel cast parts of arbitrary size and shape and have a furnace capable of vacuum firing large parts, in FY10 we plan to move from laboratory experiments to making useful laser parts. Specifically we will (1) optimize our present process, performing experiments to measure lasing and scattering on the final parts; (2) establish quality control on the raw material powder currently produced by our industrial partner; (3) scale the part sizes to over 100 × 100 × 10 mm; and (4) fabricate samples of graded ceramic parts and transparent ceramics, such as mixed cation ceramics suitable for broadband applications, from new materials.

Publications

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Fundamental Mechanisms Driving the Amorphous-to-Crystalline Phase Transformation—Nigel Browning (08-ERD-032)

Abstract

Many fast phase transformations are currently known only through before-and-after experiments coupled to theoretical models of the assumed mechanism. However, by directly correlating experiments with theory on the same time and length scales, the mechanisms actually responsible for the resulting transformed structures can be evaluated uniquely. We propose to combine unique experimental capabilities—a dynamic transmission electron microscope (DTEM) and an aberration-corrected TEM—with large-scale atomistic simulations to develop a fundamental atomic-scale understanding of reversible amorphous-to-crystalline phase transformations in materials such as $Ge_2Sb_2Te_5$, Sb_2Te, and GeSb. These alloys have tremendous technological potential as materials for next-generation nonvolatile memory devices.

The aim of this project is to understand fundamental phenomena at the heart of phase transformations in materials. This work has immediate technological implications because of our focus on phase-change semiconducting materials that are of interest for their potential in dramatically improving nonvolatile memory technology. Our work will also provide validation of modeling

tools used extensively at LLNL. This combination of advances in fundamental science and technological impact should result in papers published in leading journals.

Mission Relevance

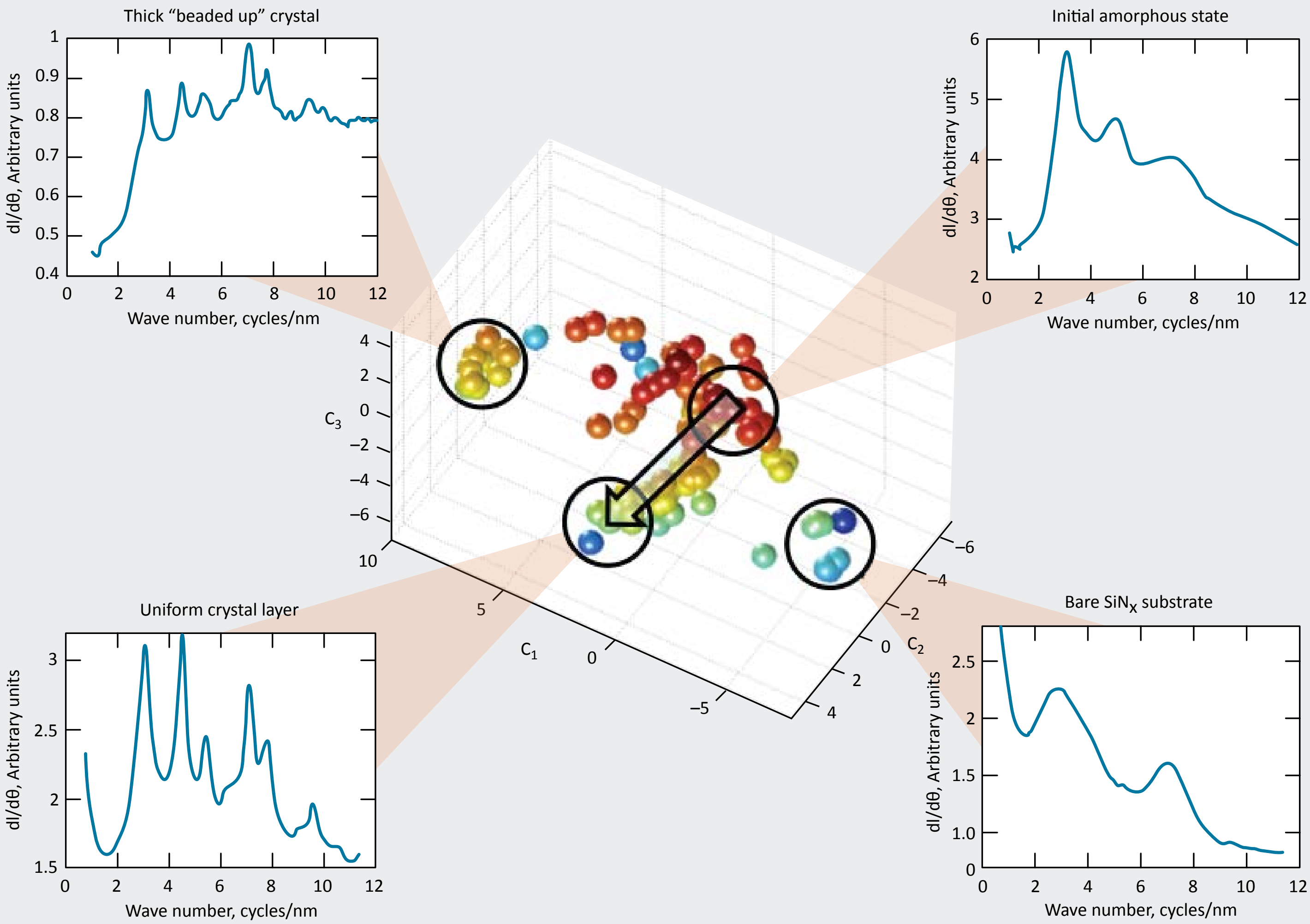
This project supports LLNL's mission in stockpile stewardship and expanding the use of DTEM for in situ diagnostics. The unprecedented overlap between experiment and theory for the materials being studied enables a robust experimental test of simulation codes used by LLNL for phase transformations in materials under extreme conditions.

FY09 Accomplishments and Results

As we developed sample preparations to study the crystalline-to-amorphous transformation, we found that nanostructured samples showed surprising spatial nonuniformity in their melt and resolidification and associated microstructural evolution, most likely caused by unexpected geometrical laser absorption effects. This is clearly relevant both to memory applications and to the basic scientific goals of the project, making it interesting enough that we chose to delay Sb_2Te_3 experiments. We found that molecular dynamics simulations predicted extremely high nucleation densities, on a scale directly observable in DTEM, and we used principal component analysis to extract independent information on nucleation, growth, and morphology changes from the nanosecond-scale diffraction data.

Proposed Work for FY10

Our FY09 results indicate that the governing kinetics are entirely dominated by grain growth, while the barrier for



Principal component analysis can extract independent information about nucleation, growth, and morphological changes in a multidimensional space while minimizing noise.

nucleation is too small to measure. Our goal in FY10 is to confirm these results and check their general applicability with different compositions. Specifically, we will (1) implement specimen geometries to study the reverse transition ex situ and in situ, (2) focus on developing increased simulation efficiency by using importance-sampling methods to concentrate the events on atoms belonging to subcritical nuclei and developing a first-principles database of configuration energies using density functional theory, and (3) perform the first large-scale simulations on the $Ge_2Sb_2Te_5$ alloy to compare with experiments.

Publications

Reed, B. W., et al., 2009. *Dynamic transmission electron microscopic investigation of telluride phase change materials.* Banff Meeting on Structural Dynamics, Banff, Alberta, Canada, Feb. 25–28, 2010. LLNL-ABS-420997.

Strain-Rate Effects on Plasticity and Defects—
James Hawreliak (08-ERD-033)

Abstract

This project will couple simulation and experiment to quantify the plastic response of dynamically compressed materials as a function of strain rate. We aim to accomplish two scientific firsts: perform large-scale molecular dynamics simulations to investigate ramp compression using the ATLAS supercomputer and measure the defect density and plastic response using in situ x-ray diffraction during the dynamic compression process. These experiments and simulations will help provide benchmarks for constitutive models of material response at ultrahigh pressures and strain rates. With development of fourth-generation x-ray sources, these techniques will position LLNL as a world leader in ultrafast materials science.

We expect that this project will result in three main accomplishments: (1) measurement of defects during dynamic compression, (2) lattice dependence of material response as a function of strain rate, and (3) microscopic understanding of plasticity in ramp compression using molecular dynamics simulations and experiments. All will be of large scientific impact—lattice behavior dependence on strain rate is an unexplored scientific field. Also, coupling of large-scale molecular dynamics simulations and x-ray diffraction experiments will provide a quantitative understanding of the fundamental physical phenomena that determine the building blocks of material properties, which is critical to creating predictive material models.

Mission Relevance

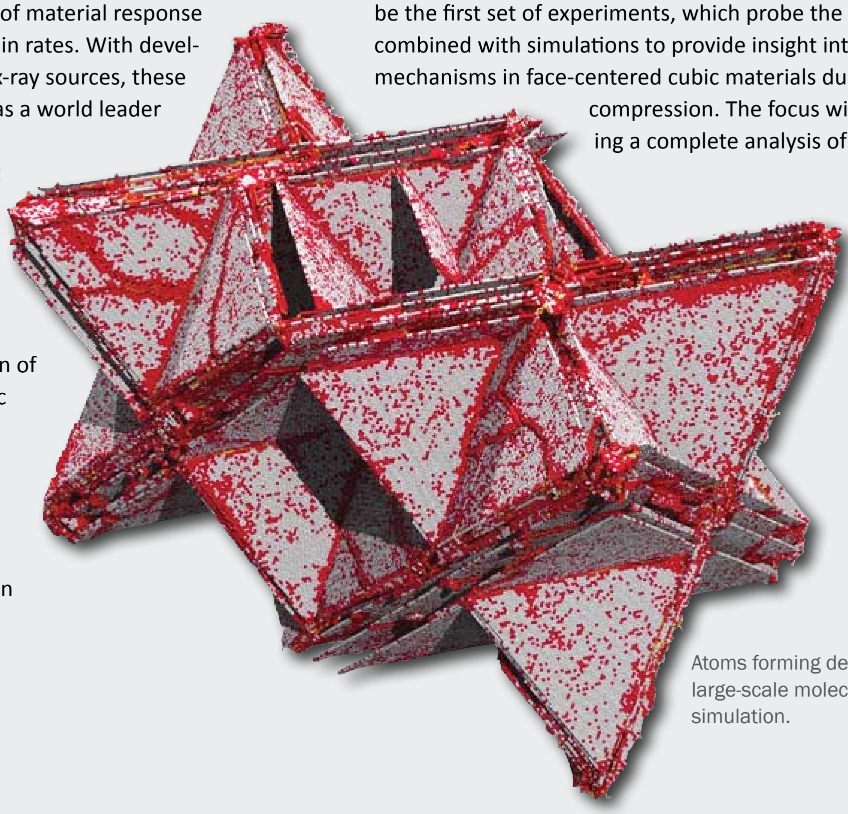
This work will aid in understanding dynamic loading of materials to high pressures. This understanding is important to Lawrence Livermore's core missions including stockpile stewardship and high-energy-density physics. Specific impact areas include advancement of ramp compression for future fusion-class laser systems, insight into atomistic properties that affect strength and equation of state, and better understanding of dislocation behavior, which is key to understanding plastic response and failure.

FY09 Accomplishments and Results

In FY09, we used tailored laser pulses on the Trident laser to ramp-compress single-crystal copper to approximately 200 Kbar in 5 ns. We used simultaneous x-ray diffraction and surface velocimetry to record both bulk and lattice response, and began analyzing the resultant data. We also continued large-scale molecular dynamics simulations, observing responses in defect generation and motion over four orders of magnitude in strain rate.

Proposed Work for FY10

In the final year of this project, the experimental and simulation results from FY09 will be analyzed and compared. This will be the first set of experiments, which probe the lattice in situ, combined with simulations to provide insight into the plastic mechanisms in face-centered cubic materials during ramp compression. The focus will be on providing a complete analysis of the large-scale



Atoms forming defects in a large-scale molecular dynamics simulation.

molecular dynamics simulations and experiments performed in FY09 to give a quantitative understanding of the microstructural dependence in copper from strain rate and provide insight into defect dependence on the loading pathway.

Publications

Hawreliak, J., 2009. *Investigating the plastic response in shock loaded solids at the lattice level using in-situ x-ray diffraction.* Intl. Conf. Plasticity 2009, St. Thomas, Virgin Islands, Jan. 3–8, 2009. LLNL-ABS-368734.

New Physical Mechanisms for Next-Generation Fusion-Laser Dynamic Sensors and Diagnostics—Evan Reed (08-ERD-034)

Abstract

Shock- and ramp-wave sensors are key to high-pressure research, but existing technologies for studying such waves have significant shortcomings. We are exploring new physical mechanisms upon which new classes of shock- and ramp-wave sensors can be based. Specifically, we will explore terahertz-frequency radiation emission as a strain-wave diagnostic. Such emission may result from piezoelectricity, optically active phase transitions, and other mechanisms. In addition to opening a fundamentally new basic-science frontier, this work may provide the scientific base for tools to address key issues in fusion-class lasers and stockpile stewardship. We will closely couple theory and experimentation to explore this relatively unexplored regime of ultrafast processes.

Our primary result will be elucidating the strain-wave processes that can be discerned from terahertz radiation emitted by the sensors, including the potentially unprecedented subpicosecond time resolution of strain waves. Existing techniques for measuring shock phenomena are limited in number and applicability. The fundamentally new technique we will explore is expected to generate publications in peer-reviewed journals.

Mission Relevance

This work supports LLNL's missions in national and energy security by providing new insight into shock-wave properties and phenomena in materials relevant to stockpile stewardship and fusion energy, and by potentially opening the door to new classes of sensors capable of spatially resolving strain or measuring strength in dynamic experiments.

FY09 Accomplishments and Results

In FY09 we conducted experiments at much higher pressures up to about 100 GPa using LLNL's Comet and Europa lasers, and we made the first observations of terahertz radiation generated from strong shocks. We also performed molecular dynamics simulations of phase transformations in piezoelectric cadmium selenide and gallium nitride to predict terahertz signals emitted when the material undergoes a phase transformation. These simulations help guide our experiments and have resulted in papers for peer-reviewed journal papers as well as invited talks.

Proposed Work for FY10

In FY10 we will conduct experiments at pressures in the 10- to 100-GPa range on materials, including gallium nitride and cadmium selenide. These experiments will determine the pressure range over which terahertz signals are reproducibly generated and can be used as diagnostics. Any evidence we find of a phase transformation from the terahertz signals will result in a publication reporting a new type of diagnostic for shock-induced materials transformations. We will document how terahertz radiation emission from shocked materials contains information about phase transformations and atomic transition pathways. This will be based on our molecular dynamics simulations of the wurtzite-to-rock-salt shock-induced phase transformation in cadmium selenide.

Publications

Armstrong, M. R., et al., in press. "Coherent THz electromagnetic radiation emission as a shock wave diagnostic and probe of ultrafast phase transformations." *Shock compression of condensed matter 2009,* American Institute of Physics, Melville, NY. LLNL-CONF-414924.

Armstrong, M. R., et al., 2009. "Observation of THz radiation coherently generated by strain waves." *Nat. Phys.* **5**, 285. LLNL-JRNL-407104.

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Reed, E. J., 2009. *Atomic transformation pathways from THz radiation generated by shock-induced phase transformations.* LLNL-JRNL-414925-DRAFT.

Do Brittle Metals Change Character Under Extreme Shock Conditions?—Damian Swift (08-ERD-038)

Abstract

When solids deform at high pressures and strain rates, different deformation mechanisms become active and existing ones are modified, changing strength properties. Physics-based models for investigating strength and tensile damage are still in their infancy. We propose to investigate the deformation of brittle metals under extreme conditions through shock-and-

release experiments on beryllium and magnesium involving in situ deformation measurements and sample recovery. We will perform shock-loading experiments in the 10- to 100-GPa regime on nanosecond time scales—where different flow behavior may occur—using laser ablation. We will obtain imaging velocity and displacement histories, along with x-ray diffraction and scattering data. In addition, simulations will be performed to complement the experiments.

We will obtain systematic measurements of compressive and tensile strength from velocity histories, and expect to measure defect densities from x-ray diffraction. Imaging records of velocity and displacement will allow the response to be related to the microstructure. Comparison with molecular and continuum dynamics simulations provides insight into changes in plastic flow mechanisms. In all, this project will provide a detailed understanding of extreme deformation at the crystal lattice level—important achievements for predictive simulations.

Mission Relevance

This project supports LLNL's missions in national and energy security by greatly improving the quantitative science underpinning predictive simulations involving compressive and tensile strength, including spall and ejecta and other important aspects of applications of dynamic loading that are foundational for stockpile stewardship and inertial-confinement fusion.

FY09 Accomplishments and Results

In FY09 we (1) used the crystal plasticity model in simulations of brittle-to-ductile transitions; (2) greatly improved the design of our shock experiments, resulting in more uniform loading and better control of pulse shape, and developed a strategy to infer defect populations from in-situ diffraction; (3) performed experiments on magnesium and beryllium at Livermore's Janus and Los Alamos' Trident lasers and, unexpectedly, recovered samples of beryllium, which we analyzed metallographically; (4) determined that magnesium shows ductile response under dynamic tension; and (5) acquired a finer pressure scan of the behavior of magnesium through the solid–solid transition.

Proposed Work for FY10

In FY10 we propose to (1) perform further experiments on magnesium and beryllium, completing our dynamic dataset, with a key goal of acquiring data on an additional orientation of magnesium crystal important for understanding the brittle–ductile transition; (2) perform metallography of recovered magnesium and beryllium samples to relate post-loading microstructure to the dynamic response; (3) measure defect densities from diffraction measurements made during dynamic loading, which will be the first direct measurements validating molecular dynamics simulations of defect generation; and (4) perform additional simulations of the experimental loading and recovery histories, which will be an initial study of the implications for inertial-confinement fusion and other extreme-loading systems.

Publications

Loomis, E., et al., 2009. "Plasticity effects in dynamically loaded nickel aluminide bicrystals." *Acta Materialia* **56**(14), 3647. LLNL-JRNL-409228.

Milathianaki, D., et al. 2009. "Shock-induced hcp to bcc phase transition in polycrystalline Mg." *Bull. Am. Phys. Soc.* **54**(8), Z2.00005. LLNL-ABS-410592.

Swift, D. C., 2009. "Flow Stress of V, Mo, Ta, and W on nanosecond time scales." *Bull. Am. Phys. Soc.* **54**(8), L3.00006. LLNL-PROC-415311.

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Swift, D. C., et al., 2009. "Shock formation and the ideal shape of ramp compression waves." *Phys. Rev. E* **78**, 066115. LLNL-JRNL-404275.

Chemical and Structural Modification and Figure Control During Glass Polishing—Tayyab Suratwala (08-ERD-055)

Abstract

The chemistry and physics involved in the controlled removal of material from a surface remains poorly understood. The objective of our proposed study is to develop a fundamental scientific understanding of chemical interactions that occur during glass polishing to help create more robust, deterministically fabricated optical surfaces. We will develop a fundamental physical understanding of material removal and the chemical and structural surface modifications that result from polishing. We will experimentally measure the removal rate and surface profile of optical surfaces as a function of various processing parameters, as well as characterize, distinguish, and potentially isolate impurities and surface structural imperfections.

This project will significantly advance our scientific knowledge of polishing and will be of general interest both to the precision optical and semiconductor industries. Specifically, the ability to deterministically finish an optical surface using a full-aperture tool will allow chip manufacturers or optical glass fabricators to achieve figure control of surface profile in a more deterministic

manner. We expect that our study also will enhance the understanding of chemical interactions that occur on the surface of glass during polishing, suggest viable post-treatments that can be used to alter or remove the chemically or structurally modified surface layer, and possibly provide post-treatment recipes to increase the damage threshold of glass surfaces.

Mission Relevance

The major benefit of this work is advances in a science-based approach to the fabrication of optical components, a critical enabling technology for high-energy, high-power, fusion-class laser systems. These lasers are essential to the Stockpile Stewardship Program's ability to understand weapons physics and materials under extreme conditions of temperature, pressure, and strain rate. The skills and scientific knowledge developed during this research will be relevant to advances in fabrication of advanced x-ray diagnostics used throughout the Stockpile Stewardship Program.

FY09 Accomplishments and Results

In FY09 we (1) modeled pressure distribution effects such as optic–lap mismatch, slope, and viscoelasticity; (2) measured the removal rate and surface profile as a function of polishing time, and repeated the measurements as a function of polishing process parameters; (3) developed a code that combines physical models for material removal to predict surface shape as a function of polishing parameters; (4) formed a science-based physical picture of the precursors of laser damage initiation—specifically, surface fractures, redeposits from etching or laser treatment, and chemical impurities in the Beilby layer; and (5) developed preliminary methods to mitigate these precursors by thermal or wet chemical means.

Proposed Work for FY10

In FY10 we will (1) complete pad and pitch polishing experiments and scale to larger optics, (2) quantify and combine phenomena affecting pressure distribution into our SurF code, which aims to predict the slope of the work piece instead of using it as a fitting parameter; (3) focus on understanding the Preston constant for the material removal process through various polishing experiments; (4) optimize the process and model for chemically etching fused silica surfaces for mitigating fracture precursors; (5) expand our mass transport model to predict performance of the etching process; (6) complete our thermal mitigation studies; and (7) measure the effect of physical parameters on the distribution of fracture surface luminescence.

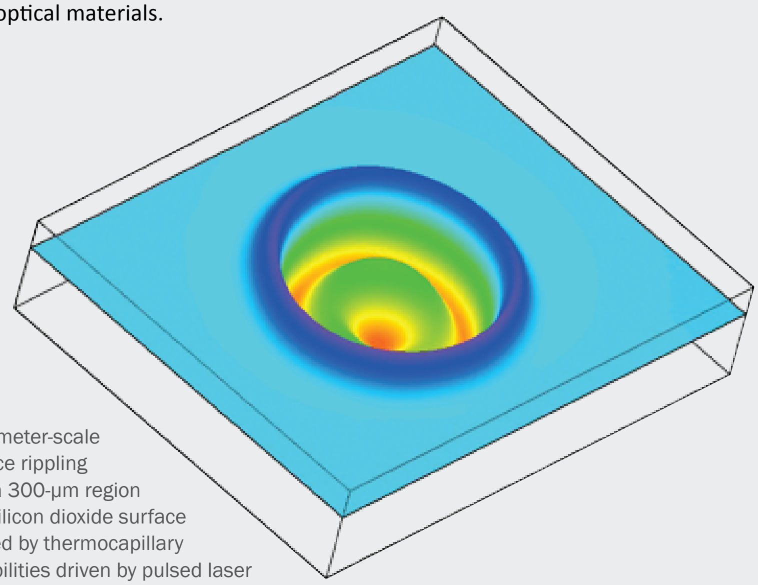
Physics of Local Reinitiation and Morphological Evolution of Mitigated Sites for Ultraviolet Optics—

Manyalibo Matthews (08-ERD-057)

Abstract

The objective of this work is to develop and implement a predictive, physics-based model to accurately control the mass transport and thermal-induced stress associated with laser-based material processing of high-fluence ultraviolet optics. Although mitigation strategies are under development, recent testing of high-fluence operations has revealed ever-more restrictive requirements for the mitigation process. In particular, mitigated site attributes associated with re-initiation, crack formation, and downstream intensification have been identified that require increasingly sophisticated physics models and experimental programs to address. The basic material science that governs these attributes is not well understood and lies outside existing predictive capabilities. We propose to integrate advanced diagnostics, materials characterization, and fundamental computational capability to clarify the origins and means to minimize or eliminate these effects.

The optics damage mitigation process employs laser-induced heating, melting, and evaporation to remove damaged material, heal subsurface cracks, smooth the surface, and anneal residual stress in the affected region. Development to date has been driven primarily by experimental work supported by empirical models that provide only rough guidance for control of temperature and material transport. Present technology has limited ability to control size, morphology, and damage threshold of a mitigated site, which fundamentally impacts yield and performance. We expect to develop a stronger scientific basis and advanced diagnostics to guide development of mitigation techniques and extend the understanding of laser interaction with optical materials.



Nanometer-scale surface rippling over a 300-μm region of a silicon dioxide surface caused by thermocapillary instabilities driven by pulsed laser heating.

Mission Relevance

High-energy laser systems are essential tools for the Stockpile Stewardship Program and other national security applications, as well as for developing inertial-confinement fusion as an advanced energy concept. High-energy lasers are also a key scientific element of high-energy-density research at LLNL. This work will provide an enabling technology for these systems to operate efficiently, reliably, and affordably with development of robust ultraviolet-optics mitigation technologies backed by reliable computational models.

FY09 Accomplishments and Results

We (1) developed an imaging technique to accurately measure the temperature and thermal conductivity of optical materials—silicon dioxide, aluminum oxide, lithium fluoride, and magnesium aluminate—heated with a carbon dioxide laser at spatial and temporal resolutions of 200 µm and 30 ms, respectively; (2) generated transient temperature maps and found them to be in excellent agreement with ALE3D thermal transport models, which included a multigroup diffusion model for radiation transport; (3) investigated microstructural evolution and residual stress in silicon dioxide caused by laser heating above glass transition using confocal Raman microscopy, achieving good agreement with predictions from ALE3D; and (4) used analytic models derived from a commercial fluid dynamics code to predict surface roughness relaxation caused by laser heating on optically damaged silicon dioxide surfaces.

Proposed Work for FY10

In FY10 we will (1) complete our combined hydrodynamics and propagation model connecting visco-capillary surface physics and evaporation on fused silica surfaces to downstream modulation of incident light, (2) develop vapor-phase transport and multigroup diffusion radiation approximations, (3) explore new approaches to mitigation involving active environments and mid-infrared irradiation using our modeling predictions, (4) probe evolution of the glass state and microstructure as it relates to residual defects and stress using characterization techniques such as confocal Raman and time-resolved photoluminescence microscopy, and (5) develop in situ diagnostics based on our thermographic probe for potential use in laser mitigation facilities.

Publications

Elhadj, S., et al., 2008. "High-temperature thermographic measurements of laser-heated silica." *J. Mater. Res.* **1137E**, 1137E00. LLNL-POST-367998.

Elhadj, S., et al., 2009. "High-temperature thermographic measurements of laser-heated silica." *Proc. SPIE* **7504**, 750419. LLNL-PRES-417032.

Guss, G. M., et al., 2009. "In situ monitoring of surface post-processing in large aperture fused silica optics with optical coherence tomography." *Appl. Optics* **47**(8), 4569. LLNL-JRNL-401368.

Matthews, M., et al., 2009. "Residual stress and damage-induced critical fracture on CO_2 laser-treated fused silica." *Proc. SPIE* **7504**, 750410. LLNL-PRES-381181.

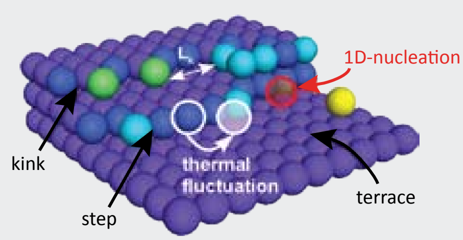
Shen, N., et al., 2009. "Study of CO_2 laser smoothing of surface roughness in fused silica." *Proc. SPIE* **7504**, 750411. LLNL-PRES-416935.

Yang, S., M. Matthews, and S. Elhadj, 2009. "Thermal transport in CO_2 laser-irradiated fused silica: In situ measurements and analysis." *J. Appl. Phys.* **106**(10), 103106. LLNL-JRNL-414595.

Kinetics of Weakly Fluctuating Crystal Surfaces: Beyond Classical Concepts—Luis Zepeda-Ruiz (08-LW-068)

Abstract

We will address a major discrepancy between the classical theory of crystal growth and molecular-scale observations of growth. We will generalize classical growth, dissolution, and ripening concepts to the case of weakly fluctuating steps on crystal faces with a unique combination of in situ atomic force microscopy experiments, kinetic Monte Carlo simulations, and analytical theory. For this generalization, we will measure and independently calculate the rate of kink nucleation and propagation (rather than their products only), step energies and propagation



Schematic representation of a terrace, step, and kinks on calcite crystal surface. Kinks are created either via movements of molecule on the step edge (thermal fluctuations) or attachment of new solute molecules from solution (1D-nucleation).

rates during crystal growth, and the dissolution of long step segments, as well as spatial and temporal correlation functions.

By building a new theoretical background, we will (1) determine the applicability limits of classical thermodynamic concepts, (2) describe kinetics in the weakly fluctuating systems beyond these limits, and (3) measure fundamental parameters directly related to molecular attachment and detachment frequencies. This project's results have direct applicability in a variety of areas such as crystal growth and epitaxy, geochemistry, mineralogy, biomineralization, and materials science concerned with coarsening, phase transitions, and dislocation phenomena.

Mission Relevance

This project supports stockpile science through predictive capabilities for high-explosive materials. It also supports energy security and environmental management through understanding mineral formation and biomolecule–mineral interactions in carbon and metals sequestration, and supports bioscience to improve human health through an understanding of the natural controls and pathologies in tissue mineralization.

FY09 Accomplishments and Results

In FY09 we (1) performed studies of calcite in aqueous solution using atomic force microscopy, (2) identified different step structures and measured kink generation and step-propagation rates, (3) compared kinetic Monte Carlo simulations with experimental results, and (4) showed that our kink-limited model offers a plausible explanation for reports of kinetic disequilibrium of trace-element signatures. Kinetic Monte Carlo simulations and high-resolution atomic force microscopy studies of step-edge structures and dynamics show that low-kink-density systems like calcite cannot be interpreted with traditional thermodynamic models based on minimization of Gibbs free energy, and also show that impurity–step interactions follow a different mechanism determined only by the kinetics of attachment and detachment.

Radiation-Tolerant Materials—Michael Fluss (09-SI-003)

Abstract

Uranium enrichment for light-water reactors and the breeding of plutonium and minor actinides are proliferation and security issues, while spent nuclear fuel is an environmental and security issue. We propose to investigate ultradeep burn-up materials that result in the minimization or elimination of fuel reprocessing from nuclear energy, sending only fission products to geological storage. For this research we intend to (1) perform ion-beam irradiations and post-irradiation characterization on nanoscale-structured radiation-resistant materials to produce atomic displacements while implanting helium and hydrogen in series or parallel, in ratios similar to that expected in the reactor environment; (2) model the ion-beam results with the purpose of extending these models to the reactor neutron environment of lower atomic-displacement rates and longer times; and (3) provide a firm scientific basis for baseline materials selections in advanced ultrahigh burn-up nuclear energy systems.

The metrics for success of this initiative are the discovery and understanding of the fundamental materials science necessary to realize ultrahigh-burn-up nuclear fission fuel and associated structural materials. The behavior of nanoscale-structured materials through modeling validated by ion-beam experiments will bridge both length scales from microscopic to macroscopic and time scales from days to decades in describing materials for ultrahigh burn-up. Key deliverables are both experimental radiation tools for the discovery of advanced radiation-resistant materials and simulation and modeling tools for the design, development, and deployment of an advanced nuclear fission-fuel technology of ultradeep burn-up.

Mission Relevance

Our proposed research supports Laboratory missions in both energy and national security. The elimination of reprocessing in the fuel cycle reduces cost and increases energy security. Materials for ultradeep burn-up of fission fuel are the key to the utilization of all the potential energy in uranium. This simple idea is the path to a sustainable nuclear fuel cycle that lowers the barriers of waste disposition, decreases the threat of proliferation, incorporates safeguards by design, and establishes economic competitiveness through sustainability and energy independence.

FY09 Accomplishments and Results

We (1) performed dual beam irradiations of oxide dispersion-strengthened specimens, iron–chromium, and iron specimens at the Joint Accelerators for Nano-science and Nuclear Simulation facility in France; (2) began analyzing these specimens using transmission electron microscopy and comparing the resultant data with that from unirradiated specimens; (3) developed techniques for fabricating micromechanical specimens; and (4) tested and installed components for irradiations at LLNL.

Proposed Work for FY10

In FY10 we will (1) characterize the microstructure that develops in oxide dispersion-strengthened materials under various ion beam radiation scenarios with helium, helium–iron, and hydrogen–helium–iron, then perform post-irradiation examination with transmission electron microscopy and micro-mechanical characterization, emphasizing a rate-theory approach to modeling the interaction of helium with the dispersed oxide particles; (2) continue advanced theory, simulation, and modeling, with emphasis on time-transcending methods and some support for continued modeling of the iron–chromium–helium ternary; and (3) perform limited validation and verification with iron and iron–chromium alloy experiments as comparison points for advanced modeling.

Publications

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Nanosecond Characterization of Dynamic Void Evolution in Porous Materials—Anthony Van Buuren (09-ERD-002)

Abstract

Very little is currently understood about how the morphology of nanofoams responds under shock conditions. Existing models of porous materials are believed to be well grounded experimentally at very low and very high levels of porosity. However, the models make inconsistent assumptions, and none have been verified in situ. Furthermore, model agreement over a broad range of compression is quite poor. We propose to characterize the morphology of nanofoams under dynamic (shocked) conditions and use these results to validate models of void evolution in the materials. We will quantify dynamic structural changes with a state-of-the-art, ultrafast, small-angle x-ray scattering system. Ultimately, we hope to obtain a predictive capability for these materials under extreme conditions as a function of initial structure and compression dynamics.

We will leverage LLNL's recent successful development of a capability for measuring small-angle x-ray scattering using a single x-ray pulse, which enables use of pump-probe experiments to measure structural changes in situ during a shock. We will apply these methods to nanofoams for the first time and expect to answer a major question: How reliable are existing theoretical models used to describe the compression of foams?

Mission Relevance

Key deliverables of this project include the ability to characterize the evolution of foam microstructures under shock conditions and validation of theoretical models, both of which are critical for future laser targets for stockpile stewardship and inertial-confinement fusion, in support of LLNL's national and energy security missions.

FY09 Accomplishments and Results

In FY09 we (1) determined initial characterization of the chemical composition and pore structure of a series of copper, gold, and carbon foams using x-ray absorption spectroscopy and small angle x-ray scattering; (2) compared the initial data to single pulse or time-resolved small-angle x-ray scattering measurements for the same carbon and copper foams—these experiments demonstrated the viability of pump-probe measurements to be preformed in FY10; and (3) established and tested a setup for laser-driven shock-loading experiments. This initial work will utilize the same methodology and equipment that will be used at the Advanced Photon Source at Argonne National Laboratory, but in a Livermore laboratory setting, giving us the ability to optimize this aspect of the experiment prior to deployment at the synchrotron.

Proposed Work for FY10

In FY10 we plan to (1) measure dynamic small-angle x-ray scattering from representative carbon foam at a single shock pressure to determine the time-dependent void evolution—this is a critical step in this project and will be used to determine if a laser upgrade of 5 to 10 J per pulse is needed, (2) compare results from the pump-probe scattering experiments to results from existing molecular dynamics and continuum simulations,

(3) calculate the expected small-angle x-ray scattering distribution from void distributions predicted by molecular dynamics simulations, and (4) measure the evolution of different types of carbon and copper foams (e.g., density and pore structure) at one shock pressure.

Understanding the Surface Properties That Lead to Optical Degradation in High-Fluence, High-Average-Power Optical Materials—Jeffrey Bude (09-ERD-003)

Abstract

Laser-induced surface damage to important optical materials limits the maximum operating fluence of fusion-class laser systems. Moreover, surface properties that limit optical performance are not well understood. The objective of this study is to develop a fundamental understanding of these surface properties in high-fluence, high-average-power optical materials. A suite of sensitive high-resolution optical techniques and advanced computational modeling will be employed to study the electronic and optical properties of dielectric surfaces at the nanoscale. We intend to clarify the links between surface properties, laser-induced surface damage, and the effects of long-term, high-fluence optical fluxes on damage resistance in optical materials.

We expect to (1) determine the physical origin of ultrafast photoluminescence from defects associated with damage in silica and determine if fast photoluminescence is a predictor of damage in other optical materials using confocal time-resolved photoluminescence imaging; (2) determine the effects of long-term, high-fluence optical exposure on the surface properties and damage resistance of optical materials; and (3) clarify the links between material properties, surface nanostructure, electronic structure, optical absorption, and high-fluence optical damage in optical materials. This work will guide development of damage-resistant optics and will help build an understanding of the limits of optical materials operated under high fluence, as well as an understanding of high-fluence, high-average-power conditions.

Mission Relevance

This research directly addresses stockpile stewardship and fusion energy challenges by optimizing large advanced laser systems. It will serve to establish science-based rules for optics reliability prediction, improve damage diagnostics, and suggest pathways to increase damage resistance in optical materials. More broadly, understanding defect-assisted absorption and material modification is a frontier problem in condensed matter physics.

FY09 Accomplishments and Results

In FY09, we made significant progress understanding electronic structure of the precursors of fast photoluminescence. Specifically, we (1) conducted initial studies on silica, quartz, potassium dihydrogen phosphate, and calcium fluoride, finding that fast photoluminescence is not unique to silica—it was detected in silica etch by-products (an important limitation for mitigation)—and identifying correlations between fast photoluminescence and damage; (2) developed a plausible, testable model for fast photoluminescence and used it to simulate and measure model systems for fast photoluminescence; (3) achieved initial results on silica fracture samples; (4) calibrated our stress platform; (5) measured micro-plasma emission during single shots; (6) performed molecular dynamics simulations of silica fracture; and (7) performed ab initio simulations of optical absorption on silica surfaces and nanoscale defect clusters.

Proposed Work for FY10

In FY10 we will (1) continue experiments and modeling that will help isolate the origin of fast photoluminescence in silica, other optical materials, and several model material systems and make correlations of fast photoluminescence to direct damage measurements; (2) perform experiments to link fracture stress intensity to fast photoluminescence and damage; (3) perform sub-damage optical stress experiments and characterize stress-induced material changes using techniques such as confocal fast photoluminescence, atomic force microscopy, scanning electron microscopy, and microplasma emission imaging; (4) continue molecular dynamics simulations of fracture in silica and extend to other materials; and (5) perform ab initio simulations of optical absorption for surfaces (including fractured surfaces) of silica and other materials.

Publications

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Laurence, T. L., et al., 2009. *Ultra-fast photoluminescence as a diagnostic for laser damage initiation.* 2009 SPIE Laser Damage Symp., Boulder, CO, Sept. 21–23, 2009. LLNL-PRES-416938.

Miller, P. E., et al., 2009. *Identification of laser damage precursors in fused silica optics.* 2009 SPIE Laser Damage Symp., Boulder, CO, Sept. 21–23, 2009. LLNL-ABS-413560

Shen, N., et al., 2009. *Isothermal anneal of damage precursors on fused silica surfaces.* 2009 SPIE Laser Damage Symp., Boulder, CO, Sept. 21–23, 2009. LLNL-POST-416936.

Multiresolution Adaptive Monte Carlo for Microstructure Simulations—Vasily Bulatov (09-ERD-005)

Abstract

The objective of our project is to extend the time and length scales of material microstructure simulations to those relevant for engineering applications. Our development will focus on the atomistic (lattice) Monte Carlo as a general and accurate framework and will rely on iron–copper and iron–chromium binary alloys as test bed material systems. Of principal interest is the kinetics of diffusive phase transformations, including nucleation and growth of precipitates, ordering, segregation, and the effects of continuous and/or pulsed irradiation drive on the same phenomena. Several novel methods will be developed that, in combination, will significantly enhance computational efficiency of microstructure simulations while maintaining or improving their accuracy.

We expect to develop a novel computational approach of multiresolution adaptive Monte Carlo that will extend the time horizon and length scales to accurate simulations of the kinetics of microstructure evolution in binary alloys. Eventually we will extend this approach to more complex materials relevant for engineering applications such as those used in nuclear reactors. Unlike existing phenomenological methods, our multiresolution approach is entirely self-consistent—on its fully refined level it reduces to a detailed atomistic representation. At the same time, our simulation approach links the fundamental mechanisms of atomic diffusion directly and seamlessly to alloy microstructure evolution on scales relevant for current and future engineering applications.

Mission Relevance

Our new simulation capability can find multiple applications in existing and emerging mission areas in which behavior of materials away from equilibrium is important, including national and energy security. For example, our new efficient methods and computer codes can be employed for computational extrapolation of material damage observed in an accelerated radiation test to the expected radiation resistance of the same material over its work life in nuclear reactors.

FY09 Accomplishments and Results

We (1) developed an exact mathematical algorithm for accelerating kinetic Monte Carlo simulations for a wide variety of systems whose evolution can be modeled as a continuous-time Markov chain process, (2) used the new algorithm to simulate diffusive phase transformations in binary metals alloys under conditions in which existing Monte Carlo simulations failed to reach relevant (long) time scales, (3) performed a large number of atomistic calculations to examine the origins of variations in atomic diffusion barriers in binary alloys as functions of local chemical composition and mechanical stress, and (4) used the results as parameters for an accurate Hamiltonian model for simulations of phase transformations in iron–copper and iron–chromium binary alloys.

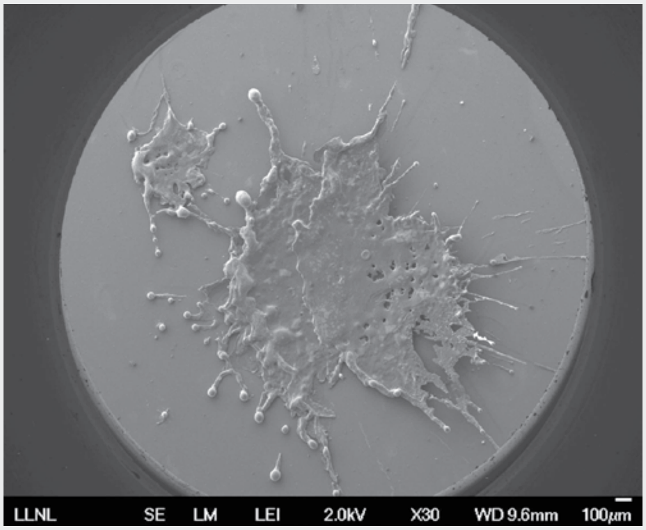
Proposed Work for FY10

In FY10 we will (1) run accelerated kinetic Monte Carlo simulations of the ABV lattice model of a binary alloy for a variety of different alloy Hamiltonians, temperatures, and alloy compositions; (2) use these simulations to select an optimal mathematical procedure for developing the lattice model as necessary for coarse-grained Monte Carlo simulations; (3) develop an algorithm and produce appropriate computer code for coarse-grained Monte Carlo, then run coarse-grained simulations, and compare the results to corresponding microscopic-lattice Monte Carlo simulations; and (4) analyze the effects of local stress on the vacancy migration barrier and compute the activation stress tensors for a binary metal alloy.

Collection of Refractory Debris from the National Ignition Facility for Stewardship-Relevant Measurements—Dawn Shaughnessy (09-ERD-026)

Abstract

Collecting solid debris from experiments conducted at the National Ignition Facility (NIF)—which has a far higher neutron flux than other facilities—will be required to measure cross sections of radiochemical detectors used to determine thermonuclear device performance. Such measurements hold



Molten debris generated at the Nevada Terawatt Facility captured on a witness plate for research into solid debris collection at Livermore's National Ignition Facility.

out the possibility of significantly reducing uncertainties in radiochemical data. This project will develop a system for collecting solid debris samples at fusion-class lasers for use in radiochemical analysis and measurement of cross sections relevant to stockpile stewardship. The distribution of the debris will first be determined through simulation and experiment. Next, several designs will be tested, and a priority list of stewardship-relevant measurements will be determined. The methodology will be benchmarked through measurement of yttrium cross sections, but ultimately a variety of radiochemical detectors will be evaluated.

If successful, this project will yield a prototype solid collector that can be fielded during early NIF shots for testing. If this new device significantly improves the acquisition and understanding of radiochemical data, as we expect, it could then be a candidate for future program support and thus be deployed in the NIF chamber for routine radiochemical measurements. Initially, we will consider several collector designs, then select the most promising ones and conduct testing at the NIF to evaluate collection efficiency and ease of insertion and extraction from this particular chamber. Once a prototype has been fully developed, measurements on the yttrium cross section will begin as ride-along experiments on other NIF shots.

Mission Relevance

This project supports LLNL's national security mission by reducing thermonuclear device uncertainties—a major goal of stockpile stewardship—by enabling solid collection to reliably measure cross sections, validate code calculations, and lower uncertainties in the interpretation of radiochemical data.

FY09 Accomplishments and Results

In FY09 we (1) began to model NIF capsule debris and test models with data we acquired from imaging and chemical analysis of disposable debris shields from the target chamber—once data are available, debris models will be adjusted, (2) evaluated the chemical nature of the debris through analyses of the disposable debris shields and blast shields that were covering other diagnostics during cryogenic shots—results show debris stays hot longer than expected and condenses as metallic species, and (3) performed sensitivity studies on potential stockpile stewardship measurements to prioritize a list of measurements. Collector designs have moved toward fielding a large plate at the end of the diagnostic instrument manipulator, and experiments on OMEGA will not be necessary if we continue to receive plates fielded in NIF.

Proposed Work for FY10

In FY10 we plan to (1) validate a final solid collection design based on viable designs obtained from our collaborators; (2) interface with NIF engineers on collector insertion and extraction options, which will likely reduce the number of viable designs once considerations for actually fielding an instrument at NIF have been made; (3) perform material compatibility tests and ablation tests on thin slat films and metal foams at appropriate photon facilities in an effort to determine the optimal materials to use for collection at NIF; and (4) construct a prototype collector for fielding at the OMEGA Laser Facility at the University of Rochester that will be used for further testing if needed.

Publications

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Magnetorheological Finishing for Large-Aperture, High-Fluence Optical Applications—Joseph Menapace (09-ERD-049)

Abstract

The goal of this project is to understand the magnetorheological finishing (MRF) processes governing the deterministic removal of material from, and achieving figure control on, optical surfaces and how these processes affect the manufacture of precise, high-fluence optics for inertial confinement fusion and other high-power laser systems. Specifically, we will (1) understand the details of MRF material removal on free-form optics so that state-of-the-art MRF protocols can be designed and developed to

make curved, meter-size optics; (2) develop new MRF polishing slurries and protocols to polish novel crystalline optical materials that are important for inertial-confinement fusion laser systems as frequency converters and lasing media; and (3) investigate the potential for using MRF to precisely polish out or mitigate flaws and damage on high-fluence optical materials.

This study will greatly enhance the scientific knowledge of MRF polishing, which has applications in precision optics, space science, and semiconductors. Specifically, the ability to deterministically finish an optical surface using a sub-aperture tool will allow optical glass fabricators to improve the figure of an optic in a more repeatable, less iterative, more economical, and more deterministic manner. We will also enhance the understanding of advanced sub-aperture polishing that can be used to remove damage and compensate for short-range internal flaws in optics artifacts that limit the suitability of small- and large-aperture optical materials in high-fluence, high-repetition-rate laser applications.

Mission Relevance

This project supports the Laboratory's missions in national and energy security by expanding the knowledge base for fabricating optical components critical to the high-energy, high-power, fusion-class laser systems used to validate complex coupled-physics computer simulations, including codes used in place of nuclear stockpile testing.

FY09 Accomplishments and Results

We (1) completed subscale free-form optics for MRF investigations; (2) designed and fabricated initial metrology fixtures and protocols; (3) performed final polishing of four off-axis aspheres; (4) obtained laser damage tests results with potassium dihydrogen phosphate (KDP) polished by MRF, achieving a fourfold improvement, in the infrared and visible-light spectra, over single-point diamond turning; (5) started tests on magnetorheological fluid stability for KDP polishing using laser-based non-contact diagnostics; (6) designed and developed a new magnetorheological fluid formulation for polishing KDP using MRF; and (7) obtained a superior optical finish—a surface roughness of only 6 Å—on KDP.

Proposed Work for FY10

In FY10 we will (1) design protocols and measure surface figure on curved, ground and polished subscale fused-silica specimens; (2) conduct MRF damage removal and final polishing using large and small MRF wheels and sub-aperture pad-polishing heads; (3) develop baseline MRF polishing processes for curved optics; (4) transition activities to large-aperture MRF; (5) refine our metrology and MRF software for polishing titanium–sapphire and KDP optics; (6) test and refine MRF fluids and delivery system stability for new nonaqueous MRF fluids; (7) damage-test optics made using new fluid formulations; and (9) begin scale-up for polishing large KDP optics.

Publications

Menapace, J. A., P. R. Ehrmann, and R. C. Bickel, 2009. *Magnetorheological finishing (MRF) of potassium dihydrogen phosphate (KDP) crystals: Nonaqueous fluids development, optical finish, and laser damage performance at 1064 nm and 532 nm.* SPIE Laser Damage Symp., Boulder, CO, Sept. 21–23, 2009. LLNL-PRES-414344.

Characterization of Tritium Uptake and Release by Inertial-Confinement Fusion Reactor Materials—James Fair (09-ERD-050)

Abstract

We will quantify the uptake and release of tritium and other key laser inertial-confinement fusion reactor materials for a range of surface preparation, exposure, and decontamination conditions expected at a typical facility. Data produced by this project will form the basis for designing and implementing tritium decontamination processes by systematically exploring tritium uptake and release in laboratory-scale packed-bed reactors and full-scale fusion-class laser optic enclosures. Key outputs will be mass transfer coefficients, other rate constants, and adsorption isotherms. The study will also characterize local electronic sensing as a method for directly measuring surface tritium activity and seek measures to maximize the availability of fusion facilities, significantly decreasing operating cost.

We expect to produce the ability to (1) predict tritium release rates under controlled decontamination conditions, (2) predict tritium uptake rates under known exposure conditions, and (3) accurately and precisely measure surface tritium concentration on inertial-confinement fusion reactor components using direct electronic sensing devices. These results will form the technical basis upon which reliable and safe tritium decontamination subsystems and processes for laser inertial-confinement fusion reactors can be efficiently developed, implemented, and controlled.

Mission Relevance

This project supports LLNL's national security mission by providing experimental data from fusion-class laser systems to validate complex coupled-physics computer simulations for stockpile stewardship, and by substantially increasing our understanding of the behavior of tritium and tritiated compounds as they interact with optical components associated with large inertial-confinement fusion laser systems.

FY09 Accomplishments and Results

In FY09 we (1) developed detailed experimental plans and codified them into formal operating procedures for a packed-bed reactor system that was built and commissioned; (2) characterized surface activity meters and found them to perform adequately and in accordance with suppliers' claims; (3) addressed challenges in obtaining suitable gold coatings for reactor interior surfaces and resolved delays in obtaining approval of the system safety analysis; (4) developed baseline models, including mass transfer coefficient estimates from computation fluid dynamics modeling, and determined they describe published inertial-confinement fusion chamber effluent tritium concentrations well; and (5) determined that the scientific literature provided good estimates of tritium isotope exchange with potassium dihydrogen phosphate, a key nonlinear optical material used for frequency conversion in inertial-confinement lasers.

Proposed Work for FY10

In FY10 we will (1) continue characterization of tritium uptake and release for a variety of materials with various surface preparations, (2) determine mass transfer coefficients for a number of inertial-confinement fusion reactor subsystems under normal purge conditions, (3) refine and tailor numerical models to specific inertial-confinement fusion reactor subsystems, and (4) explore the effects of high initial tritium concentration and surface organic contamination on tritium uptake for fusion reactor materials.

Methods for Mitigation of Damage to Multilayer Mirrors—Christopher Stolz (09-ERD-051)

Abstract

The objective of our proposed study is to develop methods to arrest damage growth in optical interference coatings. This damage is caused by laser-induced fracture and absorption from sub-stoichiometric coating materials. Advancements in increasing mirror fluence survivability have focused on material selection, absorption and defect reduction, and laser conditioning. Currently, state-of-the-art mirror coatings are limited by a few growth sites, suggesting the possibility of a localized mitigation solution. We will explore laser-based and mechanical mitigation methods coupled with an effort to understand thin-film properties, advanced electric-field modeling, and downstream-modulation modeling. We will validate site stability with laser damage testing and microscopy.

We expect to determine a thin-film mitigation process that will increase the resistance of laser transport mirrors to beam damage. Electric-field modeling will determine the proper film boundary to minimize electric field effects. Beam-modulation modeling will determine the proper mitigation geometry for a reflective component. Once this process is established, it will be validated on mirrors suitable for use on fusion-class lasers. A second phase of this proposal will be devoted to reducing defects during coating deposition and an increased understanding of the role of the substrate quality (scratches and digs) and subsurface damage on the resistance of mirrors to laser damage.

Mission Relevance

Transport mirrors are the fluence-limiting component in the fundamental wavelength section of advanced fusion-class lasers. Interest in reconfiguring these lasers to the second harmonic to realize even higher fusion gains elevates transport mirrors to the fluence-limiting optical component of the entire laser system. Fusion-class lasers are an essential tool for the Stockpile Stewardship Program and other national security applications, as well as for inertial-confinement fusion as an advanced energy concept for energy security and independence.

FY09 Accomplishments and Results

We devised a laser-based mitigation method that uses femtosecond laser machining and that does not cause damage at laser fluences up to 40 J/cm^2. This is the first coating mitigation technique that allows us to exceed the usual damage threshold (25 J/cm^2) of large-aperture mirrors. We also developed a finite-element model to evaluate the electric field within different mitigation feature shapes. A conical pit with a 30° cone angle was determined to have the lowest average light intensification.

Proposed Work for FY10

In FY10 we intend to (1) construct a rotary vane particulate filter that can be installed in a deposition chamber to reduce coating defects, (2) explore the feasibility of laser plume heating as another way to reduce coating defects, (3) determine a mitigation process with minimal cracking and absorption of the film for optimization to survive a laser intensity of 25 J/cm^2 (3 ns at 1064 nm), and (4) determine a correlation between scratch dimensions and laser stability.

Biomolecule Directed Synthesis of Highly Ordered, Nanostructured Porous Zinc Oxide—Thomas Han (09-LW-024)

Abstract

Zinc oxide (ZnO) is an important group II–IV n-type semiconductor with important optical and piezoelectric properties. Despite this promise, however, progress in using the material is limited by the current inability to control surface area and architecture. In this proposal, we aim to develop a new methodology to synthesize highly ordered, nanostructured ZnO with a high surface area. To this end, we will use a phage-display

technique employing the M13 bacteriophage to identify unique sets of small peptides that can readily bind and nucleate ZnO nanocrystals. The identified peptides will be covalently bonded to structure-directing surfactants and polymers. The newly synthesized biopolymer will be used to template ZnO nanocrystals, which will adopt the three-dimensional structure of the self-assembling biopolymer.

If successful, this project will lead to highly ordered, high-surface-area, mesoporous ZnO, which could have a significant impact in the fields of ultraviolet-light-emitting diodes, lasers, photovoltaic solar cells, gas sensors, and biosensors, among other applications. Furthermore, this novel synthetic technique can be extended to the generation of unique three-dimensional materials such as high-surface-area explosive and chemical-warfare sorbents, biocompatible porous solids for bone replacement, novel materials for fuel cells and photovoltaic solar cells, and fracture-resistance shields and armor plate materials. We also expect this work to generate publications in the peer-reviewed literature.

Mission Relevance

This project supports LLNL's national security mission by creating the capability to generate new materials for fusion targets and explosive detectors and sorbents, and supports the energy security mission by helping synthesize novel materials for photovoltaic solar and fuel cells.

FY09 Accomplishments and Results

In FY09 we successfully (1) used phase-display techniques to identify and isolate new peptide sequences that specifically bind to ZnO crystals, (2) developed optimal synthesis conditions of ZnO nanocrystals and reproducibly synthesized ZnO nanowire arrays—this platform will be the basis for studying the effects of peptides during growth of ZnO nanocrystals, and (3) synthesized ZnO nanocrystals in the presence of newly acquired peptides.

Proposed Work for FY10

In FY10 we will (1) covalently bond peptides that nucleate ZnO onto three-dimensional structure-forming polymers and Brij 58 and P123 copolymers; (2) study the self-assembling behavior of these new biopolymers; (3) develop a new scheme for synthesizing mesoporous ZnO using peptide functionalized polymers; (4) fully characterize the newly synthesized materials using x-ray diffraction, scanning electron microscopy, transmission electron microscopy, and surface area analysis; and (5) continue exploring our newly synthesized high-surface-area ZnO templated on carbon aerogel. Provided we meet all of these goals, we will make electrical measurements using mesoporous ZnO to test its suitability as a photovoltaic cell.

MATHEMATICS AND COMPUTING SCIENCES

Laboratory Directed Research and Development

A Novel Structure-Driven Approach to Sequence Pattern Definition for Remote Homology Detection—
Adam Zemla (06-ERD-059)

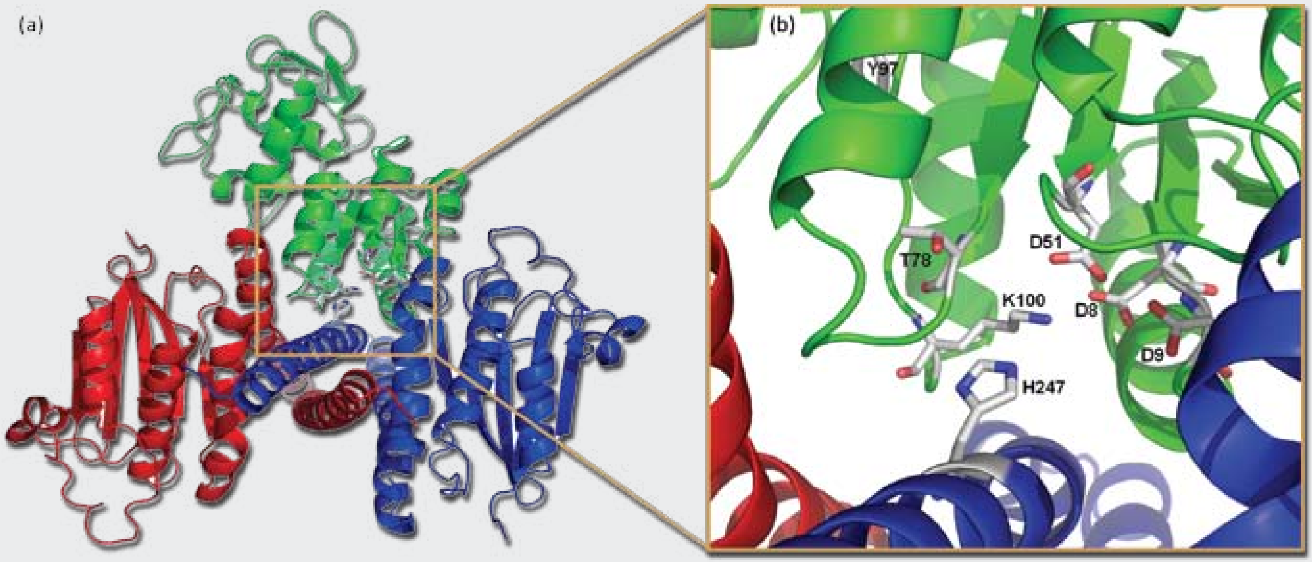
Abstract

In this project we will design, develop, test, and demonstrate an algorithm for detecting remote protein homology—an important need in protein structure modeling, functional assignment, sequence variability, and the rational design of diagnostics, therapeutics, and vaccines. This work will provide a method to assign distantly homologous proteins to structural families, and will enable efficient structure-driven identification of domain fusion proteins. We will devise sequence patterns representing structure fragments and test whether the patterns can detect known family members in the Protein Databank database, then use patterns to predict structures for up to 200 *Yersinia pestis* virulence-associated proteins. We will use laboratory methods to validate our predictions and refine the algorithm.

We will devise an algorithm for automatically generating sequence patterns that embody essential protein structure information. This achievement will immediately impact the characterization of virulence proteins from one of the most important biothreat agents, *Y. pestis*, which causes plague. A longer-term application of our algorithm is the three-dimensional modeling and characterization of proteins from all pathogens of interest in biodefense. Most significantly, this could lead to more effective signatures for identification of biothreat agents. The algorithm also will be of general use for proteins that could not otherwise be characterized.

Mission Relevance
Our work supports LLNL's mission in national security by establishing a computational capability with biodefense applications in (1) detecting and characterizing virulence proteins, (2) constructing a pathogen protein phylogeny, (3) analyzing sequence variability in rapidly evolving virus genomes, and (4) aiding the rational design of diagnostics, therapeutics, and vaccines.

FY09 Accomplishments and Results
We developed a structure-driven system for distant homology detection and domain fusion-based prediction that is capable of making links between proteins (interacting partners) that were previously difficult to identify. We also completed development of the algorithm that for any given protein structure constructs structure-driven pattern data—profiles and position-specific scoring matrices—for pattern-based homology searches and refinement of calculated alignments. Our novel algorithms for domain fusion-based predictions and pattern-based homology analysis helped several research efforts, for example to make models of a two-component (SpaK–SpaR) system and reconstruct links between interacting partners from the *Y. pestis* autoinducer-2



The domain fusion-based homology model of a SpaK–SpaR complex (a), and close-up view of interacting residues (SpaK–H247 and SpaR–D8, D9, D51) believed to mediate transfer of a phosphate group from SpaK to SpaR (b).

quorum-sensing network. These technologies will also be supported by the Defense Threat Reduction Agency for its Transformation Medical Technologies Initiative, where our algorithms will play a significant role in protein structure modeling, analysis, and annotation efforts.

Publications

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Knowledge-Based Coreference Resolution—
David Hysom (07-ERD-027)

Abstract

Extracting knowledge buried within unstructured electronic documents is becoming an increasingly critical issue to the intelligence community. Millions of such documents are created daily, but obtaining knowledge from them requires identifying relevant documents, recognizing real-world entities, determining relationships among entities, extracting events, identifying when the same event is discussed in multiple documents, and providing a summary of events contained within a collection. One critical step not being addressed by the larger community is knowledge-based, non-pronoun, non-proper-name (NPNPR) coreference resolution. This proposal will address this by leveraging the unique capabilities of LLNL, including work in graph-based entity disambiguation.

To meet our goal of making significant improvements to NPNPR coreference resolution, we will develop novel research algorithms to create concept-independent signatures from documents and graphs and to scalably compare individual signatures and decide individual equivalence. We will develop algorithms to more accurately resolve NPNPR using semantic graphs and other sources as our external knowledge base. These algorithms

will perform significantly better than state-of-the-art coreference resolution techniques and are expected to provide accuracies greater than 75% for NPNPR coreferences.

Mission Relevance

By developing advanced text-analysis algorithms that will help analysts extract knowledge from massive volumes of text documents in counterterrorism and other homeland security applications, this project supports the Laboratory's national security mission.

FY09 Accomplishments and Results

We (1) began extending entity signature development; (2) explored bootstrapping for automated annotation of training and test sets and knowledge acquisition, with an emphasis on domain independence; and (3) continued development of new algorithms to acquire external semantic knowledge. The successful conclusion of this project brought a new capability to LLNL and to the academic community through its release as open source. This project's completed code was integrated into the Laboratory's LexisNexis-related efforts and the Counterproliferation Analysis and Planning System.

Publications

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Advanced Computational Techniques for Uncertainty Quantification—Charles Tong (07-ERD-028)

Abstract

This project is aimed at developing advanced uncertainty quantification methods that can efficiently and accurately handle large-scale multiphysics simulations distinguished by large numbers of inputs and expensive evaluations. This research aligns well with Lawrence Livermore's increased emphasis on modeling and simulation, and the technologies developed will benefit many Laboratory simulation-based applications, as well as new initiatives such as the DOE Global Nuclear Energy Partnership program.

We will focus our algorithm research and development effort on (1) derivative-based global sensitivity analysis, (2) sensitivity analysis for high-dimensional problems, (3) new response surface methods, and (4) probabilistic risk analysis. We anticipate that our research results will be published in journals and conference proceedings, and the developed software will find immediate application to LLNL applications as well as to the broad scientific community.

Mission Relevance

Our project aligns well with the Laboratory's goal of advancing the state of the art in large-scale simulations, on which the Stockpile Stewardship Program is based. It also will be useful in support of the Global Nuclear Energy Partnership initiative and will help fulfill the Laboratory's mission in energy security. In addition, this research effort will leverage the Laboratory's current expertise in local and global sensitivity analyses and keep it at the forefront of high-consequence, high-fidelity, and high-dimensional simulation models.

FY09 Accomplishments and Results

In FY09 we (1) developed and implemented a mathematical framework within the PSUADE (Problem Solving Environment for Uncertainty Analysis and Design Exploration) software laboratory based on adaptive geometric refinement with application to response surface analysis and risk analysis, (2) demonstrated dimension-reduction techniques in a simulation of the effect of an earthquake upon a nuclear reactor using a soil and foundation structure interaction system—this showed that the uncertainties in soil properties are the major contributors of the output variabilities, and (3) partnered with the University of California at Santa Cruz on an extensive review of high-dimension reduction methods and use of the Bayesian additive regression tree method. The successful conclusion of this project has enabled us to apply more robust uncertainty quantification methods to important applications such as stockpile stewardship and environmental modeling. In particular, this project has demonstrated the advantages of adaptive sample refinement (i.e., add sample points only when needed) and a multi-algorithmic approach (i.e., use multiple methods to validate the uncertainty quantification analysis results) to improve efficiency and robustness of uncertainty quantification methods.

Publications

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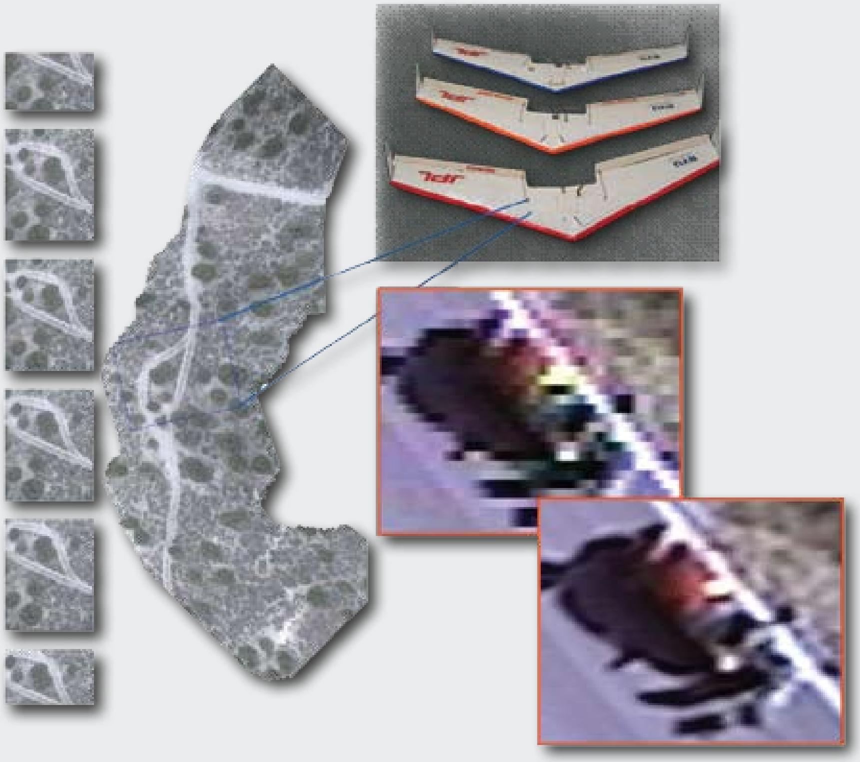
VidCharts: Real-Time Algorithms for Large-Scale Video Analysis, Compression, and Visualization—

Mark Duchaineau (07-ERD-035)

Abstract

This project aims to produce techniques for processing huge streams of imagery for national security applications. Our core technical ideas include a novel algorithm to compute dense image correspondences and a progressive, hierarchical processing framework. Leveraging large-data work done at the Laboratory in support of massive simulations, we will produce



Real-time dense correspondence enables mosaics of wilderness rescue drone videos and resolution enhancement of areas of interest. These images show single-frame and multiple-frame enhancement.

a prototype automatic visual summary and drill-down system to allow hours of video to be analyzed accurately in minutes. This technology has the potential to accelerate, by orders of magnitude, the human-analysis tasks of categorizing, indexing, annotating, and otherwise managing the petabytes of video data being generated worldwide each day.

If successful, this project will result in VidCharts, a prototype visual indexing system for huge video streams, including scene segmentation, pan/zoom/mover analysis, space–time drill-down, visualization of complex moving objects in the summary view, and three-dimensional (3D) scene and camera parameter extractions. In our system, processing speeds will be accelerated by orders of magnitude using both novel streaming hardware optimizations and the progressive, multiresolution streaming algorithm pipelines developed in LLNL's large-data research efforts. Furthermore, our system will yield over a thousand-fold compression with enhanced quality for repeated imaging of a scene from a moving camera. The project also aims to create the first scalable video content indexing and query system.

Mission Relevance

The project supports the Laboratory's national security mission, particularly arms control and nonproliferation, which are the most urgent and critical application areas for new software systems to accelerate the accurate analysis and management of huge streams of imagery. Numerous monitoring, tracking, discovery, and operational activities fall within this application area.

FY09 Accomplishments and Results

In FY09 we focused on the 3D-from-video application and introspective error analysis and feedback to the dense correspondence algorithm that has been at the heart of this project. The 3D work has resulted in a number of results, including enhanced depth estimation, camera pose estimation, silhouette extraction, camera parameter error classification, real-time super-resolution generation, and interactive mosaic generation as a visual summary of, for instance, aerial video from a search and rescue operation. This project has spawned a number of efforts supported by the Department of Defense and DOE in the areas of large-scale video processing, 3D from video, wide-area activity analysis for nonproliferation applications, and the high compression of persistent surveillance imagery.

Publications

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Software Security Analysis—Daniel Quinlan (07-ERD-057)

Abstract

Lawrence Livermore, as well as the DOE, obtains software from a wide variety of sources, both as binaries and source code. Currently, LLNL has limited ability to determine if such software is free from either intentional or unintentional security defects. Furthermore, existing security-analysis algorithms and techniques do not exploit large-scale parallelism. Leveraging LLNL's unique parallel-computing technology to address large-scale program analysis problems, we propose research on the security analysis of software in both binary and source-code form. This project will help the Laboratory build internal expertise in software security assurance, including mechanisms for the automated source-to-source transformation of vulnerable code to secure code.

We expect this project to greatly increase LLNL's ability to construct and maintain highly secure and reliable software systems. We plan to release tools developed in this project through the open-source channel so that they also benefit other researchers and tool developers in building their own binary and source-code analysis tools. At a more fundamental level, this project also will advance our understanding in building practical and effective analysis tools for binary and source-code applications. Our work builds on existing collaborations with Argonne National Laboratory and several universities to support a program-analysis framework able to handle compilation and analysis of LLNL's largest-scale Advanced Simulation and Computing applications.

Mission Relevance

This project supports LLNL's national security mission by improving the Laboratory's cybersecurity infrastructure with tools to support the general analysis and reverse engineering of outside software. Our work also will create a significant level of internal expertise in software security analysis.

FY09 Accomplishments and Results

In FY09 our work resulted in improved development of Compass for the static analysis of security vulnerabilities in source code, including developing new Compass rules in collaborations with Carnegie Mellon University. We also improved our binary analysis work in the ROSE compiler framework—for which we received an R&D 100 Award—and made it part of our collaborations with other external research groups. This project resulted in new collaborations with U.S. government cybersecurity groups focused on the general analysis of software security.

Publications

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Quinlan, D., et al., 2006. *Support for whole-program analysis and the verification of the one-definition rule in C++.* Static Analysis Summit, Gaithersburg, MA, June 29, 2006. UCRL-CONF-222122.

Verification and Validation of Radiation Hydrodynamics for Astrophysical Applications—Louis Howell (07-ERD-061)

Abstract

With this project, we intend to verify and validate an adaptive-mesh radiation hydrodynamics code with applications in astrophysics and high-energy-density physics. Verification tests will include uncomplicated problems with known or analytic solutions that will be used to determine accuracy of the numerical solutions. These tests will be applied to code units (e.g., hydrodynamics) and, as possible, to integrated radiation-hydrodynamics simulations. Verification also will include more complex tests (e.g., the crooked-pipe test). Validation will employ data from actual experiments in collaboration with Stony Brook University and the Computational Astrophysics Consortium.

The immediate result of this work will be increased understanding of simulation accuracy of the adaptive-mesh radiation–hydrodynamics code for particular astrophysics problems, including supernovae explosions, with a focus on radiating shock instabilities. These instabilities are of great interest to the Stockpile Stewardship Program. Another expected result is an advancement in methodology for validating such code.

Mission Relevance

This project supports stockpile stewardship by developing and applying new verification and validation methods for astrophysical radiation hydrodynamics to quantify the uncertainties in large-scale simulations for NNSA applications.

FY09 Accomplishments and Results

In FY09, we (1) added new radiation problems to our verification test suite, including emission from a radiating sphere and both gray and multigroup versions of a test of the coupling between fluid and radiation; (2) compared results obtained with this test suite with an analytic solution to the radiating sphere and found excellent agreement, showing that the multigroup solution of the coupling test approaches the gray solution as a limit; and (3) ran radiating-shock problems and found significant differences between published results using the ZEUS-MP code and current tests using the codes Castro and V2D. In summary, this project developed several verification tests for simulations of hydrodynamics, radiation diffusion, and coupling between the two and began to explore simulations of radiating shocks using analysis and code-to-code comparisons. These studies are particularly relevant to verification of the Castro adaptive-mesh radiation-hydrodynamics code, which is supported by the DOE Office of Science. The issues raised in this project will continue to be explored under efforts to apply Castro to simulations in astrophysics.

Storage-Intensive Supercomputing—Maya Gokhale (07-ERD-063)

Abstract
This project addresses efficient computation of data-intensive problems in national security and basic science by advancing storage-intensive supercomputing capabilities. We propose to (1) develop new algorithms and applications to solve large-scale data analytics problems on this class of architectures; (2) explore new programming models, tools, and libraries to address the difficulty in developing software applications for storage-intensive architectures; (3) develop new system architectures for storage-intensive supercomputing in partnership with industry collaborators; and (4) enable an order-of-magnitude improvement in price and performance over today's architectures for a broad range of data-intensive problems.

Across the Laboratory, and in the scientific and national security communities at large, scientists and analysts are searching for techniques, tools, and computing architectures to manage and analyze large datasets. Such data-intensive problems are particularly common in scientific simulation, defense applications, and sensor-related activities. For applications that require frequent access to storage, the traditional technology is inadequate. Our goal is to enable applications that simply cannot run on current systems and to deliver an order-of-magnitude improvement in performance and productivity over current systems.

Mission Relevance
This project will deliver a new capability to solve data-intensive problems in nonproliferation and homeland security, defense applications, and analysis of scientific simulation data. Storage-intensive architectures offer an advantage over computation-intensive architectures by optimizing access to large data sets. Example problems include analysis of stockpile stewardship simulations, large-scale graphs used to identify terrorist networks, massive astronomy datasets, and fusion-class laser optics imagery to assess damage.

FY09 Accomplishments and Results
We (1) built and evaluated a prototype query-oriented file system that stores arbitrary file attributes and relationships, enabling flexible scientific data management; (2) presented our Pianola synthetic benchmark generator at a supercomputing conference and released it to open source; (3) ported three data analytics algorithms to massively multicore co-processors, yielding a 58-fold speedup over conventional processors; (4) investigated parallel and streaming programming environments and measured performance and programmability; and (5) used advancing storage-intensive supercomputing to evaluate nonvolatile memory technology from Intel, Spansion, and FusionIO.

Proposed Work for FY10
In FY10 we will (1) deploy an operational data cluster with computer nodes augmented by nonvolatile random access memory, (2) host a novel query-oriented file system being developed in collaboration with the University of California at Santa Cruz, (3) perform co-processor research with a focus on heterogeneous multicore architectures, and (4) demonstrate applications in cybersecurity and intelligence on our new data cluster.

Publications
May, J., 2009. *Pianola: A script-based I/O benchmark.* 3rd Petascale Data Workshop, Portland, OR, Nov. 16, 2009. LLNL-CONF-407121.

Molina-Estolano, E., et al., 2009. *Mixing Hadoop and HPC workloads on parallel file systems.* 4th Petascale Data Storage Workshop, Portland, OR, Nov. 15, 2009. LLNL-CONF-416890.

Top, P., and M. Gokhale, 2009. *Application experiments: MPPA and FPGA.* Intl. Conf. Engineering of Reconfigurable Systems and Algorithms, Las Vegas, NV, July 13–16, 2009. LLNL-CONF-409662.

New Algorithms to Scale Domain Decomposition Up to Blue Gene Architectures—David Hysom (08-ERD-014)

Abstract
In recognition of the importance of advanced simulation and modeling capabilities to the DOE's science-based Stockpile Stewardship Program, we propose to develop novel mesh-partitioning algorithms and software for supercomputer simulations that are more scalable (>100K processors) and deliver higher quality results than the current state of the art. The key insight in our approach is to exploit implicit structure in three-dimensional hexahedral meshes to develop faster, more memory-efficient partitioning schemes with superior-quality domain decompositions for faster simulation times. The amount of parallelism and interprocessor communication overhead of a mesh-based simulation using partial differential equations is largely determined by the quality of the partition.

We expect to deliver production-quality code that produces higher-quality domain decompositions for applications of

Laboratory relevance and that are scalable to the full BlueGene/L machine. High quality will translate directly into better load balance and more efficient use of the machine. Multiblock partitioners will offer new features to scientists and make new guarantees about the nature of the domain assignment, such as whether or not domains can span blocks and what the maximum number of neighboring domains is. We expect our technique to extend into dynamic repartitioning, in which workload changes over time and is periodically rebalanced.

Mission Relevance

This project supports LLNL's stockpile stewardship mission by developing high-quality partitioning technology that scales to the full BlueGene/L machine, allowing simulations to run efficiently on the whole machine. This project will help assure LLNL's sustained preeminence in the field of stockpile stewardship simulations.

FY09 Accomplishments and Results

In FY09 we accomplished all proposed project objectives. Specifically, we (1) began developing adaptive repartitioning capabilities in our code and performed adaptive repartitioning in the limited case of pure multiblock meshes without degenerate zones or unstructured regions, (2) demonstrated the adaptive repartitioning capability on test cases, and (3) scaled our static partitioning capability to the full BlueGene/L and Dawn machines, refined the figures of merit we use to quantify the quality of a domain decomposition, and validated the figures of merit against full simulations.

Proposed Work for FY10

In FY10 we will (1) report figures of merit for our code on full BlueGene/L and Dawn machines (or on as many nodes as we will be permitted to operate); (2) avail our new algorithms to Laboratory weapons codes by providing an application program interface and library, rather than as a stand-alone application; and (3) prepare a final paper to detail project results.

Robust Ensemble Classifier Methods for Detection Problems with Unequal and Evolving Error Costs—

Barry Chen (08-ERD-022)

Abstract

Detection applications involving counterterrorism or nonproliferation are often characterized by unequal and evolving costs (i.e., consequences) for false alarms and missed detections as well as an imbalance in training examples. Conventional statistical classifiers do not adequately address these issues. To solve these problems, we intend to generalize individual cost-sensitive classifiers to cost-sensitive ensemble classifiers (CSECs), combining the strengths of both cost-sensitive and ensemble-classification methods. We will jointly optimize the key ensemble design factors through a novel global cost-minimization approach to deliver an unprecedented robust, high-performance, and easy-to-use solution to counterterrorism and nonproliferation detection problems.

We will develop and demonstrate a methodology for building CSECs, globally optimized over key design factors and capable of delivering robust, high-performance, easy-to-use solutions to detection problems involving unequal or evolving misclassification costs and unbalanced training data. The resulting methodology will be the first to address all of these challenges simultaneously and will significantly advance the state-of-the-art in classification technology, in terms of both detection performance and insight into the effects and interactions of design factors. The capability to solve detection problems of this type has broad applicability to many mission-relevant applications.

Mission Relevance

The ensemble classifiers developed in this project can be broadly applied to a wide range of objectives in LLNL's counterterrorism and nonproliferation missions, including the detection of hidden signals in intelligence data, radiological sources in low-intensity spectral signatures, attack signatures for site-protection applications, failing components in weapons systems, nefarious activities on computer networks, and clandestine underground nuclear explosions.

FY09 Accomplishments and Results

In FY09 we successfully completed and published our research on subspace feature sampling support-vector-machine classifiers. These classifiers, as well as those based on various decision trees, will serve as building blocks for our future research on heterogeneous ensembles that combine complementary base classifiers.

Proposed Work for FY10

For FY10 we intend to (1) develop ensemble classifiers that can adapt to changing costs without completely retraining the CSECs, (2) enhance detection robustness by developing classifiers that combine complementary base classifiers, (3) adapt and apply developed technologies to program applications burdened by imbalanced training data and unequal misclassification costs, and (4) develop software implementations of our novel CSECs, a user's manual enabling technology transfer, and peer-reviewed publications.

Publications

Chen, B. Y., T. D. Lemmond, and W. G. Hanley, 2009. "Building ultra-low false alarm rate support vector classifier ensembles using random subspaces." *Proc. IEEE Symp. Computational Intelligence and Data Mining.* LLNL-CONF-407542.

Enhanced Event Extraction from Text Via Error-Driven Aggregation Methodologies—Tracy Lemmond (08-ERD-023)

Abstract

Knowledge discovery systems construct massive data repositories via the extraction of events from text and are vulnerable to extraction errors. We propose to enhance the performance of the data-ingestion process via an aggregate meta-extraction capability, leading to reliable downstream inference in support of LLNL's counterterrorism and nonproliferation efforts, and more generally, to a critical breakthrough in natural language processing and knowledge discovery. We will begin by modeling typical extraction errors and quantifying their impact on downstream inference. We will then leverage this information to characterize and optimally combine multiple base extractors, reinforcing their individual strengths and mitigating their weaknesses.

Our research will yield a novel methodology for probabilistically characterizing the error processes underlying knowledge discovery, providing vital insight into the expected reliability of knowledge discovery systems. This will serve as the foundation for developing the aggregate meta-extraction system, which we expect to substantially improve the 60% accuracy rate of current state-of-the-art methods. The significant resources invested by LLNL and its customers over the last decade in knowledge discovery systems demand higher-quality data ingestion, along with a more thorough understanding of their reliability. Moreover, because our approach incorporates existing tools, we can readily leverage the investments made in the academic and commercial sectors.

Mission Relevance

Lawrence Livermore is developing systems to assemble information from multiple information and intelligence sources in support of its national and international security missions in counterterrorism and nonproliferation. However, errors arising from data ingestion propagate to downstream inference, making ensuing decisions or conclusions highly unreliable and unsuitable for practical use. Our methodology will boost data accuracy and provide a framework for estimating the uncertainty in downstream inference.

FY09 Accomplishments and Results

We conducted extraction error analyses that led us to a graduated approach to event aggregation, after which we developed new probabilistic, pattern-based and hybrid aggregation methodologies that focus on entity extraction but that are generalizable to multiscale, triple-event aggregation solutions. Performance estimates using four-base extractors on a variety of real data sources (including operational data), domains, and simulated real-world scenarios showed improvements of up to 120% over the best base extractor. We also implemented a development framework that will form the basis of a deployable system and also filed a record of invention describing these methodologies developed; journal papers will be submitted for publication after a provisional patent is secured.

Proposed Work for FY10

In FY10 we will extend and enhance the probabilistic aggregation methodology developed in FY09 via stochastic models that are able to more effectively leverage temporal textual information. In addition, we will continue to develop and generalize the entity aggregation methodologies to address the more-general triple extraction task. This unprecedented work will synergistically leverage insights gained from the event error analyses performed in FY08 and the entity meta-extraction research performed in FY09 to produce a state-of-the-art extensible methodology for triple aggregation. If successful, our research will represent a significant breakthrough in natural language processing and knowledge discovery.

Scalable Methods for Discrete-Ordinate Transport Algorithms on Massively Parallel Architectures—Robert Falgout (08-ERD-026)

Abstract

We propose to develop parallel multilevel solutions for the monoenergetic Boltzmann transport equations on inner neutron iteration and lambda iteration for x-rays. The Boltzmann transport equation describes the statistical distribution of one particle in a fluid, and is one of the most important equations of nonequilibrium statistical mechanics, which deals with systems far from thermodynamic equilibrium. Our algorithm would be an alternative to traditional source iteration using diffusion synthetic acceleration or transport synthetic acceleration. The goal is to develop a method that is effective over a wide range of regimes

(thin, thick, and diffusive) and that scales up to the 130,000 processors of LLNL's BlueGene/L supercomputer. We also propose to develop scalable multilevel sweeping algorithms to invert streaming operators. These algorithms have the potential to dramatically improve the Laboratory's computational transport-simulation capabilities.

We expect to develop parallel, scalable, robust algorithms to solve the linear and nonlinear systems required for the discretization of radiative transfer and neutron transport equations. The Laboratory's existing multigrid solvers have had a tremendous impact on the physics codes that employ these equations, but the solvers are currently tuned only for elliptic Poisson's diffusion equations. Our goal is to extend these solvers to significantly enhance the simulation capabilities of physics codes that involve radiation and neutron transport.

Mission Relevance

Scalable discrete ordinate transport algorithms are vital to LLNL simulation activities, particularly stockpile stewardship. The new algorithms developed in this project have the potential to greatly improve the robustness and efficiency of these codes.

FY09 Accomplishments and Results

In FY09 we developed (1) a space–angle description of the near-nullspace components of the Boltzmann equation and developed an improved sparse grid-like multiple semi-coarsening method for problems with anisotropic scattering; (2) a multigrid method for the full space–angle–energy Boltzmann equation; (3) a generic sweep algorithm that encompasses most existing algorithms used today, and used this framework to demonstrate and compare effective techniques for scaling beyond 100,000 processors; and (4) improved algorithms for sweeping on structured mesh-refined grids.

Proposed Work for FY10

In FY10 we will extend our multiple semi-coarsening method to the unstructured grid setting. The current algorithm requires operators for each coarse grid, but these may not be available or may be difficult and expensive to form using operator-dependent schemes. We will explore a number of approaches, including the idea of coarsening only in angle or to coarsen in both angle and space using the fine-sweeping operators. We will also extend our sweep algorithm work to the unstructured-grid setting.

Publications

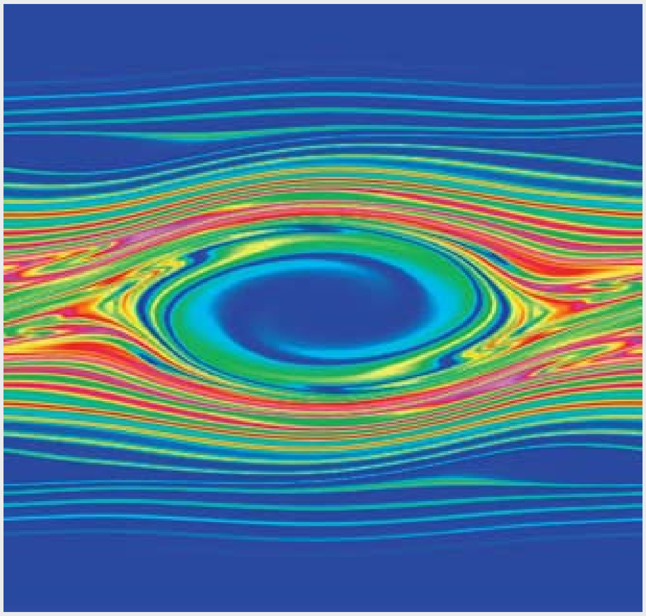
Bailey, T. S., and R. D. Falgout, 2009. "Analysis of massively parallel discrete-ordinates transport sweep algorithms with collisions." *Proc. Intl. Conf. Mathematics, Computational Methods, and Reactor Physics.* American Nuclear Society, LaGrange Park, IL. LLNL-CONF-407968.

Efficient Numerical Algorithms for Vlasov Simulation of Laser–Plasma Interactions—Jeffrey Hittinger (08-ERD-031)

Abstract

The objective of this project is to develop efficient, high-fidelity continuum algorithms for the Vlasov–Maxwell system that will facilitate routine laser–plasma interaction simulations. For more efficient designs of laser-driven high-energy-density experiments, noiseless simulations based on continuum models are required to predict the nonlinear onset and behavior of stimulated plasma instabilities. Continuum Vlasov simulations are very expensive computationally because they require discretization in a high-dimensional phase space. We will investigate the use of adaptive mesh refinement (AMR) in phase space as well as the use of nonlinear, high-order algorithms to reduce cost and improve robustness of Vlasov simulations.

We expect to be able to reduce the computational cost of four-dimensional (4D) Vlasov simulations of laser–plasma interactions by two orders of magnitude, and 6D Vlasov simulations by at least three orders of magnitude. This will enable feasible, routine 4D Vlasov simulations (12–48 h runs on 128 processors) and groundbreaking 6D Vlasov simulations on Livermore's massively parallel computers. With the ability to perform these routine simulations, in conjunction with existing particle- and fluid-plasma models, plasma physicists will be able to predict the behavior of nonlinear stimulated-plasma instabilities, leading to more optimal designs of laser-driven high-energy-density experiments at future fusion-class laser facilities.



Using our new finite-volume algorithm, we computed the density of particles as a function of space and velocity at late time for the two-stream instability problem.

Mission Relevance

Developing the algorithms required to routinely simulate laser–plasma interactions typical in high-energy-density regimes will advance experiments at future high-power lasers. These high-energy-density experiments have direct application to Laboratory missions in stockpile stewardship, fusion energy research for long-term energy needs, and fundamental science such as astrophysics.

FY09 Accomplishments and Results

In FY09 we (1) developed multidimensional, finite-volume algorithms for Vlasov discretization comparable in cost to existing schemes but with higher-fidelity results at coarser resolutions; (2) implemented our algorithms in a AMR test bed code based on the SAMRAI (Structured Adaptive Mesh Refinement Application Infrastructure) code and verified them on the Vlasov–Poisson system; and (3) used AMR to demonstrate 2D mesh reductions of 72%.

Proposed Work for FY10

In FY10 we expect to produce a single-species, fourth-order, finite-volume Vlasov–Poisson simulation capability capable of running in 2D through 4D. We will (1) generalize this code to multiple kinetic species, (2) generalize the Poisson model to an electromagnetic subset of the Maxwell equations, (3) implement the semi-Lagrangian algorithms within the adaptive mesh refinement test bed, (4) explore variants of the finite-volume algorithm, (5) develop diagnostics for physically relevant metrics, (6) generalize the implementations to 5D and 6D, (7) apply this code to physically motivated verification problems, and (8) study performance and scalability of the code.

Publications

Banks, J. W., and J. A. F. Hittinger, 2009. *Adaptive and high-order methods for laser–plasma interaction problems.* IMACS World Conference on Computational and Applied Mathematics in Science and Engineering, Athens, GA, Aug. 3–5, 2009. LLNL-ABS-413421.

Banks, J. W., et al., 2009. *VALHALLA: An adaptive, continuum Vlasov code for laser–plasma interaction.* 39th Ann. Anomalous Absorption Conf., Bodega Bay, CA, June 14–19, 2009. LLNL-POST-413664.

Cohen, B. I., et al., 2009. “Erratum: Stimulated Brillouin backscattering and ion acoustic wave secondary instability.” *Phys. Plasmas* **16**, 089902. LLNL-JRNL-412473.

Cohen, B. I., 2009. “Stimulated Brillouin backscattering and ion acoustic wave secondary instability.” *Phys. Plasmas* **16**, 032701. LLNL-JRNL-407238.

Understanding Viral Quasispecies Evolution Through Computation and Experiment—Carol Zhou (08-ERD-036)

Abstract

We propose to develop a combined predictive approach involving novel multiscale modeling and simulation along with bioinformatics analysis tools to uncover basic principles of viral evolution. Instead of focusing on a single species, however, we will design a computational simulation framework for modeling a broad group of RNA virus families with similar replication strategies. The project will advance understanding of RNA virus evolution and control, vaccine and drug resistance, and emergence of new diseases. Our new approach will enable enhanced collaborations and increased relevance for other federal agencies, industry, and academia.

We expect to develop a novel research tool that will enable us to understand how RNA viruses evolve and adapt to avoid immune response and become resistant to vaccines and antiviral drugs. Using this tool, we will be able to conduct experiments to understand the basis of viral quasispecies memory that enables reversion of vaccine strains to infectious wild types, to compare the evolutionary potentials of different viral species, and to understand mechanisms of emergence of new agents of human and animal disease. The results from our modeling and simulations will enable development of new biodefense technologies by providing key insight into how viruses mutate, adapt, and evolve under different selective pressures.

Mission Relevance

This project supports the Laboratory’s missions in homeland security and bioscience to improve human health by applying advanced computing to the identification, characterization, and simulation of virulence mechanisms to increase our understanding of virulence and the evolution of pathogenicity.

FY09 Accomplishments and Results

In FY09 we (1) completed implementation and verification of an in-cell virus replication stochastic simulation model; (2) completed the design, implementation, and verification of a cell-to-cell infection model; (3) continued development of bioinformatics tools—we completed a new algorithm for sequence variability analysis; and (4) continued a collaboration with researchers at the University of California at San Francisco in exploring polio genetics and evolution.

Proposed Work for FY10

In FY10 we propose to (1) process and analyze empirical genome data generated by our collaborator in a study of viral genetic drift in a cell culture subjected to heat shock protein 90 (Hsp90) inhibition, (2) design criteria and develop an algorithm for automated clustering and scoring of observed and predicted single-residue mutation candidates, (3) design criteria and develop algorithms for detection and clustering of coordinated-residue mutations, (4) adapt the stochastic simulation modeling code for simulations of the P1 protein and Hsp90 model system and verify and calibrate the model using empirical data provided by our collaborator, and (5) analyze the mutational propensity of the poliovirus P1 capsid precursor gene.

Hierarchical Vehicle Activity Models for Site Security—Douglas Poland (08-ERD-067)

Abstract

We propose to construct dynamic hierarchical vehicle activity models to create a system capable of detecting subtle, distributed suspect activity. We will focus on two scenarios—vehicles engaged in surveillance and those engaged in staging an attack—that are not addressed by current surveillance systems and are not feasible to address manually. Starting with vehicle tracking information from an existing system, we will construct dynamic hierarchical models of individual vehicle activity patterns and collective spatial and temporal activity patterns. This will enable us to characterize normal activity and detect anomalous activities of concern.

We will develop a quantitative understanding of the performance characteristics of video surveillance systems to use in designing stochastic models that leverage system outputs. Specifically, we will (1) produce a framework for constructing and maintaining dynamic hierarchical models of individual and collective activity, built on ensembles of sequences of discrete observations, that can be extended to other types of observations; (2) construct anomaly detection algorithms and characterize the performance of this architecture for detecting specific potential threats; (3) explore how the performance of hardware and software components impacts overall performance; and (4) document system design considerations.

Mission Relevance

This work supports the homeland security mission by enabling greater situational awareness and, therefore, faster and more effective assessment of and response to potential threats at NNSA and other relevant facilities. This project also supports the national security mission by developing and demonstrating hierarchical activity models that will significantly strengthen efforts addressing persistent surveillance and proliferation detection (i.e., site protection and monitoring).

FY09 Accomplishments and Results

We (1) finished implementing our vehicle activity model as a hierarchical dynamic Bayesian network; (2) implemented anomaly detection algorithms; (3) made substantial progress on integrating the modeling and anomaly detection functions; (4) made some infrastructure progress, bringing a three-camera license-plate-recognition location online and addressing bugs and limitations in the software; (5) continued work on our experimental test bed; (6) continued verifying our sensor error models; and (7) continued iterating the feature extraction, vehicle identification, and model learning parameters and algorithms. In this project, we formulated a strategy for tracking vehicles and identifying suspect behavior at a secure site using a combination of sparse, existing area-surveillance video cameras and high-performance license plate readers positioned at strategic entry and exit points. We applied cutting-edge statistical modeling techniques, coupling them to commercial off-the-shelf video technology, and used this new capability with simulated data to demonstrate basic model acquisition and anomaly detection capabilities. The next step would be to conduct live experiments with additional infrastructure to further validate this capability.

Supercomputing-Enabled Transformational Analytics Capability (SETAC)—Celeste Matarazzo (09-SI-013)

Abstract

We propose to develop fundamentally new analytical approaches for cyber security situational awareness for protecting and defending our nation's computing networks. Our supercomputing-enabled transformational analytics capability (SETAC) will focus on transforming the analysis process to provide real-time situational understanding by enhancing our current signature-based analysis with machine-learning behavioral analytics that can be applied as data is traveling through the network. SETAC requires considerable research in hardware that is powerful enough to apply analytic algorithms to multiple gigabit-per-second data streams and also requires new analytic algorithms that can provide a high-fidelity, real-time behavioral-view of the network through distributed "intelligent agents."

If successful, SETAC will provide real-time behavioral analytics for cyber security data. Our proposed system capabilities will include (1) identification and classification of high-volume streaming network traffic, (2) high-performance sensor nodes to increase processing capabilities and provide distributed detection across the network, (3) a distributed computing test bed to develop prototype advanced global collection and analysis approaches, and (4) system- and component-level metrics for performance assessment.

Mission Relevance

This proposal supports LLNL missions in nonproliferation and homeland security as well as supporting efforts in advanced defense capabilities. Our research will enhance the Laboratory's threat prevention and response technologies by addressing thrust areas in knowledge discovery, advanced analytics and architectures for national security and actionable situational awareness, and information dominance.

FY09 Accomplishments and Results

In FY09 we developed, deployed, and evaluated SETAC. Specifically, we (1) developed an agent framework based on the code JADE and which connected 50 hosts at LLNL; (2) deployed two classes of algorithms on Tilera hardware and one class on field-programmable gate arrays; (3) developed several behavior-based machine-learning algorithms, including Hypertext Transfer Protocol attack detection, network traffic classification, and nonparametric generative models of Internet Protocol traffic; (4) devised two approaches for finding the most vulnerable hosts; (5) created activity models for LLNL networks, using both network traffic and host process data; and (6) participated in a cybersecurity exercise with another national lab in which we successfully demonstrated reverse-engineering and supercomputer-based binary analysis.

Proposed Work for FY10

In FY10 we propose to (1) make our distributed agent framework scalable with respect to the number of host agents and deploy hundreds of agents within LLNL; (2) evaluate reliability and security of the agent framework; (3) continue to evaluate hardware architectures (Tilera and the field-programmable gate arrays) and embedded processing within Cisco routers; (4) extend our behavior-based machine-learning algorithms for cyber situational awareness and attack detection to distributed and streaming algorithms, including learning and inference; (5) develop a probabilistic activity model of hosts in our agent framework for anomaly detection; and (6) continue our collaboration with Laboratory cyber operations.

Publications

Gallagher, B., and T. Eliassi-Rad, 2009. *Classification of HTTP attacks: A study on the ECML/PKDD 2007 discovery challenge.* LLNL-TR-414570.

Gallagher, B., et al., 2009. *Guilt by association: Exploiting implicit relationships in network data for traffic classification.* LLNL-TR-414362.

Henderson, K., and T. Eliassi-Rad, 2009. *Solving the top-K problem with fixed-memory heuristic search.* LLNL-TR-410187.

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The supercomputing-enabled transformational analytics capability (SETAC) research team (left to right): Grant Johnson, Phillip Top, Brian Gallagher, William Hanley, Celeste Matarazzo, Christopher Roblee, Brenda Ng, Maya Gokhale, Tina Eliassi-Rad, Keith Henderson, Anthony Bartoletti. Not shown: Kelley Herndon-Ford.

Conf. Machine Learning and Principles and Practice of Knowledge Discovery in Databases. LLNL-JRNL-407301.

Thompson, B., and T. Eliassi-Rad, 2009. *DAPA-V10: Discovery and analysis of patterns and anomalies in volatile time-evolving networks.* 1st Workshop on Information in Networks, New York, NY, Sept. 25–26, 2009. LLNL-CONF-416785.

Tong, H., et al., 2009. *BASSET: Scalable gateway finder in large graphs.* LLNL-TR-414380.

Tong, H., et al., 2009. *BridgeFind: Fast detection of top-K bridges in large graphs.* LLNL-TR-414449.

Tong, H., et al., 2008. "Fast mining of complex time-stamped events." *Proc. 17th ACM Conf. Information and Knowledge Management.* LLNL-CONF-405539.

Quantitative Analysis of Vector Field Topology—
Peer-Timo Bremer (09-ERD-014)

Abstract

Today's computer simulations produce data of increasing complexity, resulting in an increasing need for the qualitative and quantitative analysis of complex features. Topology, a major area of mathematics concerned with spatial properties that are preserved under continuous deformations of objects, provides powerful tools to define and extract such features. This project focuses on techniques to quantitatively analyze vector fields based on their topological structure. Vector fields are often used in physics to model, for example, the speed and direction of a moving fluid throughout space, or the strength and direction of some force, such as the magnetic or gravitational force, as it changes from point to point. We will develop a mathematical framework for robustly extracting topology from sampled vector fields while maintaining rigorous error bounds. The extracted topology will allow quantitative analysis of topological structures. The hierarchical encoding we develop will allow us to analyze, simplify, and compare vector fields on multiple scales. These techniques will provide opportunities to find explicit definitions for secondary features such as vortices.

We will develop the computational theory necessary to generate complete topology of general vector fields using entirely combinatorial algorithms unaffected by numerical errors. Using metrics tailored to specific application domains, we will construct a hierarchical representation of the topology to permit multiscale analysis. Finally, we will use topological techniques to enhance the ability to track features in dynamic vector fields. The resulting tools will represent fundamentally new analysis capabilities directly applicable to the most ubiquitous form of simulated data.

Mission Relevance

Many relevant phenomena such as combustion, fluid flow, or magnetic fields are best described by vector fields. However, because of their inherent complexity, vector fields are often analyzed using derived scalar fields, which only partially describe these processes. Our direct quantitative analysis, simplification, and comparison of the structural properties of vector fields will provide LLNL with unique capabilities to more effectively analyze large simulations relevant to the national security mission areas of stockpile stewardship and global security. Our advances will also lead to new scientific insights.

FY09 Accomplishments and Results

In FY09 we (1) developed a combinatorial algorithm to detect a critical point in vector fields of arbitrary dimensions and under loose interpolation conditions; (2) shifted our focus, in response to recent developments in vector field topology, from combinatorial topology to scalar decompositions to achieve the same goals; (3) developed techniques to consistently compute vector field topology as the overlay of two multiscale complexes of forward and backward finite-time Lyapunov exponent fields; (4) developed new techniques to represent and visualize uncertainty in vector fields, the progressive drawing of streamlines, and new ridge-detection algorithms to extract features from time-dependent vector fields; and (5) reformulated the finite-time Lyapunov exponent computation in an incremental fashion in preparation for in-situ computation.

Proposed Work for FY10

In FY10 we will continue studying vector field topology on the practical and the theoretical levels. Specifically, we will (1) extend the critical-point extraction algorithm to combinatorial classification, (2) investigate formal proofs of equivalence between Lagrangian coherent structures and vector field topology, (3) continue study of the Helmholtz–Hodge decomposition as a possibility of analyzing general vector fields as the combination of several restricted fields, (4) extend the multiresolution representation to three-dimensional vector fields, and (5) work with our collaborators to compute topological information such as finite-time Lyapunov exponents during initial simulation.

Rapid Exploitation and Analysis of Documents—
David Buttler (09-ERD-017)

Abstract

The exploitation of unstructured text documents is a vital component of the national intelligence mission. There are tens of millions of existing documents relevant to that mission and a rapidly increasing rate of new ones that analysts must assess quickly. We will develop advanced analytic tools to rapidly triage documents, which will allow analysts to focus on the most

important documents quickly. This project addresses specific research gaps in identification of concepts and automatic creation of a concept hierarchy for summarizing a corpus. Documents of interest are frequently in foreign languages, where translation is a major bottleneck. Therefore, we propose to develop cross-language topic hierarchies. Lastly, analysts are overloaded with streams of documents. We will monitor analyst interests, and provide a personal ranking system.

Our research focuses on understanding approaches and techniques that promote efficient and effective discovery and analysis of large document sets given the limitations of current natural language-processing technologies. This project will work with intelligence analysts to identify the conditions when different methods assist or fail in supporting their work. Furthermore, we will identify a number of targeted research activities that cover technology gaps in document exploitation. In particular, we will explore approaches that assist in the rapid exploitation and analysis of document corpora. We expect to dramatically improve the ability of analysts to discover the most relevant documents for a particular line of inquiry.

Mission Relevance

This proposal is a step towards creating a world-class information exploitation capability for LLNL's missions in national and homeland security by boosting ability to process the increasingly massive datasets collected for nonproliferation, intelligence, and military missions. We will develop new algorithms to organize vast document sets and alert analysts of new information relevant to their analytic tasks. This capability will have direct applications for programs such as Livermore's Counterproliferation Analysis and Planning System that are of interest to the Department of Defense.

FY09 Accomplishments and Results

In FY09 we (1) began an ongoing survey of the rapidly changing field of probabilistic topic modeling and automatic hierarchical facet generation, (2) described the current major approaches and identified the leading researchers in the area, (3) implemented a prototype search system that extends state-of-the-art information retrieval capabilities with personalized feedback and generated facets, (4) demonstrated the system over relevant data sets and stressed the scale of the system, and (5) continued to improve the user interface, scalability, and accuracy of the system.

Proposed Work for FY10

In FY10 we propose to (1) measure and improve disambiguation of domain-specific terms from analyst lexicons and machine-generated topic models, (2) measure concept search ability of the faceted search system and the effects of personalized ranking on search ability, and (3) incorporate probabilistic models into corpus specific-topic facets for search. These results will provide enhanced capabilities to quickly identify the themes and trends in a corpus and preserve the capability to locate individual documents quickly and easily.

Adding Validation and Novel Multiphysics Capabilities to the First-Principles Molecular Dynamics Qbox Code—

Erik Draeger (09-ERD-019)

Abstract

The purpose of this project is to increase the accuracy and temperature and pressure range of the Qbox materials simulation code. Qbox currently relies on approximations that can break down at extreme temperatures and pressures. We will integrate Qbox with high-accuracy quantum Monte Carlo codes and develop automated validation tools to quantitatively assess these approximations on the fly. We will also develop a flexible, parallel multiphysics framework to couple different quantum simulation codes to allow researchers to easily implement and test new multiphysics algorithms. Lastly, we will use this framework to develop new multiphysics methods to overcome hurdles associated with extreme conditions such as quantum effects of light nuclei and electron exchange–correlation effects.

We expect this project to result in (1) rebuilt, sustainable quantum Monte Carlo capabilities for the Laboratory; (2) robust, on-the-fly validation tools for Qbox; (3) a flexible multiphysics framework to simplify development of new multiphysics quantum algorithms; (4) research into new multiphysics algorithms to extend predictive materials simulations capabilities at LLNL; and (5) high-quality publications of first-principles simulation methods and applications. These results will allow us to perform validated, accurate calculations of materials at extreme conditions with unprecedented accuracy. They will also pave the way for new breakthroughs in predictive materials modeling, benefiting both the Laboratory's mission and standing as a leader in world-class research.

Mission Relevance

Predictive materials simulation has long been a cornerstone of NNSA and LLNL missions. Qbox is currently being used for calculations in Stockpile Stewardship and the National Boost Initiative to the limit of its current capabilities. Increasing the accuracy, validation capabilities, and range of accessible conditions would be of direct benefit to national security efforts. As a general materials simulation tool, new capabilities would also benefit many basic research efforts performed at Lawrence Livermore.

FY09 Accomplishments and Results

In FY09, we (1) performed a detailed evaluation of open-source quantum Monte Carlo codes and selected the diffusion quantum Monte Carlo code CASINO and the path-integral Monte Carlo code PI; (2) created interfaces between Qbox and CASINO and PI using new Qbox commands and post-processing conversion scripts to enable users to quickly switch between methodologies; (3) performed detailed comparisons of deuterium with both PI and Qbox, observing significant differences in the pair correlation functions and resulting in a new path integral sampling algorithm and a state-of-the-art theoretical prediction of the deuterium Hugoniot; and (4) began transition metal comparisons using CASINO and Qbox.

Proposed Work for FY10

In FY10 we will (1) continue to develop the multiphysics framework, starting with the integration of CASINO and Qbox for on-the-fly validation of first-principles molecular dynamics calculations; (2) develop a test code using Code Co-op to assess its utility in linking the Qbox, CASINO, and PIMC codes and measure the parallel performance for a variety of parallel configurations; and (3) continue to run materials simulations to quantify areas where the current Qbox approximations fall short, and work with PIMC and CASINO developers to add new capabilities needed to fully capture the physics of systems of interest.

Role Discovery in Dynamic Semantic Graphs—

Tina Eliassi-Rad (09-ERD-021)

Abstract

Role discovery arises in many intelligence and defense applications. The objective of this project is to develop algorithms that capture the formation and evolution of roles and functions in noisy and incomplete dynamic semantic graphs. New algorithms are needed that take into account both the heterogeneity and dynamicity in data. These new algorithms will generate statistical models that combine probabilistic predictive models (that handle data heterogeneity) with stochastic process models (that handle data dynamicity). For the first time, this work will unite two modeling categories on graphs. New statistical models will be judged based on their accuracy, run time, and space complexity and tested on publicly available as well as sponsor-provided data.

If successful, the work will provide viable solutions to some of the current analysis needs in cybersecurity as well as homeland and national security. In particular, the work will produce new algorithms that (1) model both the heterogeneity and dynamicity in data, (2) allow analysts to directly examine the roles of entities in data sets, and (3) provide insights on the generative mechanisms of relationships. The discovered knowledge can subsequently be used for behavior modeling, anomaly detection, and other graph analytics problems. For instance, in the cybersecurity domain, the work will model the function of hosts over time to detect suspicious activities (e.g., an abrupt role change). These expected results are significant because they provide a different view of the asymmetric threats facing the nation.

Mission Relevance

This work supports LLNL missions in nonproliferation and homeland security, and in advanced defense capabilities. By tracking the formation and evolution of roles (i.e., functions) in dynamic semantic graphs, the roles of entities of interest can be directly examined. This abstraction contributes to the understanding of hidden hostile elements, and is well suited for identification of the asymmetric nature of threats faced in homeland and national security domains.

FY09 Accomplishments and Results

We (1) built an infrastructure for attribute prediction over time, developing and evaluating three statistical models that are highly predictive of attributes over time, even with sparse information; (2) developed and evaluated three scalable, nonparametric models for group evolution inference and ran them on Hadoop, a distributed computing framework; (3) developed and evaluated a hybrid community-detection algorithm using models for communities that were highly predictive of link structures and had low variation of information; and (4) developed and evaluated new algorithms for the fast mining of complex time-stamped events and for collective classification and statistical tests in network data, using, in all of our experiments, at least four real graphs from various domains.

Proposed Work for FY10

In FY10 we plan to study scalability with respect to inference in our probabilistic group evolution algorithm. In particular, we will develop inference techniques on distributed memory machines. This will help us analyze large graphs with millions of nodes and edges. In addition, we will develop probabilistic models for multifaceted information diffusion. For each task, we will conduct extensive empirical studies on publicly available data (which we have already identified). At the end of FY10, we expect to have all the pieces in place to conduct role discovery experiments on time-evolving graphs with a fixed set of nodes and varying edges.

Publications

Eliassi-Rad, T., and K. Henderson, 2009. “Literature search through mixed-membership community discovery.” *Proc. 1st Workshop on Information in Networks.* LLNL-CONF-416981.

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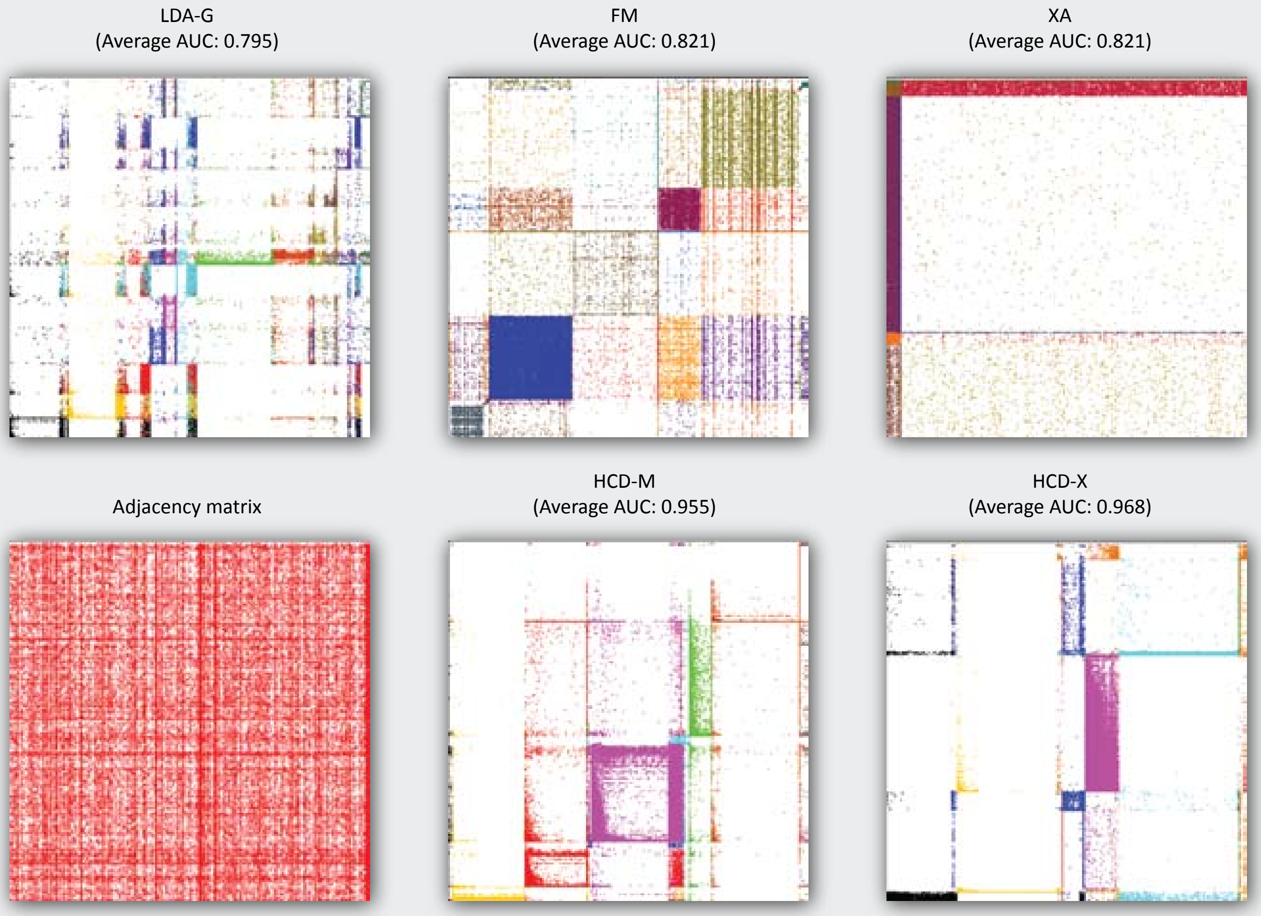
Tong, H., et al., 2008. “Fast mining of complex time-stamped events.” *Proc. 17th ACM Conf. Information and Knowledge Management*, pp. 759–768. LLNL-CONF-405539.



Adjacency matrix (bottom left) for an Internet Protocol traffic network and its corresponding community-sorted matrices. Greater white space in a matrix indicates better clustering and higher average link prediction performance—that is, area under the curve (AUC).

Modern Finite Elements for Lagrangian Hydrodynamics—Tzanio Kolev (09-ERD-034)

Abstract

The objective of this project is to develop new finite-element discretization algorithms for Lagrangian shock hydrodynamics. Our methods will be more accurate and robust than the currently used computational schemes and will address several longstanding issues with the hydrodynamics simulation codes at LLNL, including symmetry preservation on unstructured grids, exact total energy conservation, artificial viscosity discretization in multiple dimensions, and the handling of hourglass-mode instabilities. This will be achieved by applying modern high-order, multiscale, discontinuous Galerkin finite-element technology for discretizing Euler equations on a moving grid, coupled with new mathematical theory and numerical algorithms.

If successful, this project will produce new finite-element discretization schemes that will enable Lagrangian simulations with LLNL's hydrodynamics codes with a higher degree of fidelity than is currently possible. This research could also allow the finite-element methodology, which has been very successful for elliptic problems, to be extended to general systems of hyperbolic conservation laws.

Mission Relevance

Hydrodynamics simulations are of critical importance in numerous LLNL applications, including stockpile stewardship, inertial-confinement fusion, and other mission-relevant efforts. The proposed research will develop finite-element simulations technology to improve the predictive capability of these simulations while requiring fewer user-adjustable parameters. This project therefore supports LLNL's missions in national and energy security.

FY09 Accomplishments and Results

We (1) developed a high-order energy-conserving approach for Lagrangian hydrodynamics based on a novel general Lagrangian finite-element discretization framework, which has lead to new insights, including development of a finite-element-based tensor artificial viscosity; (2) demonstrated that high-order finite-element methods have important practical advantages, such as exact total energy conservation, improved radial symmetry preservation, support for curvilinear zones, and sharper resolution of the shock front (sometimes within a single zone); (3) developed a flexible Lagrangian finite-element research code where we tested the new algorithms on the Sedov blast wave, Noh implosion, and Saltzman piston problems; and (4) investigated some finite-element-based function–recovery procedures and are starting to address discontinuous Galerkin methods.

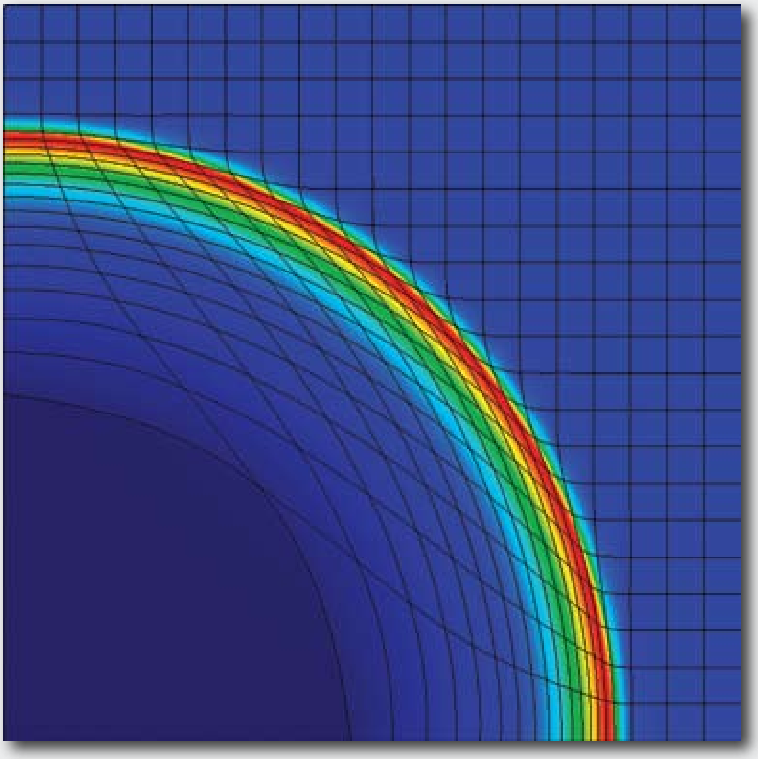
Proposed Work for FY10

In FY10 we will perform detailed theoretical and practical investigation of finite-element methods in axisymmetric settings. In particular, we will (1) explore general pairs of finite-element velocity–pressure spaces that are compatible with respect to the Rz divergence operator and consider the trade-offs in balancing momentum and energy-conservation errors for higher-order methods, (2) investigate the applicability of discontinuous Galerkin approaches for discretizing the Euler equations on a moving grid, and (3) initiate the verification, stability analysis, and integration of the most promising discretization schemes for research with Livermore's Advanced Radiographic and Energetic Systems capability.

Publications

Dobrev, V., et al., 2009. *Energy conserving finite element discretizations of Lagrangian hydrodynamics, part 1: Theoretical framework.* Numerical Methods for Multi-Material Fluids and Structures, Pavia, Italy, Sept. 21–25, 2009. LLNL-PRES-416883.

Dobrev, V., et al., 2009. *Energy conserving finite element discretizations of Lagrangian hydrodynamics, part 2: Examples and*



Sedov blast problem (formation of a blast wave from a very intense point-source explosion) using biquadratic coordinates and velocities with discontinuous bilinear density, energy, and pressure. Note the radial symmetry, curved zones, and sharply resolved shock front.

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Lagrange Multiplier Embedded Mesh Method—
Michael Puso (09-ERD-044)

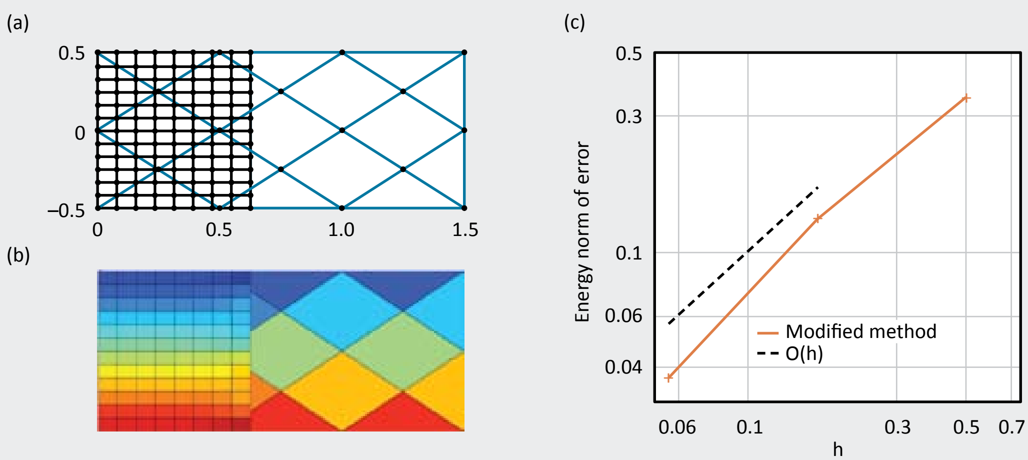
Abstract

The embedded-mesh method can drastically simplify the process of developing models and solving problems too difficult for existing tools, such as the blast rupture of shell structures and moving solid conductors in air grids (as in flux compression generators and rail guns). Our objective is to develop a new embedded-mesh method to simulate independently meshed regions with distinct physics formulations, such as the fluid–structure interaction of a Lagrange solid mesh moving through a Eulerian fluid grid. Although such methods are typically based on finite differences and place restrictions on mesh and grid sizes, we propose a mortar-based (enforcing the compatibility condition along the contact interface in a weak integral sense) Lagrange multiplier method for three-dimensional finite-element multiphysics simulations. Our surface-integration method will alleviate mesh size restrictions, and the novel application of a dual space multiplier will eliminate implicit calculation of the multipliers. Our approach will be applied to the blast rupture of shell structures and coupled electrodynamics–solid mechanics problems. We will employ both arbitrary Lagrange–Eulerian and Lagrange codes.

We will develop a computational tool in which the embedded mesh eliminates the need for a conforming mesh and thus requires no mesh motion in the types of problems considered. This general constraint tool will be built to interface with other LLNL codes such as ALE3D and Diablo solid mechanics codes, and will be demonstrated on two model problems: the blast rupture of shell structures and moving solid conductors in air grids.

Mission Relevance

The tools developed in this project will support LLNL’s national security and defense mission, such as moving solid conductors for flux-compression generation and rail guns. In addition, the proposed embedded mesh method has application to the understanding of the effects of high explosives, a core LLNL competency.



Overlapping grid model (a) used for development of our embedded mesh coupling software. The resulting stress field (physical quantities on the boundary surface) is transferred smoothly across the boundary between the two meshes, as represented by the gradual change in color at the surface (b). A convergence plot for this approach (c) demonstrates optimal accuracy and robustness of the method (red line) by showing that a measure of the computational error as a function of mesh size parameter (h) is less than the order of (h), which is superior to previous approaches.

FY09 Accomplishments and Results

In FY09 we initiated development for the FEusion embedded mesh coupling software. The data model accepts a superposed mesh (e.g., Lagrange solid) and a background mesh (e.g., ALE fluid). The software identifies overlaps, resulting voids on the background grid, and the strains on the "cut" background cells. It then generates constraint equations that enforce velocity continuity and associated transformation operators along the boundary between the two meshes. We also created an interface to Livermore's ALE3D code and wrote a developer's guide detailing the specific data structures exchanged with FEusion. A MATLAB mathematical software implementation was also developed as a numerical test bed for the new coupling methods.

Proposed Work for FY10

In FY10 work will focus on (1) developing particularization for different physics in the finite-element solver—that is, fluid and structure interaction and coupled solid-electrodynamics; (2) analyzing, using our new techniques, two model problems of blast loading on a shell structure and a moving solid projectile in a flux-compression generator or rail gun; and (3) preparing journal articles detailing our new method and results.

Petascale Computing-Enabling Technologies—

Bronis de Supinski (09-ERD-053)

Abstract

This project addresses the challenges arising from current trends in computer architectures that will soon lead to large-scale systems with many more nodes, each having chips with multiple cores. Such trends will culminate in systems with over one million processors. Furthermore, multicore chips will mean less memory and less memory bandwidth per core. In response, we will create fundamentally new approaches to cope with these memory constraints and the huge number of processors. Our integrated research agenda involves scalable algorithms, code correctness, performance analysis methodologies, and close interaction with application scientists.

This project will diagnose the problems that will be encountered in petascale computing systems. Specifically, we will design scalable, sparse linear solver algorithms; investigate a code-correctness methodology that tracks algorithmic behavior and automatically determines the cause of incorrect executions; and explore performance analysis mechanisms that identify the sources of inefficiencies. Our achievements will increase scientists' productivity and improve system utilization, thus dramatically increasing the overall scientific output of LLNL's large-scale computing resources.

Mission Relevance

By extending LLNL's expertise in system architectures, algorithms, and software tools to new architectures for applications in weapons material modeling, fusion energy, and environmental modeling, this project supports LLNL's missions in national and energy security as well as environmental management.

FY09 Accomplishments and Results

In FY09 we (1) profiled key sparse linear solver routines in the Hypre code and used these results to guide initial multicore refinements; (2) designed and implemented a new interpolation operator that better suits the smaller amount of memory per core expected in future systems; (3) developed advanced mechanisms to identify behavior equivalence class, as well as designing a technique to identify the equivalence class in which the error likely arose; and (4) explored techniques to measure and improve load imbalance in key applications. This project's work towards improving the usability of petascale systems has provided a framework to address similar issues for exascale systems.

Publications

Ahn, D. H., 2009. *Scalable temporal order analysis for large-scale debugging.* 23rd Intl. Conf. Supercomputing, Yorktown Heights, NY, June 8–12, 2009. LLNL-CONF-412227.

Gamblin, T., 2008. *Scalable performance measurement and analysis.* LLNL-TH-419482.

Gamblin, T., et al., 2008. *Scalable load balance measurement for SPMD codes.* 22nd Intl. Conf. Supercomputer, Austin, TX, Nov. 15–21, 2008. LLNL-CONF-406045.

Hilbrich, T., et al., 2009. *A graph-based approach for MPI deadlock detection.* 23rd Intl. Conf. Supercomputing, Yorktown Heights, NY, June 8–12, 2009. LLNL-CONF-411814.

Lee, G. L., et al., 2008. *Lessons learned at 208K: Towards debugging millions of cores.* 22nd Intl. Conf. Supercomputer, Austin, TX, Nov. 15–21, 2008. LLNL-CONF-402967.

Yang, U. M., in press. "On long-range interpolation operators for aggressive coarsening." *Numer. Linear Algebr.* LLNL-JRNL-413051.

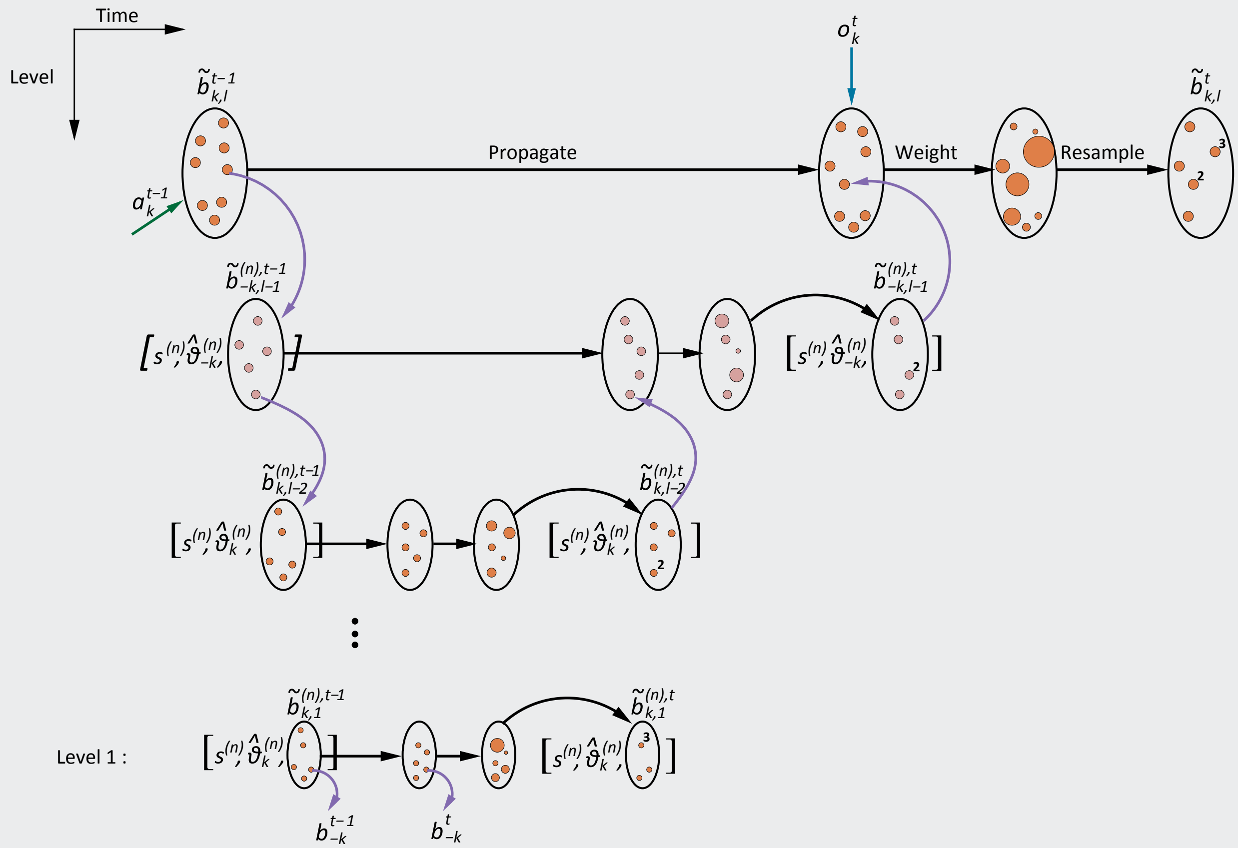
Towards Understanding Higher-Adaptive Systems—

Brenda Ng (09-LW-030)

Abstract

Countering real-world adversaries such as terrorist networks and cyber attackers involves formidable challenges such as incomplete or imperfect information, misinformation, asymmetric players, nonsequential actions, and unknown sets of actions. We will study higher-adaptive systems—systems that can modify their structure and behavior in response to detection or regulation attempts—with the ultimate goal of enhancing adversarial modeling by providing insights on representing and reasoning about disinformation and deceptive actions, which would aid in the analysis and control of real-world adversarial systems. Our plan is to develop three modules in a spiral lifecycle model: (1) an adversary system, (2) the knowledge representation of an observer system, and (3) the decision control of an observer system. We will develop a prototype system and then, through an iterative process, improve upon it in the learning and modeling of adversarial behaviors and optimal decision making.

We will focus on passive adversaries with fixed dynamics and deceptively aggressive adversaries with adaptive dynamics, and ultimately deliver a computational framework for characterizing dynamically changing, deceptive adversarial systems. This will pave the way for future studies of even more adaptive and aggressive adversarial systems, such as those that withhold resources and information from their opponents. These foundations will help advance work in artificial intelligence and game theory communities and provide the basis for addressing significant national security threats.



An agent updates its beliefs based on its anticipation of the other agent's observations, actions, and updates of its model. This results in recursive inference by particle filtering, as shown.

Mission Relevance

This project supports the Laboratory's national security mission by providing important knowledge and skills about real-world adversarial modeling and higher-adaptive systems, with applications in biological systems (e.g., regulatory networks), law enforcement (e.g., money laundering and drug trafficking), and homeland security (e.g., terrorist networks, cyber attacks, and proliferation of weapons of mass destruction).

FY09 Accomplishments and Results

We used the framework of interactive, partially observable Markov decision processes in developing a modeling and response system for countering higher-adaptive adversaries. This structure incorporates nested intent into the belief of each agent, allowing us to model the interaction of higher-adaptive agents. Employing the concrete example of money laundering, we (1) designed the first interactive, partially observable Markov decision process model to simulate the money laundering process; (2) researched and implemented algorithms for finding optimal response strategies; (3) obtained empirical results illustrating the complex interactions between asymmetric agents, which affects the efficacy of approximation schemes; and (4) submitted our results to the International Conference on Autonomous Agents and Multiagent Systems.

Proposed Work for FY10

In FY10 we will shift our focus from passive adversaries with fixed dynamics to deceptively aggressive adversaries with adaptive dynamics. We will augment the framework created in FY09 to (1) include model learning capabilities for inferring the adversary's transition, observation, and reward functions to enable learning of unknown dynamics; (2) incorporate uncertain evidence to model intentionally manipulated observations to address deception and unreliability in the adversary's observable outputs; (3) produce an enhanced computational framework to enable learning, modeling, and response for adversarial higher-adaptive systems; and (4) report our results in peer-reviewed publications and in presentations.

Publications

Ng, B., et al., 2009. *Modeling money laundering via interactive partially observable Markov decision processes.* AAMAS 2010, 9th Intl. Conf. Autonomous Agents and Multiagent Systems, Toronto, Canada, May 10–14, 2010. LLNL-CONF-418110-DRAFT.

Assessing the Feasibility of Alternative Inertial-Confinement Fusion Approaches—Max Tabak (09-FS-005)

Abstract

In the decade following the first demonstration of a working laser, a seminal 1972 article in *Nature* by Livermore's John Nuckolls predicted that nuclear fusion ignition could be achieved with laser energies of about 1 kJ. Today, the approach to achieving fusion ignition in the laboratory is coming to fruition, following a monumental science and technology effort that spans decades. Along the path to today's inertial-confinement fusion methodology, various alternative approaches to the final-stage fusion target and its environment—such as different holhraum or laser-intensity parameters—were not considered because of demonstrated or anticipated technological problems or uncertainties in laser–plasma interactions. The goal of this project is to quantitatively assess the feasibility of an alternative approach to fusion lasers using current advanced laser–plasma simulation capabilities available at Lawrence Livermore.

This study will assess the feasibility of an alternative approach to laser-driven inertial-confinement fusion that warrants a quantitative assessment: multihole hohlraum targets with small case-to-capsule ratios. We expect to determine whether or not this approach could enable inertial fusion under conditions that are advantageous from the viewpoint of laser–plasma coupling efficiency, radiation uniformity, plasma density and stability, and target chamber parameters such as illumination geometry. This project has the potential to enable a more effective approach to next-generation fusion-class laser systems. Our work is also intended to provide new insights into laser–plasma interactions and burning plasmas.

Mission Relevance

This proposal supports LLNL's missions in national security and energy security by providing physical insights into complex laser–plasma interactions in burning plasmas, central to both weapon systems and the future of energy production. Similarly, identifying potential alternative approaches for next-generation fusion-class laser systems also benefits both of these missions.

FY09 Accomplishments and Results

We designed 500-µm-radius laser entrance holes that stayed open for 30 ns with 5% of critical density inside. We determined that aluminum is a substantially hotter plasma fill material than hydrogen and would provide much higher pressure to retard hohlraum filling for a given level of plasma density, with possibly reduced plasma instability properties. The radiating volume of each radiator was about 2 mm long, and its centroid moved less than 1 mm—similar to current target hotspot motion, although still requiring further improvements to reduce this motion. This study opened new possibilities for laser-driven hohlraums that are scaleable to high gain scales, may reduce laser–plasma instabilities, and are compatible with the small-opening-angle laser irradiations envisioned in fusion reactor scenarios. We expect interest in follow-on work from DOE's Office of Fusion Energy Science.

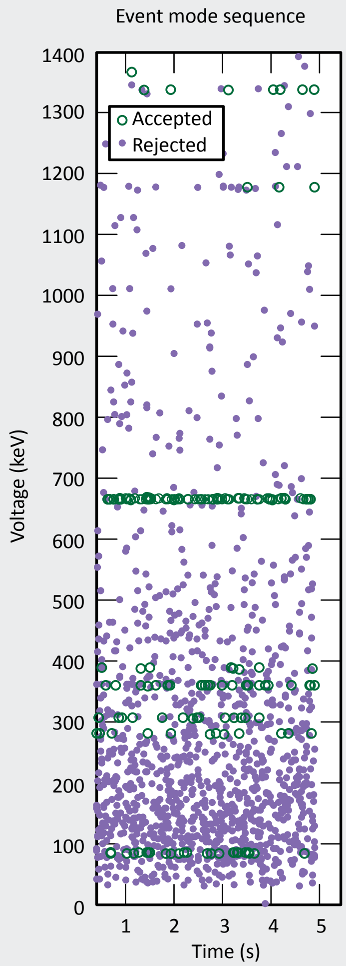
NUCLEAR SCIENCE AND ENGINEERING

Laboratory Directed Research and Development

Detection, Classification, and Estimation of Radioactive Contraband from Uncertain, Low-Count Measurements—James Candy (07-ERD-019)

Abstract

The detection of special nuclear material (SNM) smuggled into our nation is a critical issue for homeland security. Today's high-speed, high-throughput computers enable physics-based statistical models that capture the essential signatures of radionuclides to be incorporated into a sequential scheme (a Bayesian sequential processor) capable of online, real-time operation. This project is focused on the detection, classification, and estimation of illicit SNM from highly uncertain, low-count radionuclide measurements using a statistical approach based on Bayesian inference and physics-based signal processing. The effort will encompass theory, simulation, experiments, and application.



Sequential Bayesian detection and identification of photon arrivals (purple) and discrimination (green).

We expect to develop solutions for the detection, classification, and estimation of a moving SNM source, with a goal of reliably detecting kilograms of shielded plutonium with a 95% probability at a 5% false-alarm rate. The Bayesian approach will enable development of a sequential framework that will lay the foundation for future problems that are time and space varying or equivalently statistically nonstationary. This approach is applicable, in principle, to a large variety of model-based problems in many other critical areas of Laboratory work, including defect detection in the Stockpile Stewardship Program. Advanced signal- and image-processing techniques for the next generation of processors will evolve from this project.

Mission Relevance

The detection of illicit SNM is a top priority of LLNL in furthering the national security mission. Radionuclide detection, classification, and identification are critical for detecting the transportation of radiological materials by terrorists, an important goal in national and international security. This technology also supports stockpile stewardship because of its potential application in defect detection.

FY09 Accomplishments and Results

We (1) evaluated a Bayesian detection scheme using both simulated and controlled experimental data, (2) developed a signal-processing transport model based on point-to-point modeling by incorporating transport physics and validating the results with full-physics simulations, (3) developed a solution to the classification problem solution using physics-based Bayesian processors, and (4) developed a theoretical solution to the detection problem by incorporating Compton scattering physics into the processor.

Proposed Work for FY10

For FY10 we plan to (1) demonstrate the performance of the processor, including Compton processing on controlled experimental data; (2) develop a solution based on the sodium-iodide detector measurements gathered previously; (3) incorporate the estimate of the threat mass problem into our model-based scheme for threat detection; (4) demonstrate the Bayesian scheme on simulated and experimental data; and (5) evaluate performance of our approach on moving containers. We expect to develop a radiation detection system capable of processing photon arrivals in near real time, incorporating information extracted in a timely and reliable manner even with low counts.

Publications

Candy, J., et al., 2009. “Physics-based detection of radioactive contraband: A sequential Bayesian approach.” *IEEE Trans. Nucl. Sci.* **56** (6), 517. LLNL-JRNL-411357.

Candy, J., et al., 2009. “Radioactive contraband detection: A Bayesian approach.” *Proc. MTS–IEEE Oceans 2009 Conf.* LLNL-CONF-411355.

Chambers, D., 2008. “Signal-processing model for radiation transport.” *IEEE Trans. Nucl. Sci.* **1**, 150. LLNL-TR-405952.

Accelerator Mass Spectrometry of Strontium-90 for Biomonitoring and Human Health—Scott Tumey (07-ERI-002)

Abstract

A high-yield fission product, strontium-90 is one of the most hazardous constituents of nuclear waste. Being a pure beta emitter, strontium-90 is difficult to measure accurately in environmental samples because it generally occurs in the presence of other beta emitters—that is, fission products. An alternate methodology to measure strontium-90 with potentially significant advantages over radiation counting is accelerator mass spectrometry, which combines sensitivity with throughput and expediency. Consequently, we propose to develop a method to quantify strontium-90 by accelerator mass spectrometry, which, combined with the high-throughput design of the Center for Accelerator Mass Spectrometry facility, would result in an effective measurement system for this radionuclide.

The primary outcome of this project will be a robust measurement capability that will have immediate application to improved environmental monitoring and dose assessment for the Marshall Islands project. The capability will also have utility in human health studies focusing on the relationship between strontium-90 exposure and cancer rates. A potentially high-impact application that we will investigate is the possibility for strontium-90 to compliment calcium-41 as a bioindicator of bone-related diseases and as a tool for evaluating the efficacy of various treatments. Finally, analytical techniques for the detection of strontium-90 have an obvious and natural application to nuclear nonproliferation and homeland security.

Mission Relevance

This project is well aligned with the national security mission of the Laboratory because of the role of strontium-90 in homeland security and nuclear nonproliferation—almost all of this isotope is produced in the nuclear fuel cycle or past nuclear tests. Therefore, its detection in environmental samples could serve as a diagnostic for clandestine reprocessing of nuclear fuel for weapons use. In addition, the application of strontium-90 to human health studies and its potential use in detection and treatment of bone-related diseases are important contributions to science in the public interest.

FY09 Accomplishments and Results

In FY09 we successfully completed (1) an investigation of suitable methods for removing bulk quantities of calcium from real-sample matrices, (2) research of chemical purification procedures to eliminate zirconium-90 interference, and (3) validation of our sample-preparation protocols by measuring strontium-90 in standard reference materials. The successful conclusion of this project has produced a state-of-the-art measurement capability for strontium-90, and we are beginning to apply this capability in support of DOE programs such as the Marshall Islands project.

Publications

Tumey, S. J., et al., 2007. *Accelerator mass spectrometry of strontium-90 for homeland security, environmental monitoring, and human health.* 9th European Conf. Accelerators in Applied Research and Technology, Florence, Italy, Sept. 3–7, 2007. UCRL-ABS-231565.

Tumey, S. J., et al., 2009. “Further development of accelerator mass spectrometry for the measurement of Sr-90 at Lawrence Livermore National Laboratory.” *J. Radioanal. Nucl. Chem.* **282**, 821. LLNL-JRNL-414715.

Tumey, S. J., et al., 2008. *Further development of Sr-90 accelerator mass spectrometry at Lawrence Livermore National Laboratory.* AMS-11, 11th Intl. Conf. Accelerator Mass Spectrometry, Rome, Italy, Sept. 14–19, 2008. LLNL-ABS-404376.

How Carbon and Oxygen Can Be Made in Stars: An Ab Initio Approach to Nuclear Reactions—Petr Navratil (09-ERD-020)

Abstract

Stellar and nucleosynthesis modeling predictions depend strongly on knowledge of the reactions that produce carbon-12 and oxygen-16. These thermonuclear reactions determine the carbon-to-oxygen ratio during stellar helium burning, with far-reaching consequences for the production of all heavier species. Current knowledge about the reactions is far from sufficient, and a breakthrough can be reached only with a fundamental theory. We propose to develop an ab initio many-body nuclear reaction theory to accurately predict rates of the alpha-capture reactions responsible for production of the two elements. In this project, these alpha-capture rates will be calculated from first principles by means of an ab initio no-core shell model combined with the resonating-group method.

We will gradually develop formalism and codes to treat the scattering of increasingly heavier projectiles on light nuclei and perform the first-ever ab initio calculations of d(t,n)^{4}He and ^{4}He(^{3}He,gamma)^{7}Be cross-sections as intermediate steps towards addressing the alpha-capture reactions leading to formation of carbon-12 and oxygen-16. The successful completion of this project will result in (1) a long-awaited ab initio theory to explain alpha clustering in light nuclei and calculate cross sections of reactions important for astrophysics from first principles, (2) an improved accuracy of the 2-alpha(alpha,gamma)^{12}C and ^{12}C(alpha,gamma)^{16}O reaction rates, and (3) an enhancement of the predictive capability in stellar modeling.

Mission Relevance

This project will establish the capability to perform calculations of light-ion reactions relevant to LLNL missions in fusion energy generation and will result in a fundamental understanding of alpha clustering and improved alpha-burning cross sections for astrophysics, in support of the Laboratory's national security mission.

FY09 Accomplishments and Results

In FY09 we developed the deuteron-projectile formalism and performed successful deuteron–alpha and deuteron–triton elastic scattering calculations. The deuteron–alpha results reproduce known low-lying lithium-6 resonances. Depending on the nuclear interaction, the lithium-6 ground state is found weakly bound or unbound, which suggests importance of deuteron breakup channels. Our deuteron–triton scattering calculations reveal a resonance in the 3/2+ s-wave channels, while no resonance is found in the 1/2+ s-wave channel. This is explained as a consequence of the Pauli exclusion principle. In addition, we coded coupling of d+t and n+^{4}He channels needed to complete the d(t,n)^{4}He fusion calculations.

Proposed Work for FY10

In FY10 we will (1) develop the formalism for three-nucleon projectiles, necessary to describe the ^{4}He(^{3}He,gamma)^{7}Be capture reaction; (2) test the helium-3 and hydrogen-3 formalism by studying ^{3}He-alpha and ^{3}H-alpha scattering and beryllium-7 and lithium-7 bound states, respectively; and (3) perform ab initio calculations of the ^{4}He(^{3}He,gamma)^{7}Be and ^{4}He(^{3}H,gamma)^{7}Li capture reactions. The goal of these tasks is to extend ab initio many-body nuclear reaction theory from its current one- and two-nucleon projectile capability developed in FY09 to projectiles of up to four nucleons.

Publications

Navratil, P., and S. Quaglioni, 2009. "Applications of local chiral N2LO three-nucleon interaction to nuclear structure and reactions." *Bull. Am. Phys. Soc.* **54**, DH.00008. LLNL-ABS-414346.

Navratil, P., and S. Quaglioni, 2009. "Towards the first ab initio calculation of the deuterium–tritium fusion." *Bull. Am. Phys. Soc.* **54**, DM.00005. LLNL-ABS-414340.

Navratil, P., et al., 2009. "Recent developments in no-core shell-model calculations." *J. Physics G Nucl. Part. Phys.* **36**, 083101. LLNL-JRNL-411567.

Quaglioni, S., and P. Navratil, 2009. "Ab initio many-body calculations of nucleon-nucleus scattering." *Phys. Rev. C* **79**, 044606. LLNL-JRNL-409500.

Shock Temperatures from Neutron Resonance Spectroscopy—James McNaney (09-ERD-037)

Abstract

Temperature is a fundamental thermodynamic property and accurate temperatures are necessary to understand and predict processes involving thermal activation such as chemical reactions, plastic flow, and phase transitions. However, temperature is extremely difficult to measure during dynamic loading. Optical techniques such as pyrometry are widely used, but cannot probe the bulk volume of opaque materials such as metals—a major deficiency. This project seeks to develop a neutron resonance spectrometry capability for measuring temperature dynamically and in situ during shock loading. We will achieve this goal by extending and optimizing the initial proof-of-principle measure-

ments at the Los Alamos Neutron Science Center (LANSCE) and through the development of a short-pulse-laser-based neutron resonance spectrometry capability at Lawrence Livermore.

Successful completion of this work would result in a high-fidelity, time-resolved temperature measurement technique capable of probing the interior of a dynamically loaded material on the nanosecond-to-microsecond time scale. Work at LANSCE would extend the neutron resonance spectrometry technique to a wide range of opaque materials driven using standardized shock-loading techniques, such as high-explosive-driven flyers. Development of a laser-based neutron resonance spectrometry technique would represent a ground-breaking achievement with enhanced time-resolution versus the LANSCE-based capability. In addition, the technique would have diagnostic application to large-scale, fusion-class laser facilities. Measurements made using this approach would lead to a better understanding of temperature-dependent material behavior in general.

Mission Relevance

Development of a neutron resonance spectrometry capability would be of high value to Laboratory efforts in both weapons and photon science, in support of the Stockpile Stewardship Program and the national and energy security missions. In particular, the proposed work would support advanced physical model development, improved materials property understanding, advanced experiments and diagnostics, and high-neutron-flux science. This capability would have significant impact to understanding many aspects of material behavior under dynamic loading conditions, including those relevant to LLNL fundamental high-energy-density research.

FY09 Accomplishments and Results

In FY09 we focused on developing a short-pulse-laser-based neutron source. Specifically, we conducted a set of experiments at Livermore's Titan laser to investigate neutron production from short-pulse-laser-generated protons in the lithium–beryllium nuclear reaction. We demonstrated the production of 1 to 4 billion neutrons, most with energies of 1 to 3 MeV, in a 10-ps pulse. We thus identified the optimal conditions for neutron production at Titan and used that information to develop the basis for determining optimal conditions for other short-pulse-laser platforms.

Proposed Work for FY10

In FY10 we intend to continue development of our neutron source and focus efforts on optimizing the proton-to-neutron conversion. Specifically, we will (1) match the converter design, possibly using a mixture of isotopes, and the proton energy spectrum to the nuclear cross sections of interest; (2) design and evaluate compact moderator strategies for creating a neutron spectrum suitable for a neutron resonance spectrometry measurement; and (3) design a scaled-up version of the measurement suitable for use at the OMEGA Extended Performance Laser System at the University of Rochester to evaluate potential limits to the technique and its accuracy.

Publications

Higginson, D. P., et al., 2009. *Laser-generated proton beam optimization for (p,n) neutron production.* 51st Ann. Mtg. Division of Plasma Physics, Atlanta, GA, Nov. 2–6, 2009. LLNL-POST-418832.

Higginson, D. P., et al., 2009. *Manipulation of laser-generated proton beam energy distribution for (p,n) neutron production.* 51st Ann. Mtg. Division of Plasma Physics, Atlanta, GA, Nov. 2–6, 2009. LLNL-ABS-414877.

PHYSICS

Laboratory Directed Research and Development

Novel High-Energy-Density Source—James Hammer (06-SI-001)

Abstract

With this project, our objective is to develop a novel high-energy-density source of higher quality than is achievable by other pulsed-power technology. High-energy-density science, the study of matter under extreme conditions, is a key to mastery of fission and fusion science and its applications. The development of a novel source relies on a close coupling between multidimensional code simulations and experiments.

We expect to achieve a high-energy-density source that will be of broad utility to the Stockpile Stewardship Program and that will provide a capability complementary to future fusion-class lasers.

Mission Relevance

This work directly supports the Stockpile Stewardship Program at Lawrence Livermore by providing a new, high-energy-density source for experiments, as well as by validating codes used for high-energy-density modeling.

FY09 Accomplishments and Results

In FY09 we fabricated and tested a series of targets, completing the work specified in the scope of our project. Publications on instability growth related to a wide range of pulsed power experiments were completed. We also continued modeling these and earlier targets as preparation for follow-on efforts that will apply the design principles and physics we developed. In summary, this project has allowed us to transform a novel source concept for pulsed-power drivers into an experimental reality involving an entire class of high-performance, high-energy-density sources that are complementary to high-power laser sources and that will provide a basis for ongoing NNSA research in stockpile stewardship for the foreseeable future.

Publications

Miles, A. R., 2009. “Nonlinear Rayleigh–Taylor instabilities in fast Z-pinches.” *Phys. Plasmas* **16**, 032702. LLNL-JRNL-407151.

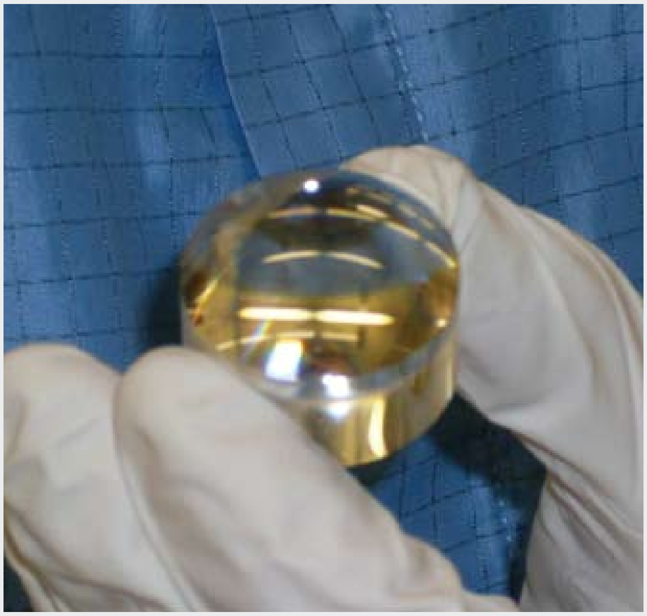
Miles, A. R., 2008. “Nonlinear Rayleigh–Taylor instabilities in fast Z-pinches.” *Proc. XII Intl. Conf. Megagauss Magnetic Field Generation.* LLNL-ABS-401934.

A Compact, High-Intensity Neutron Source Driven by Pyroelectric Crystals—Vincent Tang (06-ERD-065)

Abstract

The objective of this effort is to establish a new paradigm for active neutron-interrogation systems. We will explore the potential for achieving an extremely compact, high-intensity neutron source exploiting nuclear fusion reactions driven by pyroelectric crystals. The concept being investigated represents a revolutionary approach for accelerator-induced nuclear fusion reactions in a compact platform. Pyroelectric crystal–driven neutron sources would potentially eliminate the need for large, high-voltage power supplies and thus radically change the size and configuration of the ion accelerator, enabling a palm-sized neutron source. Therefore, this project could have a significant impact on weapons science, nuclear physics, and homeland security applications.

We will quantitatively determine the potential for scaling crystal-driven ion and neutron sources to fluxes equivalent to 10^6 deuterium–tritium neutrons per second or higher, and establish the technology and science basis for a non-isotopic, palm-size, highly mobile crystal neutron source that can be used for detection of special nuclear materials. Our technical approach is to (1) complete a modeling and experimental study of the crystal-based neutron source; (2) demonstrate experimental scaling—that is, neutron output up to three orders of magnitude greater (if deuterium–tritium is used) than initial results; and (3) construct novel nanoscale ion sources for achieving experimental scaling. Ultimately, we plan to couple an independent and controllable ion source to the crystal that will further intensify the ion beam and enable both pulsed and continuous operation.



Ultracompact shaped pyroelectric crystals such as this one provide the hundreds of kilovolts of energy required for fusion reactions when heated, and formed the basis of our palm-size neutron source experiments.

Mission Relevance

Neutron interrogation provides a noninvasive method of screening cargo and shipping containers for special nuclear materials smuggled through ports. This project supports Lawrence Livermore's national security mission by investigating a promising new technique that may enable a field version or even handheld neutron sources with the ability to interrogate targets anywhere, not just at ports. This approach offers the further possibility of a remote, autonomous neutron probe for the covert interrogation of targets and threat identification.

FY09 Accomplishments and Results

In FY09 we made notable advances in our ultracompact crystal-driven neutron source experiments. Primarily, pulsed pyrofusion was demonstrated for the first time and studied using negative high-voltage crystal targets coupled to a microelectromechanical-system-scale, palm-sized ion source. User-controlled deuterium–deuterium fusion yielding greater than 10^4 n/s was achieved with ~100-ns pulse widths, achieving peak rates greater than 10^{11} n/s. In addition, a new system model of crystal voltage and neutron production was constructed and compared with new voltage measurements of negatively biased crystals, showing quantitative agreement and providing understanding of pulsed pyrofusion system scaling. The successful conclusion of this project enabled new possibilities in the remote detection of explosives and special nuclear material through the development of ultracompact, pulseable ferroelectric-crystal-driven neutron source technology. The Defense Advanced Research Projects Agency will support this new capability to research the use of ferroelectric high-voltage materials for compact directional neutron sources; we also expect support from other sponsors to further develop our sources for special nuclear material detection.

Publications

Tang, V., et al., 2008. "Crystal driven neutron source: A new paradigm for miniature neutron sources." *AIP Conference Proceedings* **1099**, 870–73. LLNL-PROC-406224.

Tang, V., et al., 2008. *Experimental investigation and simulations of liquid driven pyroelectric voltage sources for compact accelerators.* 20th Intl. Conf. Application of Accelerators in Research and Industry, Ft. Worth, TX, Aug. 10–15, 2008. LLNL-ABS-403201.

Tang, V., et al., 2009. *Fusion neutron sources for energy and national security applications.* LLNL-ABS 411131.

Tang, V., et al., 2009. "Intense pulsed neutron emission from a compact pyroelectric driven accelerator." *J. Appl. Phys.* **105**, 026103. LLNL-JRNL-407763.

Tang, V., et al., 2008. *Nano-structure ion sources for neutron production.* 20th Intl. Conf. Application of Accelerators in Research and Industry, Ft. Worth, TX, Aug. 10–15, 2008. LLNL-ABS-403195.

Tang, V., et al., 2008. "Neutron production from feedback controlled thermal cycling of a pyroelectric crystal stack." *Rev. Sci. Instrum.* **78**, 123504. UCRL-JRNL-233604.

Tang, V., et al., 2008. *Pulsed neutron emission from a compact spark plasma driven pyroelectric accelerator.* 50th Ann. Mtg. Division of Plasma Physics, Dallas, TX, Nov. 17–21, 2008. LLNL-ABS-408696.

Multipulse, High-Energy Backlighting for a Compton-Radiography Ignition Diagnostic for High-Power Lasers—Riccardo Tommasini (07-ERD-004)

Abstract

We intend to develop the capability for multipulse Compton radiography to obtain an ultrahigh-speed movie of the compressed deuterium–tritium (DT) fuel in laser ignition capsules as they evolve through ignition time. In addition, we will develop the ability to produce multiple radiographs over long delays (tens of nanoseconds), for a single, high-power laser shot. Such a capsule-implosion diagnostic would provide an unprecedented, time-resolved view of the DT fuel shape at peak compression, which will be an invaluable aid in achieving ignition. The large-delay, multipulsed radiographs would greatly decrease the number of laser shots required to achieve a given scientific result.

We expect to achieve a multipulse, high-energy radiography capability over a time interval of approximately 0.1 ns for high-power laser ignition experiments, and over tens of nanoseconds for high-energy-density physics experiments. In addition, we will develop a K-alpha backlighter with a high signal-to-noise ratio at approximately 80 keV for Compton radiography and at approximately 40 keV for high-energy-density physics experiments. Such experiments will benefit from multiple radiographs over long interframe delays (~20 ns) on a single fusion-class laser shot, greatly reducing the number of shots needed for high-pressure strength experiments. High-power laser experiments will benefit

from multipulse backlighting at approximately 80 keV over a time span of a few hundreds of picoseconds for Compton radiographs of ignition capsules as they evolve through ignition time, allowing the hohlraum to be tuned to maximize capsule symmetry.

Mission Relevance

Our proposal is exceptionally well aligned with the stockpile stewardship and energy security missions of the Laboratory, by developing a unique Compton radiography ignition diagnostic for fusion-class lasers, as well as a multipulse, high-energy radiography capability to increase the accuracy of measurements and reduce the number of experimental laser shots. The Compton radiography diagnostic will greatly improve our ability to achieve ignition on fusion-class lasers, giving a time sequence of two-dimensional images of the compressed DT fuel.

FY09 Accomplishments and Results

In FY09 we (1) measured the conversion efficiency for the 100 to 200-keV broadband Bremsstrahlung backlighters, which exceeded 1 part in 10^4 and approached 1 part in 10^3; (2) demonstrated source sizes of about 6 µm for x-ray photon energies greater than 100 keV using 5-µm-thick gold foils and wires; (3) demonstrated radiographs based on Compton scattering using thick carbon–hydrogen samples; (4) performed experiments on the OMEGA Extended Performance (EP) laser at the University of Rochester, where we extended the results obtained on Livermore's Titan system to higher energies and obtained two-dimensional radiographs of tungsten spheres at photon energies exceeding 100 keV using gold micro-wire backlighters; (5) demonstrated two-dimensional Compton radiography on imploding deuterium–deuterium-filled plastic shells at OMEGA and OMEGA EP; (6) finalized the design of backlighter targets and shielding for the National Ignition Facility; and (7) predicted Compton radiography performance as a function of implosion yield and associated background. The successful completion of this project allowed us to develop efficient Bremsstrahlung backlighters and to record, for the first time, two-dimensional radiographs of imploding shells near peak compression. These radiographs have spatial and temporal resolution of 10 µm and 10 ps, respectively, and demonstrate a novel technique of x-ray backlighting and areal density measurements for inertial-confinement fusion experiments and for applications in plasma physics. Our novel technique is now being adapted to programmatic measurements for the National Ignition Facility.

Publications

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Cladding-Pumped Raman Fiber Lasers—Jay Dawson (07-ERD-005)

Abstract

We propose to develop a cladding-pumped Raman fiber amplifier. This device will enable us to generate extremely high-energy pulses in multimode, rare-earth-doped fiber amplifiers and efficiently convert that light to a diffraction-limited laser beam with tens of millijoule pulse energies and hundreds of watts of power. This new capability will enable applications of interest to the Laboratory such as x-ray generation; very high-energy, short-pulse laser front ends; and high-speed cutting and welding in compact, robust all-fiber formats. We believe this technology will scale several orders of magnitude beyond the current state of the art in fiber pulse energy with diffraction-limited beam quality.

We expect to demonstrate a cladding-pumped Raman laser with greater than 200-kW peak power pulses in a short length of

optical fiber. This will show that it is possible to construct short and efficient cladding-pumped Raman lasers with good beam quality. This will result in one or more publications and possibly significant intellectual property. We further expect to investigate theoretically the scaling properties of such a laser. The laser proposed here would be capable of accessing new regimes of pulse energy and average power in a compact and robust format not available in other types of systems. The inherent bandwidth of the Raman transition would also enable short-pulse applications of the system.

Mission Relevance

High-average-power, high-energy laser systems support our national security mission along a broad front of applications. These include materials processing such as laser peening to strengthen aircraft engines and airframes, x-ray generation such as backlighters for future fusion-class laser experiments and for pulse-probe shock experiments, and remote sensing of chemical-absorption signatures to determine the presence and distance of chemicals relevant to nonproliferation and homeland security.

FY09 Accomplishments and Results

In FY09 we (1) achieved a brightness enhancement of 192 with output pulse energies of 20 µJ from the fiber laser system, (2) designed the desired specialty optical fiber needed to suppress the second Stokes scattering line of the Raman process, and (3) developed a comprehensive oscillator model showing that with the correct waveguide design, this process can directly convert diode laser light to a diffraction-limited laser beam. In summary, this project's experimental and theoretical work has shown that the process developed can be used to directly convert diode laser light to a diffraction-limited beam with high efficiency. This process should find many practical applications.

Publications

Sridharan, A., et al., 2009. "Brightness enhancement in a high peak power cladding pumped Raman fiber lasers." *Optic. Lett.* **34**, 2234. LLNL-JRNL-412359.

Maximizing the Science from Astrophysical, Time-Domain Surveys: Targeted Follow-Up—

Kem Cook (07-ERD-014)

Abstract

Lawrence Livermore has created the field of modern, wide-field, time-resolved astronomy through the Massive Compact Halo Objects (MACHO) project, and continues to expand this field in current surveys such as SuperMACHO, the Probing Lensing Anomalies Network (PLANET), the Lowell Observatory Near-Earth Object Search (LONEOS), and the Taiwanese American Occultation Survey (TAOS), which are producing tens of terabytes of image data. In this project, we will use these data to extract science and prioritize follow-up observations in several research avenues, including (1) searching for extrasolar planets, (2) probing dark energy, (3) characterizing historic supernovae through light echo spectroscopy, (4) investigating galactic structure and formation history, and (5) constraining stellar physics. The appropriate follow-up observations will be staged at leading telescope facilities such as Keck, Gemini, and Boyden and will extend and leverage the data already in archives.

We will address some of the most important questions in astronomy and physics today. Are there planetary systems similar to our own? What is the fate of the universe? In addition, we will produce new results in several fields of astrophysics, including (1) finding extrasolar planets representative of those in our solar system; (2) reducing uncertainties in the dark energy equation of state; (3) characterizing the historical rate of type Ia supernovae through light echo spectroscopy; (4) obtaining galactic halo structure and formation history from LONEOS RR Lyr stars; (5) determining the delta Scuti distance to the Large Magellanic Cloud, which is a key rung in the cosmic distance ladder; (6) exploring stellar physics such as limb darkening via microlensing; and (7) determining the time evolution of stellar pulsations and their effect on mass loss.

Mission Relevance

The project is related to Laboratory research efforts in exploration and use of space, which benefit LLNL missions in national security and fundamental science. Determining the abundance of planets in the galaxy will showcase Livermore's scientific and computing capabilities, which helps retain and recruit the best scientific and technical minds. This project will demonstrate how coordinated follow-up to a wide-field, time-domain survey such as the Large-Area Synoptic Survey Telescope can greatly enhance its scientific payoff.

FY09 Accomplishments and Results

We have successfully completed the optimization of follow-up observations from a variety of wide-field, time-domain surveys and have published numerous exciting scientific results from this research. Specifically, in FY09 we (1) successfully applied for time for more imaging light echo observations and spectroscopy of the new light echos; (2) collected data on light echos from Cas A, Tycho, 3C 58, and Crab supernovae; (3) determined delta-Scuti variables found in the Large Magellanic Cloud by mining SuperMACHO data; (4) analyzed data on the unusually bright supernova and active galactic nuclei behind the Large Magellanic

Cloud; (5) collected Hubble Space Telescope imaging of all the SuperMACHO microlensing candidates—results on microlensing detection efficiency were combined with the Hubble Space Telescope data to generate estimates of the baryonic content of the Milky Way's halo; and (6) continued analyzing PLANET microlensing results. LONEOS and MACHO follow-up studies were not pursued because of lack of funding.

Publications

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Discovery of a Light Higgs Boson with b Quarks—
David Lange (07-ERD-015)

Abstract

A new era in particle physics will begin when the Large Hadron Collider (LHC) comes fully online and advances the high-energy frontier to a center-of-mass energy of 14 TeV. We propose to develop a technique that may discover the Higgs boson by enhancing detection of b quarks in the first data samples produced from experiments at the LHC. We will develop the particle-identification techniques, trigger algorithms, and

analysis codes to search for the Higgs boson in its dominant decay mode. We are focused on the first data sample, where we will commission our apparatus and measure backgrounds to confirm our simulations. These measurements will result in one of the first-ever analyses of the dominant decay mode at the LHC.

Discovery of the Higgs boson would represent the beginning of a new era in particle physics—understanding new phenomena at the teraelectronvolt scale. Understanding the light Higgs sector will be one of the first physics goals of the LHC, and we will play a leading role in the search for the Higgs boson with b quarks, leveraging LLNL's B-Factory expertise in b-quark decay kinematics and event-filtering technologies to discover this decay channel.

Mission Relevance

The data-mining, analysis, and computing capabilities developed in this project for collider physics have direct application in homeland security applications for detecting subtle patterns in massive sets of disparate data. This work also supports the Laboratory's mission in breakthrough science by enabling LLNL to play an important role in discoveries that will have a profound impact on particle physics. In addition, this research will also be an exceptional recruiting tool for outstanding young scientists with both radiation-detection and computer-simulations capability required for the Laboratory's nonproliferation and homeland security work.

FY09 Accomplishments and Results

Using the Compact Muon Solenoid and simulated events, we completed our analysis for measuring the event characteristics of Z bosons produced with two or more particle jets by the LHC. Although the first LHC run began too late to carry out this data analysis, we were able to carry out additional work in commissioning the detector for its first physics run. We led efforts both to deploy high-level trigger algorithms in the data acquisition system and to integrate improved reconstruction algorithms into the FY09 effort to collect data based on cosmic rays. The successful completion of project enabled the development of LLNL analysis techniques for the discovery of new phenomena from the first LHC data and for significant advancements in experimental techniques in the operation of the high-level trigger for the Compact Muon Solenoid. We anticipate DOE Office of Science support in applying the techniques developed in this project to the first LHC data.

Publications

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A New Approach to Simulating Inhomogeneous Plasmas for Inertial Fusion Energy and Other Applications—

David Grote (07-ERD-016)

Abstract

We propose to develop a novel approach to simulating inhomogeneous magnetized plasmas and to begin applying this new method to problems of importance to Lawrence Livermore. Numerical simulations of such plasmas—which arise in fast ignition, magnetic fusion energy, and space sciences—are challenging. The newly developed drift-Lorentz particle mover has proven very effective for heavy-ion fusion by enabling the use of significantly larger time steps. The goal of our research is to extend this invention, combining it with implicitness and collisions, so that it can be applied to fast ignition for inertial fusion and a broad range of other significant problems relevant to Laboratory missions.

If the project is successful, we expect to demonstrate an advanced plasma simulation capability that substantially reduces the computational effort needed for simulations of inhomogeneous, magnetized plasmas, based on a novel method that differs qualitatively from anything now available. For fast ignition, this should enable more robust calculations, with a more accurate treatment of interparticle collisions. This approach may also prove a simpler alternative to the gyrokinetic formulation widely used in magnetic fusion energy core-turbulence studies, which becomes complex when applied to edge plasmas. When completed, our project would place LLNL in a better position to assess the promise of this idea. The new capability could benefit other areas as well, such as space plasmas.

Mission Relevance

This project is designed to strengthen LLNL's capabilities in fast ignition for inertial fusion energy, a longstanding Laboratory strategic goal. With a strong foundation created for magnetic fusion energy and heavy-ion fusion, we seek to build capabilities as interest in inertial fusion energy increases. This capability therefore supports the Laboratory's missions in energy security and breakthroughs in fundamental science and technology, as well as advancing the supercomputing environment on which stockpile stewardship is based.

FY09 Accomplishments and Results

In FY09 we further developed and tested the electrostatic version of the drift-Lorentz algorithm in the context of the electrostatic particle-in-cell code WARP. We discovered during testing that a multidimensional implicit sheath model at material boundaries was necessary to take advantage of our algorithm. Implementing this physics phenomenon into the code was a significant effort beyond the scope of this project. However, we were successful in our second major goal, to implement the Langevin collision operator in codes used for modeling plasmas. This algorithm underwent extensive testing and is now used extensively in fast-ignition research at the Laboratory. This has proved to be an important part of the study of deposition of energy from the laser-generated electron beam into the target.

Publications

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Techniques for Supernova Cosmology with the Large Synoptic Survey Telescope—Scot Olivier (07-ERD-023)

Abstract

We propose to develop and test techniques for precisely quantifying the properties of cosmic dark energy using observations of supernovae with the Large Synoptic Survey Telescope (LSST). The LSST, a large-aperture optical-imaging facility, will be the most powerful astronomical survey instrument of the next decade. It was designed to address fundamental questions concerning the structure and evolution of the universe. Leveraging LLNL's leadership position in LSST-related research, we intend to establish the Laboratory's preeminent scientific leadership in supernova cosmology by elucidating the nature of the mysterious dark energy that is driving acceleration of the cosmic expansion.

The discovery of the accelerated expansion of the universe is based on less than 100 Type Ia supernovae, indicating their importance as distance indicators. In contrast, LSST will discover approximately 2.5 million Type Ia supernovae out to a redshift of approximately 0.8. Even a small subset of these supernovae, if properly observed, will allow for a precise map of cosmic expansion with unprecedented constraints on the equation of state of dark energy of the universe. Our goal is to develop tools to simulate the capability of LSST in discovering distant supernovae and to optimize strategies for controlling systematic errors.

Mission Relevance

This project will help make important advances in astrophysics and space science with national security applications by leveraging the Laboratory's expertise in high-energy-density physics, nuclear fusion, instrumentation and diagnostics, and scientific computing and data management. In particular, large-scale data management and image analysis techniques have specific relevance to similar efforts in nonproliferation and homeland security.

FY09 Accomplishments and Results

In FY09 we (1) completed an analysis of the accuracy of redshift estimates from supernova light curves (photometric redshifts) and the resulting accuracy of measurements of cosmological parameters, allowing us to define the baseline LSST capability for supernova cosmology; (2) completed an evaluation of the effect of optical errors in the LSST design; (3) analyzed observations of supernovae to quantify characteristics that limit their accuracy as standard candles; and (4) incorporated models of supernovae into the comprehensive LSST data management, simulation, and visualization framework. This successful project enabled a fundamental understanding of the baseline LSST capability for supernova cosmology. The National Science Foundation and the DOE Office of Science will continue supporting this aspect of research and development for the LSST.

Publications

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Electronic Anomalies in Ordered and Disordered Cerium at High Pressures and Temperatures—Magnus Lipp (07-ERD-029)

Abstract

Because of strong electron correlation, cerium exhibits unusual behavior as a function of pressure and temperature—it undergoes a large anomalous volume collapse ending at a critical point, unique among the elements, and shows a melt line with a pronounced minimum. In addition, the magnetic susceptibility switches from the Curie type to Pauli paramagnetism across the

transition. However, large gaps exist in our knowledge of cerium. Its phase diagram is not well understood, and only little data exist above the critical point. Moreover, the mechanism hypothesized to underlie volume collapse is controversial. Our proposed experimental and theoretical study addresses these intensely debated issues by determining the structure of solid and liquid cerium with high precision using high-energy x-ray scattering and by measuring susceptibility in a large-volume diamond anvil cell. Building on these accomplishments, we intend to extend these studies to another f-metal, curium.

This project will increase our understanding of the behavior of cerium, including (1) if its anomalous transition is not isostructural but rather a second-order transition extending from the critical point to the melt-line minimum, (2) whether a remnant of this transition continues into the melt and separate liquids of different density, and (3) if the change in entropy across the transition is because of electrons alone, which is an assumption recently challenged because of the neutron scattering of phonons. Our experiments will interface heavily with theoretical efforts centering on the different mechanisms proposed to cause the anomalous transition.

Mission Relevance

The physics of f-electron correlation in the lanthanides and actinides is central to the Stockpile Stewardship Program. Such research will provide crucial data in support of the Laboratory's national security and stockpile stewardship missions.

FY09 Accomplishments and Results

In FY09 we (1) investigated the bare (magnetic) moment of cerium by x-ray emission, revealing a surprisingly large drop in the intensity of the satellite structure across the volume collapse; (2) performed several x-ray scattering experiments on liquid cerium and bismuth under conditions of high pressure and temperature; and (3) began measurements of cerium susceptibility using a designer diamond anvil cell. The experimental techniques developed and tested during this project—to achieve simultaneous conditions of high pressure and high temperature for the study of the volume collapse of cerium in a safe and efficient manner—have been adopted at the Laboratory for experiments on radioactive actinides.

Publications

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Quantum Properties of Plutonium and Plutonium Compounds—Michael Fluss (07-ERD-048)

Abstract

The anomalous properties of plutonium and plutonium alloys arise from correlation effects, but the organizing principle and the order parameter are unknown. We are using negative-pressure tuning with americium and performing physical property measurements of plutonium at low temperatures using low-specific-activity plutonium-244 to understand the element's ground state. Recent collaboration has provided unique experimental measurements of the phonon density of states of alpha and delta plutonium, which enhances our understanding of interatomic potentials and thermodynamics. We have added dynamical mean field theory calculations of plutonium to quantitatively correlate with experiments.

Our goal is to understand how plutonium's quantum properties are connected to its unusual physical properties. This project will result in an improved physical picture of the electronic structure of plutonium and a concomitant understanding of the consequences of real-world effects such as impurities, radiation damage, radiogenic products, pressure, and temperature. Measurement of the spin-pairing mechanism will identify the underlying basis for many of plutonium's properties. In a scientifically broader sense, significant progress in this area will result in an improved physical picture for many other complex materials such as copper oxide superconductors. Successful processing and use of plutonium-244 metal in scientific studies create important new skills and knowledge for Lawrence Livermore that open the door to a completely new class of experimentation on plutonium.

Mission Relevance

This project sustains and nurtures the Laboratory's expertise in fundamental plutonium science by focusing on a 21st century solid-state challenge—understanding 4f and 5f elements in the vicinity of f-electron localization. The project will result in new skills and usher in a new class of plutonium research using low-activity plutonium-244 to perform experiments previously not possible. The research proposed here, if successful, has the potential to profoundly change our understanding of the fundamental properties of plutonium and plutonium compounds, an important effort that supports the Laboratory's mission in stockpile stewardship and the ability to create breakthroughs in fundamental science and technology.

FY09 Accomplishments and Results

In FY09 we completed resistivity and the associated magnetoresistive measurements for delta plutonium and a plutonium–americium alloy—we observed differences in the magnetoresistivity, while Hall effect measurements provided insight into the electronic structure. Our radiation damage studies provided new information about several annealing stages, including the kinetics, and represent a significant departure from current molecular dynamics models. In addition, we extended dynamical mean field theory coupled with density functional theory to look at vacancies and interstitials in both alpha and delta plutonium, with the results showing significant changes to the f-electron count that predict changes in the physical properties. These are consistent with our experimental measurements. The successful conclusion of this project resulted in the development of new tools for working with small samples of plutonium, an increased understanding of the fundamental physical properties of plutonium, insight into the nature of radiation damage in these materials, and extension of dynamical mean field theory to plutonium, its alloys, and the influence of impurities and vacancies.

Publications

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A Plasma Amplifier Toward Zettawatt Laser Powers—
Robert Kirkwood (07-ERI-004)

Abstract

We propose to develop a technique to increase laser power with three-wave stimulated mixing and pulse compression in a plasma. The goal is to demonstrate pulse compression that will allow existing laser facilities to operate with as much as a thousand times higher output powers than can be obtained with conventional approaches. This advantage is possible because of the much higher power-handling limits of a plasma (<10^{14} W/cm^2) than of conventional solid-state optics (<10^{11} W/cm^2). This project is a critical step in enhancing the high-power operating regime for fusion-class lasers, and has applications in inertial fusion, radiation sources, and particle accelerators as well as providing critical data on the saturation of stimulated Raman scattering.

We expect that experiments with Livermore's Janus and COMET laser systems will demonstrate depletion of the Janus beam by the Raman amplification of the 1-ps COMET beam for a duration of greater than 10 ps, thereby demonstrating pulse compression of a 1-ns beam in a plasma. We intend to further establish the intensity and plasma conditions necessary to compress an entire 1-ns pump in future experiments. In addition, we will obtain measurements of the saturated levels of seeded, stimulated Raman scattering to verify models of wave saturation, on a time scale too fast for ion wave motions. We also will perform experiments combining pump beams for pulse compression of multiple beams. We expect our results will lead to publications in peer-reviewed journals.

Mission Relevance

The success of this research will support Laboratory missions in both stockpile stewardship and energy security, and open up new opportunities in high-energy-density science by substantially increasing the power of many existing lasers. The success of these experiments would leverage the existing petawatt beam program aimed at opening new, high-power operating regimes, and would enable study of laser–plasma interactions on the short time scale necessary to identify electron and ion saturation processes.

FY09 Accomplishments and Results

In FY09 we performed experiments in which a frequency-shifted, short-pulse seed beam interacted with a 20-ps Janus pulse. Amplification factors as high as 60-fold at low seed energy were demonstrated. As the seed energy increased, the amplification factor was observed to decrease more rapidly than our pre-experiment one-dimensional particle-in-cell simulations, limiting the maximum output seed power to 4 x 10^9 W. This demonstrated a window in which nonlinear effects nearly suppress scattering. Data with 0.5- and 3.5-ps duration seeds confirmed that the nonlinear effects scaled with power. This data is providing a benchmark for ongoing two-dimensional particle-in-cell simulations that will be used to design plasma amplifiers and take advantage of suppressed scattering to improve coupling in National Ignition Campaign targets. The successful conclusion of this project has provided a database for designing Raman amplifiers and pulse compressors in hot plasmas and controlling their effects in multibeam ignition experiments. In particular, the data identified high-dimensional nonlinear effects that limit Raman amplification and will determine amplifier and compressor design in the future. In addition, our research will allow for improved coupling in central hot spot ignition targets for the National Ignition Campaign. This campaign, in collaboration with Los Alamos National Laboratory, is developing a two-dimensional simulation model from the data obtained in these experiments. The model will be used to design future experiments that optimize coupling in hohlraums in the presence of Raman re-amplification from multiple intersecting laser beams.

Publications

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Kirkwood, R. K., et al., 2009. *Amplification of light by Langmuir waves in a hot, strongly damped plasma and its relevance to ignition and pulse compression.* 39th Ann. Anomalous Absorption Conf., Bodega Bay, CA, June 14–19, 2009. LLNL-ABS-412263.

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Kirkwood, R. K., et al., 2009. "Light amplification by seeded stimulated Raman scattering of a crossing beam and its saturation as is relevant to ignition." *Bull. Am. Phys. Soc.* **54**(15), J05.6. LLNL-ABS-405480.

Kirkwood, R. K., et al., 2009. *Observation of amplification of light by Langmuir waves and its saturation on the electron kinetic time scale.* LLNL-JRNL-413257.

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Ping, Y., et al., 2008. *Progress in laser pulse amplification by stimulated Raman scattering in a plasma.* 50th Ann. Mtg. Division of Plasma Physics, Dallas, TX, Nov 17–21, 2008. LLNL-ABS-405599.

Uncovering Supersymmetric Leptons at the Large Hadron Collider—Jeffrey Gronberg (07-LW-037)

Abstract

A new era in particle physics will begin when the Large Hadron Collider (LHC) at the CERN particle physics laboratory near Geneva, Switzerland, comes fully online. The LHC will be the first collider to reach the energy regime where current theory predicts an entirely new realm of particle physics. Although expected to enable discovery of new fundamental particles, the LHC will be blind to an entire class of new particles—supersymmetric leptons. We propose to develop a novel triggering technique based on exploiting photon–photon interactions of beam protons, which would allow discovery of the new particles. We will study the analogous process of dimuon production in photon–photon events from actual data to determine if a supersymmetric lepton trigger would be successful.

The LHC experiments, as currently designed, will miss a significant piece of the puzzle necessary to discover fundamental physics occurring at the teraelectronvolt scale. To complete the picture, experimentalists will need the capability to observe and study supersymmetric leptons. In this project, we will analyze dimuon production and, using these results, determine the feasibility of a supersymmetric lepton trigger. A trigger upgrade allowing supersymmetric leptons to be discovered would be a major enhancement to the LHC physics program, leading to major physics results, carving out a scientific leadership role for LLNL, and resulting in papers published in high-profile, peer-reviewed journals.

Mission Relevance

By providing access to the latest developments in detector technology, data processing, and data mining, this project furthers LLNL's missions in nonproliferation and homeland security, which heavily utilize all three of these capabilities. This project also will help recruit scientific talent in high-energy physics, whose expertise is applicable to radiation detection and other cutting-edge national security work.

FY09 Accomplishments and Results

In FY09, we participated in the cosmic ray run at the LHC's Compact Muon Solenoid using the full muon detector and used the resultant data to validate our calorimeter analysis technique for separating inclusive and exclusive events in dimuon analysis. We also adapted our analysis technique for the measurement of Standard Model dimuons to work at a center-of-mass energy of 10 TeV (as well as at 14 Tev). This was necessary after the LHC's accelerator accident, which delayed initial data taking by one year and lowered the initial energy. In this project, our design study demonstrated that a supersymmetric lepton trigger was worth pursuing with new forward detectors. Partly because of our achievements, LLNL's measurement of Standard Model dimuon production was selected for expedited publication with the first dataset, and a group was formed within the larger collaboration to develop and implement new forward detectors for the supersymmetric lepton trigger. We expect DOE's Office of Science to support the application of this newly developed expertise to development of the required precision timing system.

Publications

Gronberg, J., and J. Hollar, 2008. *Exclusive dilepton production at CMS.* LLNL-POST-405855.

Hollar, J. J., 2008. "Photon physics at CMS." *Proc. 12th Intl. Conf. Elastic and Diffractive Scattering.* LLNL-PROC-418602.

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Hollar, J., X. Rouby, and S. Ovyn, 2008. "Exclusive $\gamma\gamma \rightarrow l^+l^-$ and $\gamma p \rightarrow \Upsilon \rightarrow l^+l^-$ production." *Nucl. Phys. Proc. Suppl.* **179**, 237. LLNL-MI-402370.

Hollar, J., X. Rouby, and S. Ovyn, 2008. *Forward physics triggers.* LLNL-TR-402528.

Fast-Ignition Proof-of-Principle Experiments—

Pravesh Patel (08-SI-001)

Abstract

Our objective with this project is to investigate the feasibility of a new approach to laser ignition. Fast ignition directly compresses the fusion fuel to high densities and then ignites it with a separate laser beam. This is a scientifically and technologically challenging approach that if successful, offers the potential for large advances in efficiency over the potential baseline approach. We will design and undertake integrated fast-ignition experiments that will measure and optimize the laser-to-ignition hotspot-energy-coupling efficiency for a fuel assembly of the scale required for high-gain fast ignition. Our work will define the requirements for fast ignition and provide the pathway to robust 100-MJ yield platforms for experimental access to extreme high-energy-density environments.

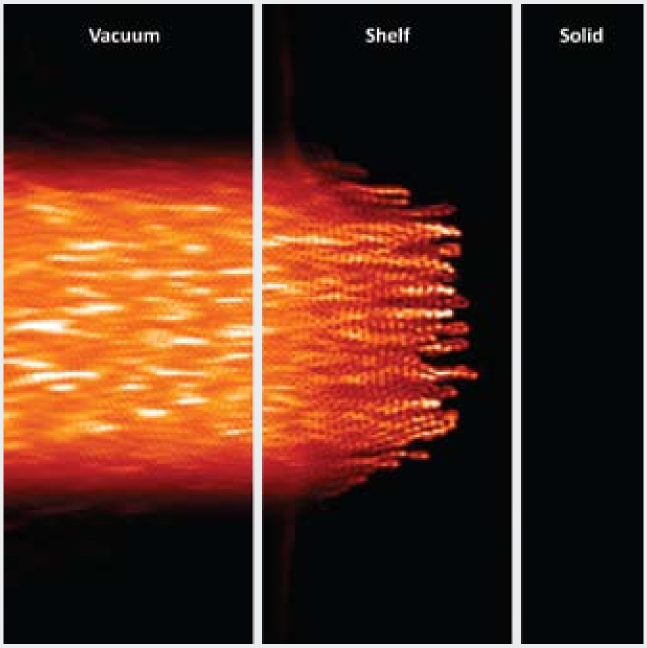
This project will define the requirements for high-gain fast ignition for future fusion-class laser systems. In particular, we will optimize isochoric fuel assembly in the presence of a cone and understand and optimize both ultra-intense laser–plasma interactions and energy transport by relativistic electrons to measure the short-pulse energy required to obtain high-gain fast ignition. This project will resolve the key physics uncertainties in fast ignition. Applications of robust, 100-MJ fast-ignition platforms will have broad implications for the Laboratory in high-energy-density science far beyond this specific project.

Mission Relevance

Ready access to the high-neutron and charged-particle fluxes produced by fast-ignition targets will enable a broad range of applications supporting LLNL's missions in stockpile stewardship and energy security, and allow access to new regimes of excited-state nuclear physics and basic science. Increased gain from fast ignition will enable an inertial fusion path to energy security. These challenging problems are at the forefront of the new scientific frontiers opened by new fusion-class laser facilities such as the National Ignition Facility (NIF), and will be important in recruiting and retaining exceptional scientists for the Laboratory.

FY09 Accomplishments and Results

We (1) completed a revised point design for the NIF integrated fast ignition experiment, combining two-dimensional radiation hydrodynamics calculations of shell implosion around a cone, short-pulse laser–plasma interaction, and fast electron transport; (2) designed risk-mitigation experiments for the OMEGA laser at the University of Rochester, which are scheduled for FY10; (3) performed two electron source experiments at Livermore's Titan laser; (4) performed simulations with new particle-in-cell, plasma simulation, and laser shock-processing codes; (5) tested our K-alpha imaging diagnostic on the Titan laser; and (6) performed numerous test bed validations of the NIF Advanced Radiographic Capability (ARC) adaptive optics and pointing system.



Particle-in-cell simulation of a high-intensity short-pulse beam interacting with a solid target at the National Ignition Facility Advanced Radiographic Capability.

Proposed Work for FY10

In FY10 we will (1) design and execute energetics, symmetry, and shock-timing campaigns at NIF to tune our spherical capsule implosion designs; (2) develop a two-dimensional design that optimizes fuel assembly around the cone tip; (3) develop an integrated point design with a self-consistent hydrodynamics assembly, NIF ARC beam interaction and electron generation, and electron transport and energy deposition; (4) perform sensitivity analysis of the point design; (5) perform experiments on OMEGA to validate new tuning strategies for deuterated polystyrene shells and single-shock pulse shapes; (6) design ARC radiography experiments to measure peak density and areal density around the cone tip; and (7) establish deuterated polystyrene shell experiments as a surrogate for full-scale deuterium–tritium shell fast-ignition experiments.

Publications

Akli, K., 2009. *Measurements of high-intensity, short-pulse laser–generated electron beam flux.* IFSA2009, 6th Intl. Conf. Inertial Fusion Sciences and Applications, San Francisco, CA, Sept. 6–11, 2009. LLNL-ABS-412303.

Chen, C. D., 2009. "Bremsstrahlung and Kalpha flurorescence measurements for inferring conversion efficiencies into fast ignition relevant hot electrons." *Phys. Plasmas* **16**, 082705. LLNL-JRNL-415191.

Kemp, A. J., 2009. *Full-scale kinetic modeling of short-pulse interaction and electron transport in cone target experiments.* IFSA2009, 6th Intl. Conf. Inertial Fusion Sciences and Applications, San Francisco, CA, Sept. 6–11, 2009. LLNL-ABS-411899.

Ma, T., 2009. *Effects of laser prepulse on hot electron production and transport in hollow-cone targets.* APiP2009, 16th Intl. Conf. Atomic Processes in Plasmas, Monterey, CA, Mar. 22–26, 2009. LLNL-ABS-409819.

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Mackinnon, A. J., 2009. *Progress in fast ignition studies with electrons and protons.* APiP2009, 16th Intl. Conf. Atomic Processes in Plasmas, Monterey, CA, Mar. 22–26, 2009. LLNL-ABS-409835.

MacPhee, A. G., 2009. *Explaining the effects of laser prepulse on hot electron generation in cones.* IFSA2009, 6th Intl. Conf. Inertial Fusion Sciences and Applications, San Francisco, CA, Sept. 6–11, 2009. LLNL-ABS-412374.

Patel, P. K., 2009. *Design of fast ignition core heating experiments with full scale hydrodynamic fuel assembly.* IFSA2009, 6th Intl. Conf. Inertial Fusion Sciences and Applications, San Francisco, CA, Sept. 6–11, 2009. LLNL-ABS-413395.

Tabak, M., 2009. *Features of a point design for fast ignition.* IFSA2009, 6th Intl. Conf. Inertial Fusion Sciences and Applications, San Francisco, CA, Sept. 6–11, 2009. LLNL-ABS-412196.

Nonequilibrium Electron Dynamics in Warm Dense Matter—Yuan Ping (08-ERD-005)

Abstract

Recent discoveries in the behavior of warm dense matter cannot be explained by existing theory because it ignores nonequilibrium and nonadiabatic effects. Our goal is to understand dynamic electron behavior under nonequilibrium extreme conditions and to advance condensed matter theory beyond adiabatic approximation. This will be an integrated experimental and theoretical effort, which will overcome a fundamental barrier in condensed matter physics by measuring temporal evolution of the electron density of states and introducing nonequilibrium electron distribution and nonadiabatic electron–phonon coupling in calculations. Measurements will be made using optical and x-ray probes, and theory development will be based on an extension of the Ehrenfest equation.

We will obtain temporal evolution of carrier density and dielectric function from optical measurements and temporal evolution of the N-edge and 4p–5d absorption line from x-ray measurements. These will be the first data on the behavior of electron density of states under nonequilibrium extreme conditions, serving not only as a phenomenological guide to model development, but also as a quantitative benchmark of theory. Our theory effort will yield calculations of nonequilibrium and nonadiabatic effects on carrier density, dielectric function, and x-ray absorption cross-section pertinent to our experimental program. The combined outcome will be the first step in advancing our understanding of condensed matter physics in a nonequilibrium extreme regime and beyond the adiabatic approximation.

Mission Relevance

The study of electron dynamics under nonequilibrium extreme conditions advances material science and supports Laboratory efforts in stockpile stewardship, while large-scale quantum molecular dynamics simulation advances the Laboratory's supercomputing efforts.

FY09 Accomplishments and Results

In FY09, we made a key discovery about electron degeneracy in warm dense matter produced by isochoric laser heating—that under nonequilibrium conditions, electron degeneracy leads to charge non-neutrality in a gold nanofoil. The new finding is crucial for proper understanding of the unique nature of nonequilibrium warm dense matter. An important manifestation of the phenomenon was its effect on dielectric function, which was consistent with our earlier measurements. We also obtained systematic single-shot data by chirped pulse measurements with an 800-nm pump pulse on warm dense gold. Preliminary analysis showed different electron dynamics with a 800-nm pump compared to 400-nm pump, demonstrating the concept of selective excitation.

Proposed Work for FY10

In FY10 we will complete systematic study of selective excitation of warm dense gold by a 800-nm pump via one- and two-photon absorption. The demonstration of selective excitation in controlling the resulting state of a warm dense solid would be a potential breakthrough because it is fundamental to extend isochoric heating to other excitation sources including free-electron lasers, energetic electrons, and ions as a universal platform in high-energy-density research. We will also design and perform an experiment to verify non-neutrality and complete time-resolved x-ray absorption spectroscopy at the Advanced Light Source at the Lawrence Berkeley National Laboratory. Our key theoretical efforts will be development of a practical method to introduce energy dissipation for electron–phonon coupling in simulations to assess nonadiabatic effects.

Publications

Ping, Y., 2009. *Dielectric function of non-equilibrium warm dense gold.* APS Topical Conf. Shock Compression of Condensed Matter, Nashville, TN, June 29–July 3, 2009, LLNL-ABS-410925.

Ping, Y., 2009. *Warm dense matter created by laser isochoric heating.* 2nd Intl. Conf. High Energy Density Physics, Austin, TX, May 19–22, 2009. LLNL-ABS-412082.

Ping, Y., et al., 2009. *Electron dynamics in warm dense gold under selective excitation.* Intl. Workshop on Warm Dense Matter, Hakone, Japan, Mar. 16–19, 2009. LLNL-ABS-410924.

Studying Reactions on Excited Nuclear States—
Lee Bernstein (08-ERD-008)

Abstract

The formation of heavy elements in stellar interiors involves reactions on both ground and excited nuclear states in the stellar high-energy-density (HED) plasma environment. Fusion-class lasers will offer an unprecedented opportunity to observe reactions on excited nuclear states because of the exceptionally short time over which the “burn” occurs and the nuclear–plasma interactions that occur in the HED plasma environment. We will study the nuclear–plasma interactions that take place in an HED plasma and the effect of the population of excited nuclear states on the nucleosynthesis reactions through an accelerator-based nuclear science program. In addition, we will develop a plan to carry out a new class of scientific experiments investigating these nuclear states at the National Ignition Facility (NIF).

This project will result in an increased understanding of both plasma–nuclear interactions and the effects that excited nuclear states, through these interactions, have on reactions in both stellar and stockpile stewardship environments. We will also produce an experimental plan for performing astrophysically relevant excited-state reaction experiments using fusion-class lasers such as the NIF. This work will be coordinated with the LDRD-supported program to develop nuclear diagnostic capabilities for fusion-class lasers and act to integrate the scientific capabilities needed for our unique work into the diagnostics being developed. This work will also result in high-profile publications and encourage greater involvement by the nuclear science community in fusion-class laser experiments.

Mission Relevance

This project’s insight into reactions on excited states will improve the interpretation of radiochemical data, which are a key nuclear weapons diagnostic used in both stockpile stewardship and homeland security (nonproliferation) applications. This project also supports the Laboratory’s mission in breakthrough science by improving interpretation of the radiochemical data relevant to formation of elements in astrophysical environments.

FY09 Accomplishments and Results

In FY09 we (1) performed a scoping experiment using Livermore’s Electron Beam Ion Trap to observe, for the first time, inverse internal conversion, which is a nuclear–plasma interaction relevant to astrophysical nucleosynthesis; (2) measured the ability of highly excited nuclear states to absorb photons from a high-energy-density plasma environment at Lawrence Berkeley Laboratory; (3) analyzed data from the molybdenum-93 and molybdenum-94 Silicon Telescope Array for Reaction Studies at Yale University and the Livermore Berkeley Array for Collaborative Experiments in collaboration with the nuclear physics group from the University of Oslo, who have determined the photon strength function and level density in these nuclei; (4) continued development of s-process nucleosynthesis measurements at the University of Rochester OMEGA and Livermore NIF laser facilities and submitted a draft proposal for a first experiment on NIF, and (5) prepared a manuscript for *Physical Review Letters* describing our results of nuclear–plasma interactions on highly excited states, with implications of this process for supernova-driven nucleosynthesis and prospective NIF experiments.

Proposed Work for FY10

In FY10 we will (1) perform a follow-on to the experiment at Lawrence Berkeley Laboratory , (2) complete a second manuscript describing measurements of cross sections of s-process branch-point nuclei using NIF, and (3) establish collaborations for NIF experiments with researchers from the Bruyères-le-Châtel nuclear research center in France and GSI's accelerator complex in Darmstadt, Germany.

Publications

Bernstein, L. A., et al., 2009. *Reactions on nuclei in high energy density plasmas.* 2nd Workshop Level Density and Gamma Strength, Oslo, Norway, May 11–15, 2009. LLNL-ABS-412220.

Bernstein, L. A., et al., 2009. *Studying reactions on excited states using NIF.* Fall Mtg. American Chemical Society, Washington, DC, Aug. 16–20, 2009. LLNL-ABS-411365.

Wiedeking, M., et al., 2009. *Determining lifetimes of highly excited nuclear states.* LLNL-PRES-417198.

Exploration of Laser–Plasma Interactions for High-Performance Laser-Fusion Targets—David Strozzi (08-ERD-017)

Abstract

We will use kinetic simulation and analytic theory to study nonlinear laser–plasma interactions relevant to advanced, future laser-fusion targets. For many planned laser applications, laser–plasma interactions (such as Raman and Brillouin scattering) are expected to be in a nonlinear regime, and uncertainty regarding these interactions has led to several conservative design choices. Better understanding of the interactions may reduce these constraints and expand future laser capabilities (e.g., enable the use of higher-energy "green" laser light). For our project, we will use the three-dimensional (3D) particle-in-cell code Z3 and the one-dimensional Eulerian Vlasov code Sapristi, and, if available, a two-dimensional Vlasov code currently in development.

Our research will advance the knowledge of nonlinear laser–plasma effects, including particle trapping, the Langmuir decay instability, and Coulomb collisions. Moreover, we will understand how these phenomena interact and how they develop in the multidimensional geometry of a finite laser speckle. We expect to elucidate the mechanisms that saturate laser–plasma interactions in regimes of interest, as well as potential enhancement of these interactions such as by Raman "inflation." More broadly, we will advance kinetic plasma simulation and theory, and expand the knowledge of multidimensional, kinetic codes for laser–plasma interactions. We anticipate our research will result in high-level, peer-reviewed publications and attract a talented postdoctoral researcher.

Mission Relevance

An enhanced laser–plasma interaction predictive capability will greatly benefit experimental design by allowing future fusion-class lasers to operate in regimes currently being avoided, greatly increasing available laser energy. Large, high-power laser systems are essential tools for studying weapons physics for stockpile stewardship and inertial-confinement fusion, in support of Lawrence Livermore's national and energy security missions.

FY09 Accomplishments and Results

In FY09 we (1) extended our kinetic analysis of Langmuir decay instability to the filamentation and modulation of plasma waves; (2) performed particle-in-cell simulations of Raman scattering in conditions in ignition targets; (3) continued work on the bounce-number figure of merit for trapping nonlinearity; (4) conducted 1D Vlasov simulations of Raman re-amplification in crossing laser beams; (5) calculated the fully relativistic Thomson scattering cross-section, which agreed with previous LLNL experiments; (6) participated in the modeling of secondary ion-wave instabilities in Brillouin scatter; and (7) studied the nonlinear aspects of experimental Raman spectra, side scatter, and the two-plasmon decay of Raman light.

Proposed Work for FY10

In FY10 we will (1) validate a reduced model of nonlinear Raman scattering in the pF3D code against 1D Vlasov and 2D and 3D particle-in-cell calculations and apply it to OMEGA Laser System experiments and advanced laser-fusion designs; (2) apply our Langmuir decay instability threshold condition to laser-fusion designs and assess the relative importance of instability and electron trapping; (3) study nonlinear aspects of the two-plasmon decay—such as saturation, conversion efficiency, and hot electron spectrum—with a 2D particle-in-cell code, (4) use the Vlasov code Sapristi to study Brillouin scattering with kinetic electrons; and (5) investigate Raman scattering in the presence of multiple Langmuir waves, such as in the laser entry hole of a hohlraum target.

Publications

Benisti, D., et al., 2009. "Nonlinear Landau damping rate of a driven plasma wave." *Phys. Rev. Lett.* **103**, 155002. LLNL-JRNL-418707.

Cohen, B. I., et al., 2009. "Stimulated Brillouin backscattering and ion acoustic wave secondary instability." *Phys. Plasmas* **16**, 032701. LLNL-JRNL-407238.

Kruer, W. L., 2008. *Assessing the two-plasmon decay instability in ignition-scale hohlraums.* 50th Ann. Mtg. Division of Plasma Physics, Dallas, TX, Nov. 17–21, 2008. LLNL-PRES-408928.

Palastro, J. P., et al., 2009. *Kinetic dispersion of Langmuir waves.* 39th Ann. Anomalous Absorption Conf., Bodega Bay, CA, June 14–19, 2009. LLNL-ABS-402824.

Palastro, J. P., et al., 2009. *Kinetic dispersion of Langmuir waves.* IFSA2009, Inertial Fusion Sciences and Applications, San Francisco, CA, Sept. 6–11, 2009. LLNL-PRES-413869.

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Palastro, J. P., et al., 2009. *Kinetic dispersion of the Langmuir decay instability and its relevance for ignition plasmas.* 50th Ann. Mtg. Division of Plasma Physics Meeting, Dallas, TX, Nov. 17–21, 2008. LLNL-PRES-418722.

Strozzi, D. J., et al., 2009. *Role of electron trapping in SRS on NIF ignition targets.* 39th Ann. Anomalous Absorption Conf., Bodega Bay, CA, June 14–19, 2009. LLNL-PRES-413928.

Towards a Universal Description of Nuclei with Monte Carlo Methods—William Ormand (08-ERD-018)

Abstract

We propose to investigate the application of Monte Carlo methods to develop a universal picture of nuclei spanning the periodic table. We will accomplish this by building on our recent breakthrough on the "sign problem" and applying auxiliary field Monte Carlo (AFMC). The AFMC method can provide exact results for systems with extraordinarily large dimensions, thus enabling for the first time, the basic capability needed to address the nuclear many-body problem. We will first apply our unique AFMC capability to large-scale problems with existing nuclear interactions and the Hubbard model. Then we will couple AFMC with mean-field methods to develop the first truly microscopic and universal picture of nuclei. This work will have broad scientific and programmatic impact.

The extreme complexity of the nuclear many-body problem has limited the description of nuclei heavier than iron to mean-field pictures that lack the full range of quantum correlations. Defeating the sign problem with the AFMC method will enable us, for the first time, to address previously impossible problems in nuclear theory and to deliver a universal picture for nuclei with unsurpassed predictive power. This will allow us to accurately describe very exotic nuclei far from the valley of stability, which are crucial to the synthesis of elements in the cosmos and will be the focus of DOE's next-generation accelerators in nuclear physics.

Mission Relevance

This project will utilize LLNL's high-performance computational capability to deliver a universal theory for nuclei. Our research will provide LLNL with the unique theoretical foundation to substantially improve nuclear structure inputs required by reaction theories, which in turn will significantly reduce uncertainties in nuclear data important to the Stockpile Stewardship Program.

FY09 Accomplishments and Results

In FY09 we (1) completed implementation of the shifted-contour method in the original Caltech AFMC codes, (2) examined application of the shifted-contour method on an analytic model, (3) developed codes to use Monte Carlo methods to determine basis states with angular-momentum projection and successfully demonstrated this approach for the ground state of a test case—this establishes a formalism for applications to a wide range of nuclei, and (4) established a collaboration with Oak Ridge National Laboratory to begin coupling of the new approach to mean-field methods.

Proposed Work for FY10

With the hybrid AFMC configuration-interaction code completed and tested, in FY10 we will (1) apply the code to perform nuclear structure studies with conventional shell-model interactions, but for systems beyond current computational capability; (2) explore the evolution of shell structure for nickel isotopes along the assumed neutron shell boundary; (3) couple the AFMC configuration-interaction method to mean-field methods employed by the LLNL density functional theory effort; and (4) explore the viability of coupling quantum correlations with mean-field methods to develop a more universal picture of nuclei. This would be the first attempt to include the full effect of quantum correlations within a mean-field picture for a wide range of nuclei.

Publications

Ormand, W. E., 2008. "Microscopic approaches to nuclear structure: Configuration interaction." *Eur. Phys. J. Special Topics* **156**(1), 13. UCRL-PROC-234913.

Stoitcheva, G., et al., 2007. "Tackling the fermionic sign problem in the auxiliary-field Monte Carlo method." *arXiv*, 0708.2945 v1. UCRL-JRNL-233254.

Innovative Divertors for Future Fusion Devices—Dmitri Ryutov (08-ERD-019)

Abstract

This project will attempt to resolve the critically important problem of reducing thermal loads in heat exhaust systems (divertors) of tokamak-based fusion reactors and neutron test facilities to a level below 10 MW/m^2. We have identified several solutions based on novel divertor configurations that would lead to enhancement of turbulent and convective plasma spreading over the divertor plate. We also envision the use of magnetic

materials and toroidally asymmetric coatings of divertor plates. Combining novel approaches to design, new materials, analytical theory we have developed, and numerical simulations based on Livermore BOUT and UEDGE computer codes, we will determine optimal divertor concepts for the next generation of U.S. fusion facilities.

We will develop a set of divertor concepts suitable for the planned National High-Power Advanced Torus Experiment and Component Test Facility at Princeton and the General Atomics Fusion Test Facility, as well as for future commercial reactors. We will devise appropriate tests on existing fusion devices at General Atomics and Princeton, and expect to produce journal publications, patents, and preliminary design specifications. Successful completion of this project will mean the solution of a problem of critical importance for toroidal fusion reactors. Lawrence Livermore will be well-positioned to become a leader in one of the key areas of fusion research and development at a time when funding of U.S. projects is expected to increase because of the International Thermonuclear Experimental Reactor tokamak consortium and completion of their fusion-research reactor construction phase.

Mission Relevance

Harnessing fusion energy would be a tremendous breakthrough in ensuring a safe energy future for the nation and mitigating possible international tensions over energy resources. In addition, the proposed research and development in the fusion energy area will lead to significant progress in plasma physics and material science, which supports the Laboratory's mission in stockpile stewardship.

FY09 Accomplishments and Results

We (1) performed an analytical assessment of the feasibility of inducing magnetic stochasticity using plasma-driven currents in the tokamak, showing that such stochasticity is possible for present-day devices; (2) performed UEDGE analysis of a snowflake divertor in the radiative mode, showing that the snowflake performs better than the standard divertor; (3) conducted BOUT simulations of the induced convection for tilted divertor plates; and (4) began, in collaboration with Princeton and General Atomics, experiments suitable for benchmarking the BOUT results.

Proposed Work for FY10

In FY10 we will (1) analyze the impact of the snowflake divertor on magnetohydrodynamic edge stability and charged-particle drift orbits; (2) extend the UEDGE analysis to quantify the performance of a range of possible magnetic divertor geometries, including the snowflake and Super-X setups for future devices; (3) perform BOUT simulations of the induced convection for various types of surface perturbations of divertor plates; (4) continue collaboration with Princeton and General Atomics to devise and analyze experiments using the snowflake and other possible configurations; and (5) identify best materials for induced convection and induced currents approaches to reducing heat loads.

Publications

Joseph, I., 2009. "Driving toroidally asymmetric current through the tokamak scrape-off layer, part II: Magnetic field structure and spectrum." *Phys. Plasmas* **16**, 052511. LLNL-JRNL-412074.

Joseph, I., 2009. *Driving toroidally asymmetric current through the tokamak scrape-off layer to suppress edge localized modes.* Intl. Sherwood Fusion Theory Conf., Denver, CO, May 3–5, 2009. LLNL-ABS-409785.

Joseph, I., in press. "Magnetic spectrum produced by non-axisymmetric scrape-off layer current in the two-wire model and the strike point shadow." *Contrib. Plasma Phys.* LLNL-JRNL-416576.

Joseph, I., R. H. Cohen, and D. D. Ryutov, 2009. "Driving toroidally asymmetric current through the tokamak scrape-off layer, part I: Potential for ELM suppression." *Phys. Plasmas* **16**, 052510. LLNL-JRNL-411897.

Ryutov, D. D., 2009. *The dynamics of coherent scrape-off layer structures in a snowflake divertor.* 50th Ann. Mtg. Division of Plasma Physics, Dallas, TX, Nov. 17–21, 2008. LLNL-ABS-405443.

Ryutov, D. D., and M. V. Umansky, in press. "Ion drifts in a snowflake divertor." *Phys. Plasmas.* LLNL-JRNL-418155.

Ryutov, D. D., et al., 2008. "A snowflake divertor: A possible way of improving the power handling in future fusion facilities." *Proc. 2008 Fusion Energy Conf.*, LLNL-CONF-407193.

Umansky, M. V., et al., 2009. "Analysis of geometric variations in high-power tokamak divertors." *Nucl. Fusion* **49**, 075005. LLNL-JRNL-410565.

Umansky, M. V., et al., in press. "Edge plasma in a snowflake divertor." *Contrib. Plasma Phys.* LLNL-CONF-416151.

Zweben, S. J., R. H. Cohen, and D. D. Ryutov, 2009. "Local scrape-off layer control using biased electrodes in NSTX." *Plasma Phys. Contr. Fusion* **51**, 105012. LLNL-JRNL-414426.

High-Temperature Thermal X-Radiation Sources at Short-Pulse Lasers—Marilyn Schneider (08-ERD-024)

Abstract

Data from experiments measuring the material properties of dense matter at high temperatures and in local thermodynamic equilibrium are important to the advancement of high-energy-density science. Such data benchmark the radiation-transport, opacity, equation-of-state, and atomic physics codes used to simulate astrophysical objects, weapons, and inertial-confinement fusion targets. We propose to create a thermal x-ray radiation

source by heating a few micrometers of bulk material to high temperatures. The bulk material can be heated by the heat wave diffusing into it, by refluxing of hot electrons, or by return currents balancing the charge of escaping hot electrons. The source will be created by optimizing the conversion of short-pulse laser energy into thermal x rays.

If successful, this project will impact high-energy-density physics by (1) creating an understanding of the fundamental physics of heating of bulk material by short-pulse lasers, (2) developing the ability to use the high radiation field in the thermal source as a broadband backlighter for short-pulse laser experiments that probe the configurations and charge states of materials under extreme conditions, and (3) coupling the short-pulse laser heating of bulk materials with long-pulse lasers to produce a true "hot" hohlraum at laser facilities. These achievements will open the door to experimental platforms that generate new data and benchmark high-energy-density plasma physics codes.

Mission Relevance

This project will enable laboratory-based experiments on materials important to the Stockpile Stewardship Program. This project also supports the LLNL mission of breakthroughs in fundamental science and technology by optimizing the conversion of laser energy into x rays—a fundamental high-energy-density physics problem.

FY09 Accomplishments and Results

In FY09 we (1) measured soft x-ray spectra and hot electron spectra as a function of pulse length, laser polarization, target layers and thickness, and prepulse—preliminary analysis indicates radiation temperature gradients with radiation temperatures of 200 to 300 eV and electron temperatures of about 10 to 12 keV, with some electrons reaching temperatures as high as 40 to 60 keV; (2) measured the heated soft x-ray spot size as a function of these parameters—the combination of spot size and spectra show the fraction of absorbed energy that heats the copper is about 0.01; and (3) determined that laser coupling can be increased by controlling pre-pulse, decreasing laser intensity, and smoothing the beam.

Proposed Work for FY10

Our work in FY10 will optimize the conversion efficiency of laser light into soft x rays. Specifically, we will (1) use modeling results to guide the next round of experiments on pre-pulse and spot size and intensity, (2) use soft x-ray spectroscopy on layered targets to study the heating mechanism of a bulk piece of copper, and (3) measure the time history for heating bulk copper targets using a soft x-ray spectrometer with a fast streak camera and improved triggers at the Livermore Titan laser facility.

Publications

Cone, K., 2009. *Development of a hot, thermal x-radiation source using short pulse lasers.* IFSA 2009, 6th Intl. Conf. Inertial Fusion Science and Applications, San Francisco, CA, Sept. 6–11, 2009. LLNL-PROP-413345.

Stafford, D., 2009. *Time-integrated soft x-ray imaging in high intensity laser experiments.* Master's Thesis, University of California, Davis. LLNL-TH-416616.

Advanced Computation and Experimental Analysis of Plasma Equations of State and Transport—Brian Wilson (08-ERD-027)

Abstract

We propose to develop, apply, and experimentally validate a finite-temperature, multi-ion-center code for understanding amorphous warm dense systems such as shock-heated aluminum, foams, and plasma mixtures. This work will significantly advance the study of warm dense matter by including multicenter scattering effects in finite-temperature ensembles. As a consequence, both equilibrium and macroscopic transport quantities will be calculated in the warm dense matter regime.

Our novel computational approach will greatly improve our ability to calculate and understand the equilibrium and transport properties of warm dense plasma systems at a fundamental level. More realistic treatment of continuum lowering and pressure ionization in simple systems such as aluminum—as well as complex mixtures such as copper–beryllium ablators relevant to fusion laser ignition—will be calculated, as will conductivities of dense, amorphous, ionized systems. Shock experiments, in addition to providing an initial key code benchmark for aluminum by measuring the occupancies of quasi-bound states, will be a widely applicable advance in the general ability to measure microscopic features of shocked systems.

Mission Relevance

In addition to supporting basic science breakthroughs, our new multicenter scattering code for warm dense matter equation-of-state and transport calculations will be applicable to a wide variety of Laboratory missions that involve dense plasmas in support of stockpile stewardship and long-term energy needs. The new laser experimental methods being developed to validate this code also will find wide applicability in LLNL's high-energy-density and warm dense matter research efforts.

FY09 Accomplishments and Results

We conducted preliminary calculations with an improved version of MECCA (Multiple-Scattering Electronic-Structure Code for Complex Applications) on Al_3Ni_2 mixtures at cold and warmer (5-eV) temperatures and made comparisons with density-of-state results obtained with the ion-in-helium equation-of-state models currently employed at the Laboratory. Extension to a "full potential" (i.e., nonspherically symmetric) approach was not possible because of slow convergence in angular momentum channel contributions, and so we pursued alternative numerical methods involving numerical quadrature of spherically truncated tetrahedral regions.

Proposed Work for FY10

For FY10 we will continue to develop a new Green's function contour integration that separates single-site and multiple scattering contributions to handle high densities and finite temperatures for use in MECCA. In addition, we will continue our development of a multicenter but nonspherically symmetric potential extension of a plasma equation of state, using as a first approximation, orbital-free density functional methods.

Impurity and Alloying Effects on Material Strength from First Principles—Robert Rudd (08-ERD-035)

Abstract

We will pioneer the theory and computational framework for a first-principles–based predictive description of impurity and alloying effects on the constitutive behavior of materials under extreme deformation. To date, strength modeling at LLNL using ab initio methods has focused exclusively on pure, pristine materials. This proposal will begin to develop the capability for predictive strength modeling of alloyed or "dirty" materials, using quantum mechanical techniques to study three strength-related phenomena: solute mobility, impurity strengthening, and alloy core-structure modification. The project will be both computational and experimental, with development and application of novel ab initio theory and advanced diamond anvil cell experiments to produce validated models.

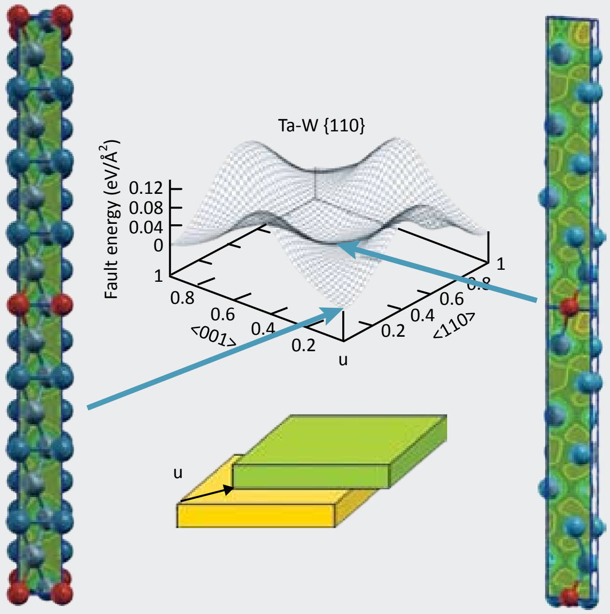
This project will develop the basic science of how alloying and impurities affect strength through modified interatomic interactions. The successful conclusion of this project will entail calculation of the effect of alloying and impurities on solute mobility, impurity strengthening, and alloy core modification. Diamond anvil cell experiments conducted as part of the project will provide validation for the impurity strengthening and help develop strength techniques; other results will be validated with existing experimental data. The principal significance of these achievements will be an ability to model the effect of isostructural alloying and impurities on strength from first principles. We expect to publish results of our findings in high-profile peer-reviewed journals.

Mission Relevance

Computational modeling of equation of state and related constitutive properties is a core competency of Lawrence Livermore. While techniques for modeling the equation of state of impure materials are well in hand, the techniques for alloy strength are largely empirical. A validated approach for development of predictive models of alloy strength (beyond the case where alloying causes new phases to form) would be a significant advance in capabilities in support of the Laboratory's mission in stockpile science.

FY09 Accomplishments and Results

We used first-principles theory and diamond anvil cell experiments to study the strength of body-centered-cubic tantalum–tungsten and vanadium alloys. In particular, we (1) conducted first-principle density functional theory calculations of the gamma surface and elastic constants of tantalum–tungsten alloys from ambient pressure up to 2.5 Mbar to construct a Peierls–Nabarro model; (2) conducted diamond anvil cell experiments to measure the strength of tantalum–tungsten alloys using the radial pressure gradient technique; (3) carried out density functional theory calculations on vanadium alloys, finding a



We conducted first-principles supercomputer calculations of the gamma surface of tantalum–tungsten alloys. The gamma surface (energy to slip) and the unit cells with and without slip are shown.

promising effect; and (4) began designing diamond anvil experiments on vanadium alloys.

Proposed Work for FY10

In FY10 we will continue to develop theoretical and experimental techniques for determining the strength of metal alloys. We will (1) use large-scale density functional theory calculations of the energy of tantalum–tungsten dislocation cores under stress to calculate the Peierls stress and verify the results of our approximate models, (2) complete calculations of the row deformation energy in tantalum–tungsten alloys and compare with the gamma surface results, and (3) complete measurements of the strength of tantalum–tungsten and possibly vanadium alloys at high pressure using the pressure-gradient technique and a diamond anvil cell.

Publications

Klepeis, J.-H., et al., in press. “DAC measurement of high-pressure yield strength of vanadium using in situ thickness determination.” *Phys. Rev. B.* LLNL-JRNL-414905.

Rudd, R. E., and J. E. Klepeis, 2008. “Multiphase improved Steinberg–Guinan model for vanadium.” *J. Appl. Phys.* **104**, 093528. LLNL-JRNL-406789.

Linking Quantum Chromodymamics to Experimental Data—Ron Soltz (08-ERD-046)

Abstract

Calculating the nonperturbative properties of quantum chromodymamics (QCD) and its implications for both high- and low-temperature phenomena have been longstanding goals of lattice QCD since its inception. Recent advances in high-performance computing, such as LLNL’s BlueGene/L supercomputer, has put this understanding—and a corresponding experimental validation of it—within reach. Partnering with university collaborators and with Los Alamos and Berkeley national laboratories, we will perform lattice QCD calculations of the equation of state and low-energy nuclear observables relevant to nuclear reactions and make detailed comparisons to data from heavy ion collisions and nuclear scattering experiments.

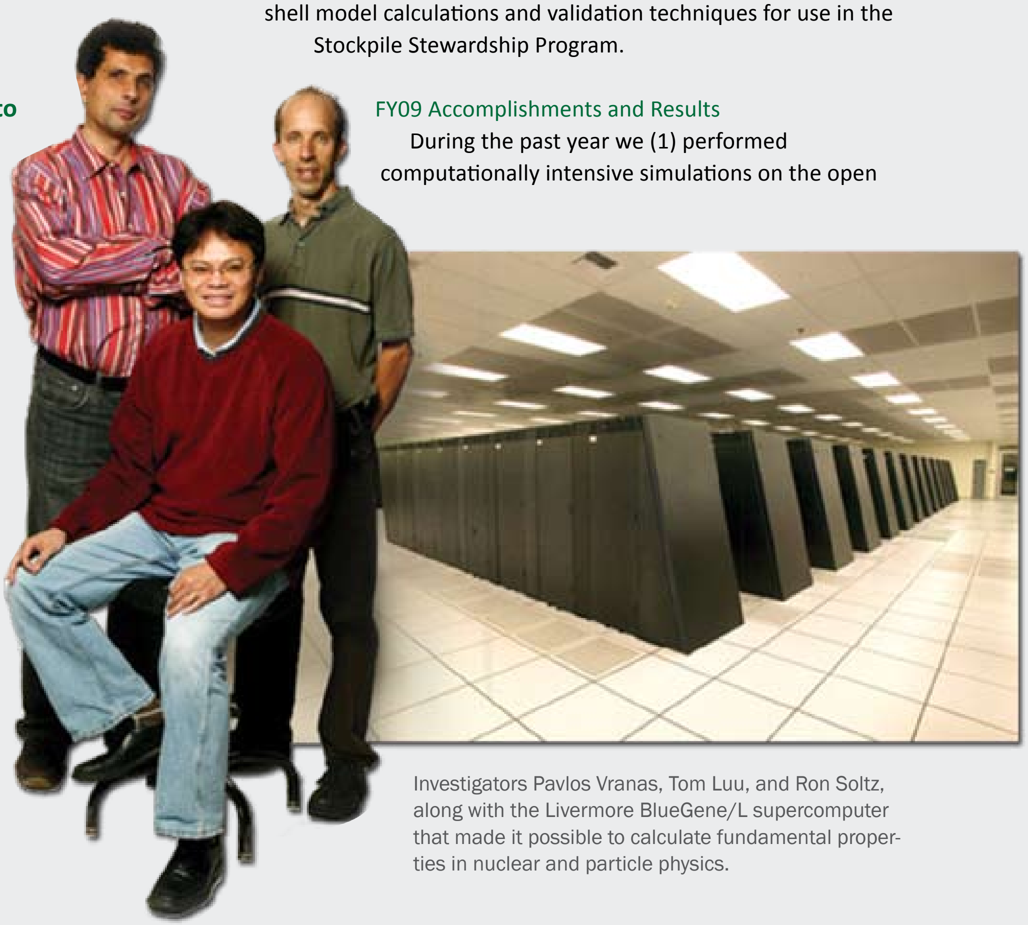
This project, if successful, would result in first-principle calculations of (1) the equation of state of nuclear matter, (2) the nucleon–nucleon phase shifts, (3) three-nucleon systems using quark degrees of freedom, and (4) strong dynamics extensions to the Standard Model. The computation of equation of state would be a significant advance in the area of high-temperature lattice QCD and will be crucial for understanding data from the Relativistic Heavy Ion Collider at Brookhaven National Laboratory and Large Hadron Collider near Geneva, Switzerland. The results of our nucleon–nucleon calculations will help benchmark low-energy QCD with experiments and calculate properties of the nuclear force that are not currently accessible experimentally. The results of our strong dynamics calculations will be crucial inputs to phenomenology at the Large Hadron Collider and possibly have direct predictive power for experiments there.

Mission Relevance

This project will enhance LLNL’s expertise in the calculation of the three-nucleon force, which will lead to improved no-core shell model calculations and validation techniques for use in the Stockpile Stewardship Program.

FY09 Accomplishments and Results

During the past year we (1) performed computationally intensive simulations on the open



Investigators Pavlos Vranas, Tom Luu, and Ron Soltz, along with the Livermore BlueGene/L supercomputer that made it possible to calculate fundamental properties in nuclear and particle physics.

BlueGene/L supercomputer in excess of 170 million core hours; (2) calculated the equation of state for QCD and inserted it into hydrodynamic models; (3) calculated nuclear phase shifts with implications to both the nuclear equation of state for supernovae and nuclear reactions; (4) completed the three-body formalism within lattice QCD, and have extracted for the first time a non-zero pure three-body interaction between pions; (5) formed a lattice strong dynamics collaboration to study the strongly interacting sector at the terraelectronvolt scale; and (6) completed a detailed study of the spectrum and coupling properties of the six techni-quark theory.

Proposed Work for FY10

For FY10 we will (1) complete our study of the QCD transition; (2) calculate the equation of state at higher temperatures to uncover a new physics regime and compare with the heavy-ion, high-temperature experiments at the Large Hadron Collider; (3) calculate detailed plasma properties using the vacuum states of our ensembles; (4) address calculations at finite density for comparison with the upcoming Relativistic Heavy Ion Collider experiments; (5) complete calculations on three-nucleon scattering parameters and potential and apply the results to nuclear few-body systems; and (6) study the eight and ten techni-quark teraelectronvolt theory, where significant effects on the mechanism of mass generation are expected.

Publications

Applequist, T., et al., 2009. *Toward TeV conformality.* LLNL-JRNL-420581.

Beane, S., et al., 2009. “High statistics analysis using anisotropic clover lattices: (I) Single hadron correlation functions.” *Phys. Rev. D* **79**, 114502. LLNL-JRNL-411560.

Beane, S., et al., 2009. “High statistics analysis using anisotropic clover lattices: (II) Three-baryond systems.” *Phys. Rev. D* **80**, 074501. LLNL-JRNL-413127.

Beane, S., et al., 2009. “Meson-baryon scattering lengths from mixed-action lattice QCD.” LLNL-JRNL-416867.

Cheng, M., et al., 2009. “Equation of state and QCD transition temperature at finite temperature.” *Phys. Rev. D* **80**, 014504. LLNL-JRNL-411569.

Detmold, W., et al., 2008. “Multipion states in lattice QCD and the charged pion condensate.” *Phys. Rev. D* **78**, 014507. LLNL-JRNL-402365.

Giedt, J., et al., 2009. “Lattice super Yang–Mills using domain wall fermions in the chiral limit.” *Phys. Rev. D* **79**, 025015. LLNL-JRNL-420849.

Soltz, R. A., 2009. “The hot QCD equation of state.” *Nucl. Phys. A* **830**, 752c. LLNL-JRNL-416214.

Three-Dimensions-Plus-Time Analysis of Plasma Microturbulence Simulations—William Nevins (08-ERD-048)

Abstract

Plasma microturbulence is the dominant mechanism of heat loss in tokamaks and will determine the fusion gain of tokamak fusion reactors. A fundamental issue is energy flow: Turbulent energy is produced by instabilities at low radial wave number. The conventional theory is that this energy scatters to high radial wave number, where it is damped. However, analysis in two dimensions (2D) plus time demonstrates insufficient energy flow to high radial wave numbers. We will develop and employ a 3D-plus-time analysis capability to investigate an alternate hypothesis—that turbulent energy is scattered to, and damped at, high parallel wave numbers.

We will develop a 3D-plus-time data analysis capability and used it to explore the above-mentioned hypothesis of energy flow in plasma microturbulence, resulting in a data-analysis code and two publications—one describing the code and another describing the energy flow in plasma microturbulence.

Mission Relevance

This project supports LLNL’s mission in energy security by enhancing our understanding of plasma microturbulence, an important heat-loss mechanism that can limit fusion gain in magnetic fusion reactors. Maximizing fusion gain is critical to the success of magnetic fusion because it will determine how much fusion power can be produced.

FY09 Accomplishments and Results

In FY09 we (1) hired a postdoctoral researcher; (2) completed data importation routines for the GENE and GYRO gyrokinetic simulation codes, thereby completing our 3D-plus-time data analysis package in serial mode; and (3) used this package to analyze data sets from both electrostatic and electromagnetic simulations, increasing our understanding of the radial propagation of plasma microturbulence and demonstrating that the magnetic field becomes “tangled” on the microscale in electromagnetic simulations of plasma microturbulence, thus opening a new channel for heat transport. Our experience in serial 3D-plus-time data analysis has motivated an extension to parallel data analysis to increase computational throughput, which will be a major effort in FY10.

Proposed Work for FY10

In FY10 we will focus on using our 3D-plus-time data analysis package to analyze data sets from plasma microturbulence simulations. This will include analysis of electromagnetic data sets obtained from the DOE Scientific Discovery through Advanced Computing program Center for the Study of Plasma Microturbulence, in which variation of the plasma pressure results in substantial changes in both the turbulence and transport levels.

Publications

Nevins, W. M., and E. Wang, 2009. *Analysis of 3D plus time microturbulence simulation data.* Transport Task Force Workshop, San Diego, CA, May 28–June 1, 2009. LLNL-PRES-412568.

Nevins, W. M., et al., 2009. *Turbulence driven magnetic reconnection.* 51st Ann. Mtg. Division of Plasma Physics, Atlanta, GA, Nov. 2–6, 2009. LLNL-PRES-418962.

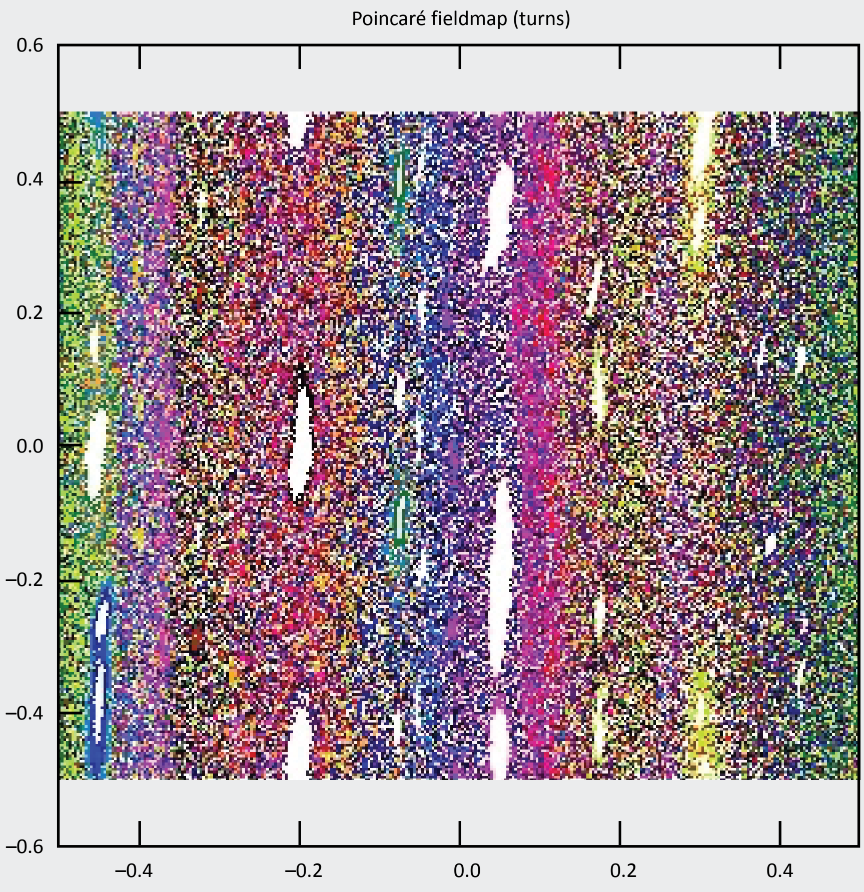
Wang, E., and W. M. Nevins, 2009. *Radial propagation in the ITG CYCLONE base case.* 51st Ann. Mtg. Division of Plasma Physics, Atlanta, GA, Nov. 2–6, 2009. LLNL-POST-419067-DRAFT.

Cryogenic Bolometers for Double Beta-Decay Experiments—Nicholas Scielzo (08-ERD-049)

Abstract

The Cryogenic Underground Observatory for Rare Events (CUORE) will be a large detector designed to search for the neutrinoless double beta-decay of tellurium-130 (^{130}Te). Observation of this decay mode would prove that neutrinos are their own antiparticles and would establish the absolute scale of neutrino masses. We propose a project on data analysis, tellurium dioxide crystal bolometer production, and background reduction that will improve the performance of CUORE, and thus improve its sensitivity to neutrinoless double beta-decay.

We will analyze our existing data from the CUORICINO experiment (a pilot-scale experiment for CUORE) to observe or establish the world's most sensitive limits on zero-neutrino double beta-decay and two-neutrino double beta-decay of ^{130}Te to both the ground and excited states of xenon-130 (^{130}Xe), as well as the



This Poincaré surface-of-section plot demonstrates that plasma microturbulence causes the magnetic field to become tangled on the microscale, opening a new channel for heat transport.

two-neutrino electron capture and beta-plus decay of ^{130}Te. We will develop procedures for producing tellurium dioxide crystals to meet CUORE's stringent requirements on radio-purity, uniformity, and surface finish. We expect to identify materials with lower radioactive contamination than those used previously. In addition, we will prepare scientific papers and technical reports summarizing the results of each of these studies, and expect these efforts to position LLNL as a leader in the CUORE project.

Mission Relevance

This project will provide expertise with large cryogenic bolometers that will be useful in many future nuclear and high-energy-physics projects in support of stockpile stewardship. Low-background counting techniques that will be refined as part of this effort also will be of relevance for detecting minute amounts of radioactive materials in a wide variety of settings in support of Laboratory missions in nonproliferation and counterproliferation. In addition, this project will attract highly qualified student researchers to the Laboratory.

FY09 Accomplishments and Results

During FY09, we (1) developed procedures that yielded bolometer detectors with extremely low backgrounds and improved energy resolution, (2) used scintillator detectors to determine that muon-induced backgrounds are negligible at CUORE's underground site, (3) developed analyses to understand background contributions and perform searches for rare nuclear decays, (4) began searches for the decay of ^{130}Te to excited states of ^{130}Xe, (5) nearly completed our ^{130}Te half-life measurement, and (6) demonstrated the most stringent limits on ^{120}Te decay obtained to date.

Proposed Work for FY10

In FY10 we plan to (1) integrate our bolometer crystal instrument with the rest of the systems that have been designed by our collaborators for CUORE-0; (2) assemble the CUORE-0 detector array and begin operation of this small-scale CUORE detector; (3) further study methods, using this detector array, to refine background elimination techniques and obtain better sensitivity to searches for double-beta decay and other rare decay modes; and (4) perform improved searches for the double-beta decay of ^{130}Te to excited states of ^{130}Xe, and measure the half-life of ^{130}Te.

Publications

Arnaboldi, C., et al., 2008. "Results from a search for the neutrinoless double beta decay of Te-130." *Phys. Rev. C* **78**, 041601. LLNL-JRNL-408037.

Dolinski, M. J., 2008. *Neutron interactions in the CUORE neutrinoless double beta decay experiment.* LLNL-TH-408040.

Norman, E. B., 2009. "Prospects for and status of CUORE—the Cryogenic Underground Observatory for Rare Events." *AIP Conf. Proc.* **1165**, 411. LLNL-PROC-414765.

Pedretti, M., et al., in press. "A ton-scale bolometric detector for the search for neutrinoless double beta decay." *AIP Conf. Proc.* LLNL-ABS-407544.

Pedretti, M., et al., 2008. "CUORE Experiment: The search for neutrinoless double beta decay." *Int. J. Mod. Phys. A* **23**, 3395. LLNL-JRNL-414692.

Partition-of-Unity Finite-Element Method for Large-Scale Quantum Molecular Dynamics on Massively Parallel Computational Platforms—John Pask (08-ERD-052)

Abstract

First-principles quantum mechanical (QM) materials calculations now account for a significant fraction of large-scale computations. However, solving such QM equations is resource intensive, which has severely limited the range of physical systems that can be investigated. We will push back those limits by developing and implementing a new approach to solving QM equations. Our partition-of-unity finite-element (PUFE) analysis could achieve an order-of-magnitude improvement over current state-of-the-art approaches, which would change the way the largest, most complex QM calculations are solved and enable important QM investigations not previously possible. We will demonstrate the unique power of our method by using it to perform the largest-ever quantum molecular dynamics simulations of d- and f-electron metals under pressure. This work is also expected to generate a series of high-profile publications.

If successful, our finite-element-based code will speed up large-scale electronic structure calculations by an order of magnitude or more, with resulting increases in computational throughput and in the size and complexity of problems that can be computationally addressed.

Mission Relevance

This project will advance QM materials calculations in general, but will have a particular impact on stockpile stewardship by providing key understanding and predictions of current and future stockpile materials.

FY09 Accomplishments and Results

In FY09 we (1) formulated QM forces for the PUFE method and implemented the forces in our PUFE code, (2) completed initial parallelization of system matrix construction and eigenproblem solution, (3) undertook QM relaxed calculations of systems with dilute impurities, and (4) initiated a collaboration with the University of California at Davis on the development of eigensolvers for the PUFE method.

Proposed Work for FY10

In FY10 we propose to (1) implement quantum molecular dynamics, (2) continue parallel optimizations, (3) commence large-scale quantum molecular dynamics simulations of d- and f-electron metals for molybdenum or tantalum under pressure, and (4) submit additional manuscripts for publication.

Publications

Sukumar, N., and J. E. Pask, 2009. "Classical and enriched finite element formulations for Bloch-periodic boundary conditions." *Int. J. Numer. Meth. Eng.* **77**, 1121. LLNL-JRNL-403676.

Measurement and Prediction of Laser-Induced Damage in the Presence of Multiple Simultaneous Wavelengths—Mike Nostrand (08-ERD-054)

Abstract

Accurate predictions of laser-induced optical damage are critical for experimentation where damage limits performance and timely recycling of optical components is necessary for efficient laser operation. Predictions of damage in high-energy laser systems based on small-scale laboratory experiments have been very poor in the past. We will create an improved predictive capability with measurements and modeling that give particular attention to the effects of multiple simultaneous wavelengths and pulse-shape variations. This will also include studies of behavior in mitigated damage sites, damage probability of process-induced flaws, and studies of short-pulse damage to gratings and mirrors. We will collect laser damage data, and then develop a predictive computational capability for describing the damage expected on an inertial-confinement fusion laser beamline. We will compare our predictions against large-aperture laser observations.

We will create the capability to precisely predict the highest level of laser performance that can be achieved at acceptable cost. (Less-accurate predictions would necessitate a larger safety margin and hence reduced laser performance.) We will also determine iterative feedback between predictive performance modeling, full-aperture damage observations, and the physical mechanisms underlying optical damage. This feedback will provide further understanding of damage mechanisms, thus providing better insight for improved optics performance and, therefore, improved laser performance.

Mission Relevance

By developing protocols to extend the useful lifetime of critical silicone dioxide and crystalline potassium dihydrogen phosphate (KDP) and deuterated KDP components used in large, fusion-class lasers, this project will benefit stockpile stewardship and inertial-confinement fusion, in support of LLNL's missions in national and energy security.

FY09 Accomplishments and Results

We have (1) increased our ability to predict the growth rate of laser-induced damage sites by showing that pulse shape, duration, and damage site size are relevant to growth; (2) incorporated these findings into new growth models; (3) developed a description of how pulse shape affects growth rate in the presence of multiple simultaneous wavelengths; (4) incorporated pulse shape and site size into our rules; (5) designed, coded, and tested laser-management software that incorporates the latest damage and operation rules and is capable of multishot predictions, with more efficient load-leveling of optic recycling and maintenance; (6) developed damage probability curves versus scratch-damage length and width; (7) tested laser and chemical mitigation protocols; and (8) collected data and began analysis of short-pulse damage.

Proposed Work for FY10

In FY10 we will (1) refine rules for the effect of pulse shape on the growth rate for a single wavelength; (2) expand pulse-shape scaling rules on growth pulses to additional pulse shapes; (3) generalize multiple-wavelength growth threshold rules to additional pulse shapes; (4) expand initiation pulse-shape scaling to multiple simultaneous wavelengths; (5) develop the predictive modeling tools to fully automate damage evaluations based on full-scale, online data and predictions; (6) incorporate damage prediction data into tools that will evaluate campaign cost metrics and make supply-and-demand operating decisions; and (7) expand predictive capability to longer intervals of months or years.

Publications

Negres, R. A., et al., 2009. "The effect of pulse duration on the growth rate of laser-induced damage sites at 351 nm on fused silica surfaces." *Proc. SPIE* **7504**, 750412. LLNL-PRES-416873.

Liao, Z. M., et al., 2009. "Using absorption distribution model to predict optimal laser conditioning for DKDP crystals." *Nonlinear optics: Materials, fundamentals and applications*, paper NWC7. Optical Society of America, Washington, DC. LLNL-PRES-414644.

Mesoscale Studies of Hydrodynamic Instability Growth in the Presence of Electric and Magnetic Fields—
Peter Amendt (08-ERD-062)

Abstract

Recent proton backlighting data on laser-driven imploded capsules and rippled foils indicate the presence of strong self-generated electric (~1 GV/m) and magnetic (~1 MG) fields. Understanding their origin has potential relevance toward planned demonstrations of inertial-confinement fusion. Elucidating the nature of these fields and their effects on interfacial instability growth will require an approach that departs from standard single-fluid hydrodynamics and instead treats the system as an aggregate of coupled electron-ion fluids—that is, as a plasma. This project will explore such plasma effects on important hydrodynamic instabilities such as Rayleigh–Taylor and Richtmyer–Meshkov.

The main deliverables of this project will be an evaluation of electric and magnetic field effects in imploding systems, an understanding of their origin and magnitude, and suggested remedial measures if the effects are deemed significant. Initially, we will evaluate methods to understand the underlying physics—both analytical and computational—and to interpret the growing database for benchmarking our models and techniques. This research will potentially have an impact not only for ignition on fusion-class lasers, but also for many high-energy-density studies with national security mission relevance.

Mission Relevance

This project supports LLNL's energy security mission by furthering the goal of robust ignition designs for inertial-confinement fusion, and also supports the national security mission by contributing to investigations of high-energy-density imploding systems.

FY09 Accomplishments and Results

Breakthrough research in FY09 included (1) the first scoping studies of a three-dimensional magnetohydrodynamic package in the radiation-hydrodynamics code HYDRA, (2) the first particle-in-cell simulations of electric fields in a shock front, (3) the study of possible field effects in explaining a longstanding anomaly from hohlraum experiments on Livermore's Nova laser, (4) a compelling theoretical basis for explaining recent proton backlighting data from the OMEGA laser at the University of Rochester in terms of shock-front generation of the observed electric field, and (5) a potential explanation of the widely known deuterium and helium-3 neutron anomaly based on barotropic diffusion across a plasma shock front in the presence of electric fields.

Proposed Work for FY10

In FY10 we will concentrate on (1) finalizing a suite of analytical tools for gauging the effects of electric and magnetic fields on instability growth, (2) testing and exercising three-dimensional radiation-hydrodynamics capabilities with magnetic field generation, (3) applying particle-in-cell simulation techniques to identify and understand mechanisms underlying the observed electric-field generation in experiments at the Massachusetts Institute of Technology, and (4) collaborate on designing and interpreting future experiments. We expect continued progress on applying analytic techniques to magnetic fields, validating the magnetic-field generation package, and developing necessary particle-in-cell techniques for understanding the evolution and distribution of electric-field generation in imploding capsules.

Publications

Amendt, P. A., 2008. "Effects of ionization gradients on inertial-confinement-fusion capsule hydrodynamic stability." *Phys. Rev. Lett.* **101**, 115004. LLNL-JRNL-403824.

Amendt, P. A., et al., 2009. "Electric field and ionization-gradient effects on inertial-confinement-fusion implosions." *Plasma Phys. Contr. Fusion* **51**(12), 12404. LLNL-CONF-413857.

Li, C. K., et al., 2009. "Observations of electromagnetic fields and plasma flow in hohlraums with proton radiography." *Phys. Rev. Lett.* **102**, 205001. LLNL-JRNL-410658.

Li, C. K., et al., 2009. "Pressure-driven MHD interchange instabilities in laser-produced HED plasmas." *Phys. Rev. E* **80**, 016407. LLNL-JRNL-423131.

Li, C. K., et al., 2009. "Proton radiography of dynamic electric and magnetic fields in high-energy-density plasmas." *Phys. Plasma.* **16**, 056304. LLNL-JRNL-423130.

Li, C. K., et al., 2009. "Study of direct-drive capsule implosions in inertial confinement fusion with proton radiography." *Plasma Phys. Contr. Fusion* **51**, 014003. LLNL-JRNL-423129.

Nuclear Astrophysics at the National Ignition Facility: Feasibility of Studying the Reactions of the Stars on Earth—Richard Boyd (08-ERD-066)

Abstract

Our objective is to develop the technical approach for nuclear astrophysics experiments to be conducted at the National Ignition Facility (NIF) to study nucleosynthesis in stars and stellar evolution. Because these experiments can only be performed at NIF at its full energy, our work will focus on studies that must precede these experiments. Target simulations will be performed using Livermore's radiation-hydrodynamics HYDRA code for several reactions, some of which are believed to be viable candidates for study at NIF, and others whose viability needs to be established. In addition, simulations of NIF ignition shots, using the

standard deuterium–tritium target but configuring the NIF laser to operate in "polar direct drive" and without the hohlraum, will be performed with an eye to a future experiment to test aspects of Big Bang nucleosynthesis. The diagnostics required to produce meaningful data will also be studied.

This project will yield the optimal designs of NIF target pellets for several experiments, along with an estimate of reaction yields, which will determine the feasibility of each experiment and will be optimized by varying parameters such as pellet design, laser energy, and laser profile. We will also determine the diagnostics required for future shots, including if existing diagnostics will provide the required information during laser shots. If new diagnostic devices are required, their properties will be determined, which would lay the groundwork for future design work.

Mission Relevance

The project furthers the Laboratory's national security mission by paving the way for NIF astrophysics experiments that will lead to advances in understanding nuclear reactions relevant to stockpile stewardship.

FY09 Accomplishments and Results

In FY09 we (1) considered, in collaboration with the Colorado School of Mines, various possible nuclear reaction tracer nuclei for carbon–hydrogen targets that would enable diagnostic assessments of NIF shots—lithium and boron isotopes are viable candidates, although their background levels need to be considered; (2) initiated efforts to determine what is needed to permit external collaborators to perform simulations of NIF shots with the HYDRA computer code; (3) developed, in collaboration with Ohio University, a theoretical formalism that allowed consideration of the effects of nonthermal particles produced during Big Bang nucleosynthesis on the reaction products of that nucleosynthesis; and (4) initiated development of a Big Bang nucleosynthesis experiment for NIF that would test some aspects of the Big Bang reaction network. Preliminary simulations have been performed for these shots, with the result that detecting the abundances of lithium isotopes produced appears feasible.

Proposed Work for FY10

In the context of the combined theoretical and experimental work on Big Bang nucleosynthesis, in FY10 we plan to (1) add several new reactions and the capability for including nonthermal reactions to the Big Bang nucleosynthesis code—we hope that these additions will address difficulties of the theory in producing correct abundances for lithium isotopes; (2) work to develop a NIF shot that can test the veracity of the theoretical nucleosynthesis description, as well as some aspects of the accuracy of NIF codes; (3) continue development of NIF parameters for several reactions in nuclear astrophysics; and (4) continue efforts to design and develop NIF diagnostic devices for collection of shot debris for subsequent analysis.

Publications

Boyd, R. N., 2009. "The National Ignition Facility: Studying the stars in the laboratory." *Proc. 10th Symp. Nuclei in the Cosmos*, Proceedings of Science, Trieste, Italy. LLNL-PRES-420500.

Boyd, R. N., L. Bernstein, and C. Brune, 2009. "Studying nuclear astrophysics at NIF." *Phys. Today* **62**(8), 60. LLNL-JRNL-414484.

Moses, E. I., et al., 2009. "The National Ignition Facility: Ushering in a new age for high energy density science." *Phys. Plasma.* **16**, 041006. LLNL-JRNL-406652.

Study of Kelvin–Helmholtz Instability in High-Energy-Density Hydrodynamic Processes—Hye-Sook Park (08-ERD-069)

Abstract

An unanswered question in high-energy-density hydrodynamics is whether Kelvin–Helmholtz instability can be studied in a controlled fashion. A controlled Kelvin–Helmholtz experiment would be a valuable step towards demonstrating the ability to field a number of science studies on future fusion-class lasers, including eventual supernova experiments. In this project, we will conduct Kelvin–Helmholtz and related supernova experiments on the OMEGA laser, leveraging LLNL expertise in target design, simulation, diagnostics, and other fields. This project will be conducted in collaboration with the University of Michigan.

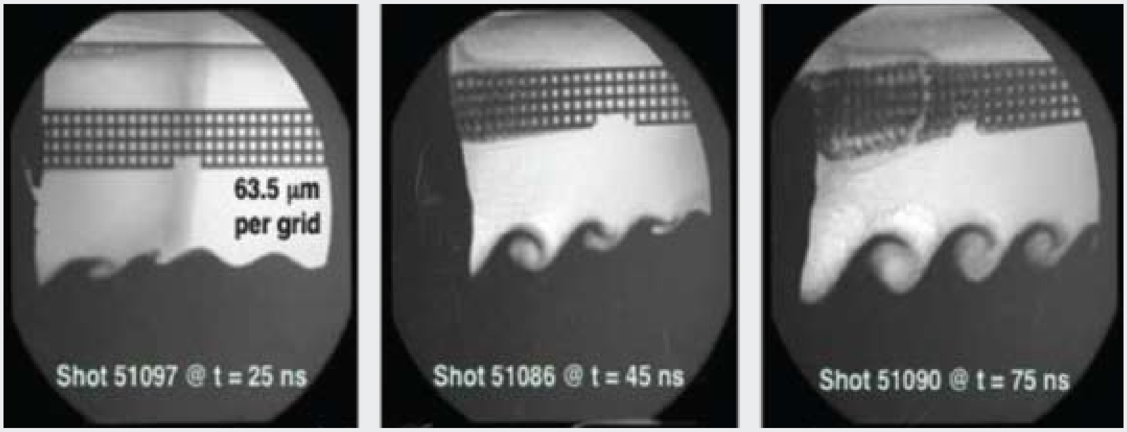
If successful, this project will deliver an x-ray radiograph of a material's controlled Kelvin–Helmholtz roll-up, demonstrating whether hydrodynamics experiments can resolve multiple interspersed layers of x-ray-absorbing and x-ray-transmitting materials, or if these layers are too adversely affected by turbulent mixing and the recently observed phenomenon of mass stripping to serve as valid diagnostics.

Mission Relevance

Understanding Kelvin–Helmholtz instability is central to many hydrodynamic processes important to Livermore's Stockpile Stewardship Program. This project supports the Laboratory's national security mission by potentially producing an entirely new type of experimental data for the validation of stockpile stewardship codes.

FY09 Accomplishments and Results

In FY09 we (1) analyzed the data obtained from previous experiments, (2) designed a new set of Kelvin–Helmholtz experiments to be performed in FY10 on the OMEGA laser at the University of Rochester, and (3) began designing hydrodynamic astrophysics experiments that can be performed at Livermore's National Ignition Facility (NIF).



Radiography images of the time development of Kelvin–Helmholtz instability at 25, 45, and 75 ns, respectively. The experiment was performed on the OMEGA laser at the University of Rochester.

Proposed Work for FY10

In FY10 we will (1) perform more Kelvin–Helmholtz experiments with new targets, which will show their reproducibility and their sensitivity to foam density; (2) design and model the Michigan-led supernova experiments for NIF (supernovae are thought to have very strong Rayleigh–Taylor and Kelvin–Helmholtz instabilities in their explosion dynamics, which are believed to cause astronomical observables such as the supernova SN1987A); and (3) design and develop a prototype of a new diagnostic technique, a very bright “x-ray sheet” probe that will image instability features, which may be feasible with the OMEGA Extended Performance (EP) Laser System and NIF. If so, we will test our prototype on the OMEGA laser.

Publications

Harding, E. E., et al., 2009. “Observation of a Kelvin–Helmholtz instability in a high-energy-density plasma on the OMEGA laser.” *Phys. Rev. Lett.* **103**, 045005. LLNL-POST-417686-DRAFT.

Hurricane, O. A., et al., “A high-energy-density shock-driven Kelvin–Helmholtz shear layer experiment.” *Phys. Plasmas* **16**, 056305. LLNL-JRNL-410680.

X-Ray Scattering on Compressed Matter—
Siegfried Glenzer (08-ERI-002)

Abstract

We propose to use LLNL’s Advanced Radiographic Capability to characterize shock-compressed matter. Specifically, we will compress hydrogen and beryllium to extremely dense states of matter, approaching 1000 g/cm^3, and directly measure density from the broadening of the Compton-scattered spectrum. Our approach combines the recently demonstrated x-ray scattering technique with K-alpha radiation produced by the ultrashort-pulse laser at the Advanced Radiographic Capability to investigate shock-compressed high-density plasmas. We will develop the new combined technique in a series of experiments conducted on high-power lasers and at free-electron laser facilities—the Linac Coherent Light Source at Stanford and the FLASH facility in Germany.

We will combine the techniques of x-ray scattering and K-alpha radiation, and our academic collaborations will ensure that our new method is adopted widely throughout the scientific community. We will also produce data important to several key areas of Laboratory research, including critical data on the compressibility and pressure ionization of dense matter, as well as new data on dense hydrogen, which are expected to resolve the ongoing equation-of-state controversy and provide a direct measure of compressibility. The project will also generate highly visible publications in physics journals.

Mission Relevance

This project will develop x-ray scattering techniques for fusion-class lasers and at the same time provide a critical test for hydrodynamic and equation-of-state modeling important to high-energy-density physics in support of stockpile stewardship. This project will also train the next generation of young scientists in a field of high importance to the Laboratory.

FY09 Accomplishments and Results

The FY09 experiments have been very successful in providing experimental x-ray Thomson scattering data on shock-compressed matter including lithium hydride from Livermore’s Titan laser, cryogenic hydrogen from Livermore’s Janus and the University of Rochester’s OMEGA lasers, and shocked beryllium in two-dimensional and spherical-driven geometry OMEGA experiments. These experiments will allow us to plan fielding x-ray Thomson scattering at the National Ignition Facility (NIF). They have tested equation-of-state models for beryllium and ion structure factors for lithium hydride. These results have validated Livermore's equation-of-state data used to model ignition targets on NIF and demonstrated screening effects in shock-compressed matter.

Proposed Work for FY10

In FY10 we will analyze the experimental results from our hydrogen and boron shock-compressed-matter experiments. Our goal is to test the plasma dispersion and equation of state in dense matter. In addition, we will perform new experiments with hydrogen and beryllium on the large OMEGA and OMEGA Extended Performance (EP) laser facilities. The latter will include ultrafast probing of fast-electron heated matter that provides information on detailed balance and relaxation. With successful OMEGA EP experiments, this technique will be ready for implementation at NIF. Several highly visible publications from this work will be published in FY10.

Publications

Fortney, J. J., et al., 2009. "Frontiers of the physics of dense plasmas and planetary interiors: Experiments, theory, and applications." *Phys. Plasma.* **16**, 041003. LLNL-JRNL-407191.

Kritcher, A. L., et al., 2009. "Ultrafast K alpha x-ray Thomson scattering from shock compressed lithium hydride." *Phys. Plasma.* **16**, 1. UCRL-JRNL-227913.

Lee, H. J., et al., 2009. "X-ray Thomson-scattering measurements of density and temperature in shock-compressed beryllium." *Phys. Rev. Lett.* **102**, 115001. LLNL-JRNL-406683.

Proton Fast Ignition—Pravesh Patel (08-ERI-004)

Abstract

We will explore proton fast ignition, from its conceptual phase to proof-of-principle subscale demonstration experiments. We propose to perform systematic experiments on the 350-J Titan laser at Livermore and the 5.2-kJ OMEGA Extended Performance (EP) laser at the University of Rochester to determine the optimal laser and target design parameters for subscale proton fast ignition, validate LLNL's short-pulse integrated modeling capability, and resolve outstanding physics issues related to proton conversion efficiency scaling, ballistic focusing, and stopping in dense plasma. The final deliverable will be an integrated demonstration experiment using the 30-kJ OMEGA implosion facility and a 5.2-kJ ignitor pulse to establish the viability of full-scale proton fast ignition on fusion-scale lasers.

Through experiments and modeling, we will establish the feasibility of full-scale proton fast ignition. The outstanding physics issues we will adress experimentally include (1) maximum conversion efficiency through optimized target designs; (2) minimum ballistically focused spot size; (3) scaling of conversion efficiency with pulse length; (4) validation of the integrated hydrodynamic, particle-in-cell (PIC) and hybrid PIC codes used to model the entire proton fast-ignition process; and (5) new physics effects in a 100-kJ full-scale fast-ignition scenario. Our final deliverable—the results of a proof-of-principle proton fast-ignition experiment on OMEGA EP—would be of momentous significance for the entire U.S. fast-ignition endeavor.

Mission Relevance

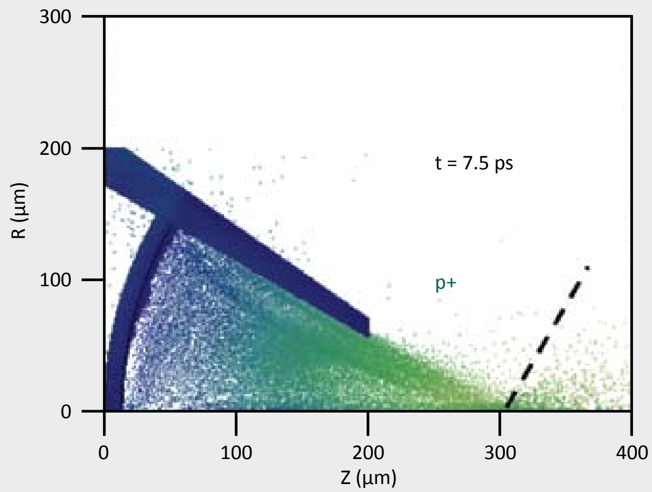
This project will provide the scientific groundwork for demonstration of proton fast ignition on fusion-class fast-pulse lasers, in support of the Laboratory's missions in national and energy security.

FY09 Accomplishments and Results

In FY09 we (1) performed a proton focusing experiment on the Trident laser at Los Alamos National Laboratory, which is similar to Livermore's Titan laser, and made measurements of the focused spot as a function of proton energy, finding it within the acceptable limit of 40 µm required for fast ignition; (2) investigated scaling with target thickness; (3) began study of target design variations using the Large-Scale Plasma (LSP) code; (4) performed LSP simulations to benchmark proton conversion efficiencies and focusing; and (5) performed shots on the OMEGA EP laser to measure proton conversion efficiency at higher energy and pulse length and analyzed the data.

Proposed Work for FY10

In FY10 we will use three weeks of time obtained on the Trident laser at Los Alamos for an experiment to study dynamics of proton focusing. Specifically, we will study the dependence of the laser spot size and hemisphere target diameter on the size



Large-Scale Plasma simulation of proton focusing from a hemispherical laser target embedded in a fast-ignition cone.

and intensity of the focused proton beam. These are the critical parameters for fast ignition. Simulations predict an optimum spot size can be obtained with large-area uniform laser irradiation. If successful, we will extend our measurements to fast-ignition laser conditions on the OMEGA EP. We will also complete a proton fast-ignition point design using the LSP simulation code to establish scaling of our subscale experiments to full-scale fast ignition.

Publications

Hey, D., 2009. *Laser-accelerated proton conversion efficiency thickness scaling.* IFSA 2009, 6th Intl. Conf. Inertial Fusion Sciences and Applications, San Francisco, CA, Sept. 6–11, 2009. LLNL-ABS-412620.

Mackinnon, A. J., 2009. *Progress in fast ignition studies.* APiP 2009, 16th Intl. Conf. Atomic Processes in Plasmas, Monterey, CA, Mar. 22–26, 2009. LLNL-ABS-409835.

Conductivity in Warm Dense Matter—Siegfried Glenzer (08-LW-004)

Abstract

Conductivity in warm dense hydrogen is a critically important quantity affecting calculations of Rayleigh–Taylor growth in inertial-confinement fusion capsules, the performance of materials compressed by laser-driven foils, equation-of-state data, and primary weapon performance, for instance. We propose to develop an x-ray scattering technique to determine conductivity in warm dense matter. Our approach is to first demonstrate proof-of-principle measurements of plasmons that are broadened by electron–ion collisions in well-characterized, isochorically heated solid-density plasmas. We will subsequently apply plasmon measurements to resolve the key technical question of conductivity in dense (cryogenic) deuterium plasmas.

This project will establish an x-ray scattering technique for determining conductivity in warm dense matter, and deliver definite data on conductivity in dense hydrogen under well-characterized conditions.

Mission Relevance

This project supports the Laboratory's missions in national security (specifically stockpile stewardship) and energy security by developing a new experimental technique and definite data on conductivity in dense hydrogen. We expect that the technique will be adopted by our academic collaborators and their students, thus helping to train the next generation of young scientists in a field of high importance to the Laboratory.

FY09 Accomplishments and Results

In FY09 we successfully measured and modeled the plasmon data from cryogenic hydrogen heated by a free-electron laser. Our experiments have shown that plasmon shift is sensitive to density and temperature while the plasmon broadening is small, indicating electron–ion collision rates on the small end of predictions from conductivity calculations.

Publications

Garcia Saiz, E., et al., 2008. "Probing warm dense lithium by inelastic x-ray scattering." *Nat. Phys.* **4**, 940. LLNL-ABS-406742.

Kritcher, A. L., et al., 2008. "Ultrafast x-ray Thomson scattering of shock-compressed matter." *Science* **322**(5898), 69. LLNL-JRNL-404372.

Lee, H. J., et al., 2009. "X-ray Thomson scattering measurements of density and temperature in shock-compressed beryllium." *Phys. Rev. Lett.* **102**(11), 115001. LLNL-JRNL-406683.

Zero-Order Phased Fiber Arrays—Michael Messerly (08-LW-052)

Abstract

The next avenue for power-scaling optical fiber lasers is to combine the outputs of many fibers into a single beam. Current approaches do not preserve the spectral properties of the constituent fibers and are thus not applicable to the highest-power fiber lasers—they work for 150-W unit cells, but not for 6-kW cells. This project will pursue what may be the only way to overcome this shortcoming—to control the laser's relative phases while at the same time controlling their absolute lengths to within a few wavelengths, making what we call a "zero-order" phased array.

Our strategy is to open the door to joule-class pulsed-fiber sources and to novel applications such as resonant amplifiers and pulse stacking. We will demonstrate techniques for monitoring and controlling the relative lengths of four fiber laser sources to within one part in a million. We will focus on monitoring the power and stability of the aggregate output at several narrow wavelength bands across their gain bandwidth, and will close the

loop using techniques already established and refined for mode-locked fiber oscillators. Another expected result is to either refute or verify claims of self-organization in fiber arrays.

Mission Relevance

By opening a path to compact, reliable joule-class fiber sources, this project will lead to more powerful x-ray sources, such as Thomson-radiated extreme x rays, as well as to techniques for the coherent generation of fusion-class laser pulses and 100-kW-class fiber lasers, in support of LLNL's missions in national and energy security. This project could lead to tenfold more energetic and powerful sources for machining and welding, in support of the Laboratory's mission in breakthrough science and technology.

FY09 Accomplishments and Results

In FY09 we developed a high-repetition-rate mode-locked oscillator (broadband source), suitable for co-phasing pulses in separate fibers as well as co-phasing pulses from a single fiber (pulse stacking). The oscillator achieved a repetition rate of 80 MHz, twice the rate of other oscillators we have previously developed, allowing for single-fiber co-phasing in 1.9-m-length cavities. The resulting pulses were combined in two separate fiber amplifier chains, whose lengths were tuned to within 0.1 ps, allowing for combination of pulses having a bandwidth of 30 nm. The amplifier chains have demonstrated amplification to 100-nJ pulses. In addition, we worked to compress the recombined pulses and determine the pulse energy at which nonlinear distortions limit the technique. The coherent combination of multiple short-pulse fiber-based lasers remains a promising path for increasing fiber energies beyond 10 mJ, as exemplified by recent interest from the Defense Advanced Research Projects Agency.

Publications

Messerly, M. J., J. W. Dawson, and P. H. Pax, 2009. *Limits to the manufacturability and scalability of large-mode optical fibers.* SPIE Photonics West, San Jose, CA, Jan. 24–29, 2009. LLNL-CONF-410235.

Relativistic Electron–Positron Jets—Scott Wilks (08-LW-058)

Abstract

Relativistic electron–positron jets are thought to play key roles in some astrophysical objects but do not exist naturally on Earth. We will experimentally demonstrate, for the first time, a dense relativistic electron–positron jet using ultra-intense laser pulses interacting with solids. We will also demonstrate the focusing of this jet to high densities. We will conduct our experiments first on LLNL's Titan laser, then demonstrate how the jet scales with energy by moving the experiment to the OMEGA Extended Performance (EP) laser. This project will leverage LLNL's laser diagnostics and is supported by a theory suggesting that choosing a specialized target will enable the focusing of electron–positron jets. This work will be conducted in partnership with university collaborators.

If the proposed research is successful, we will characterize the first dense relativistic electron–positron plasma jet ever created in a laboratory. We will measure the directionality, number density, and energy spectrum of the jets and compare our results with theoretical predictions. This will provide LLNL with a new test bed for exotic jets that are currently impossible to study in a laboratory setting. In addition, we also expect to focus the jet—something unimaginable as recently as last year. We expect several publications in high-profile journals such as *Nature* and *Physical Review Letters.*

Mission Relevance

This project is important to work related to high-energy-density physics and ultra-intense lasers and therefore supports the Laboratory's mission in stockpile stewardship and energy security. Our breakthrough, high-profile achievement will also help to recruit leading scientists in this cutting-edge field.

FY09 Accomplishments and Results

In FY09 we analyzed electron and positron data from experimental campaigns on both Titan and OMEGA EP laser systems. Specifically, we (1) estimated the expected number of pairs, and then measured the positron creation rate using an improved positron spectrometer, which compared well with our predictions; (2) succeeded in obtaining the highest positron creation rate ever recorded in the laboratory, and observed electron–positron jet-like behavior; (3) compared the experimental results with theoretical predictions and discovered an accelerating mechanism for positrons exiting the target that creates a nearly monoenergetic beam of positrons; and (4) fielded high-energy bremsstrahlung and annihilation radiation detectors for the first time on Titan to measure high-energy x rays. This project successfully achieved its goal of characterizing the first dense electron–positron jet created in the laboratory by ultra-intense lasers interacting with matter. We laid the foundation for a current LDRD project that will attempt to determine the feasibility of this method of positron creation as a new, intense source of positrons suitable for a wide range of scientific inquiry.

Publications

Chen, H., et al., 2009. "Electron energy distributions from ultra-intense laser solid interactions." *Phys. Plasma.* **16**, 020705. LLNL-JRNL-407653.

Chen, H., et al., 2008. *Positron creation using the Titan short pulse laser.* 50th Ann. Mtg. Division of Plasma Physics, Dallas, TX, Nov. 17–21, 2008. LLNL-ABS-405592.

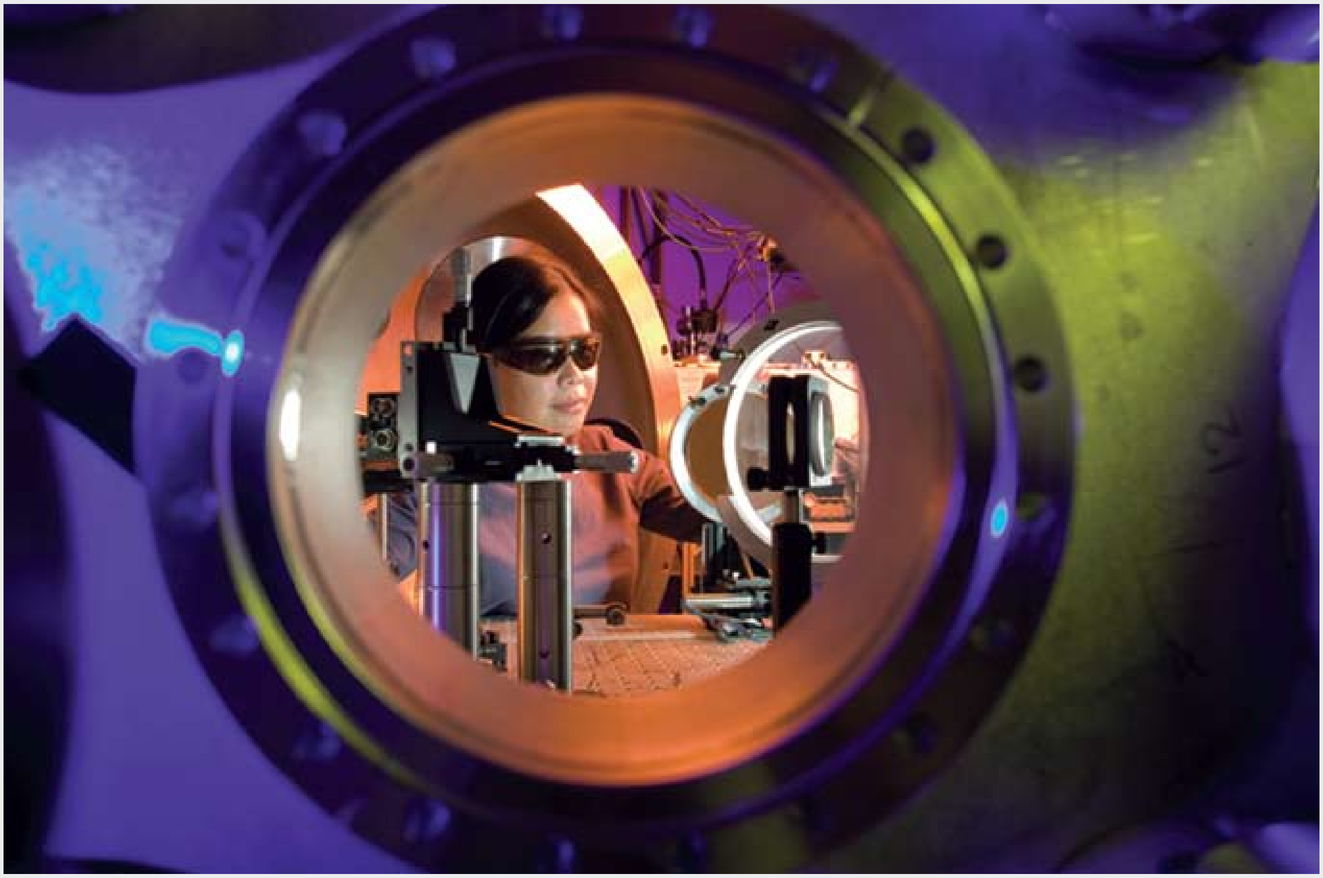
Chen, H., et al., 2009. "Relativistic positron creation using ultra-intense short pulse lasers." *Phys. Rev. Lett.* **102**, 105001. LLNL-JRNL-406720.

Meissner, C., 2009. "Mass producing positrons." *Science and Technology Review* July/August 2009, 18. UCRL-TR-52000-09-7/8.

Wilks, S. C., et al., 2008. *Generation mechanisms of multi-MeV electrons in ultra-intense laser plasma interactions and applications.* 50th Ann. Mtg. Division of Plasma Physics, Dallas, TX, Nov. 17– 21, 2008. LLNL-ABS-405449.

Wilks, S. C., et al., 2009. *Positron jets from ultra-intense laser-matter interactions.* 6th Int. Conf. Inertial Fusion Sciences and Applications, San Francisco, CA, Sept. 6–11, 2009. LLNL-ABS-412627.

Wilks, S. C., et al., 2009. *Simulations of relativistic positron creation using ultra-intense, short pulse lasers.* 51st Ann. Mtg. Division of Plasma Physics, Atlanta, GA, Nov. 2–6, 2009. LLNL-ABS-414748.



Experimentalist Hui Chen looks into the vacuum chamber where the first electron–positron jet experiments using Livermore's Titan laser were performed.

Plasma Waveguide for Electron Acceleration—

Dustin Froula (08-LW-070)

Abstract

We will develop a novel scheme for guiding laser beams in plasmas. This scalable platform will be directly applicable to wakefield acceleration and the amplification of short-pulse lasers. In our scheme, an external magnetic field will be used to prevent radial heat transport, resulting in a temperature gradient and therefore a density gradient, which will act as an optical plasma waveguide. This plasma platform will yield a significant increase in electron beam energy (up to 10 GeV) and beam current. This proposed tabletop wakefield electron accelerator is well-suited for driving pulsed radiation sources with femtosecond-duration bunches, such as free-electron lasers and tunable x-ray radiation through Thomson upshift.

We will demonstrate a plasma channel that is inherently scaleable to produce greater than 10-GeV electrons and the next generation of high-power, short-pulse laser beams. Our novel concept will not only be scalable to electron beam energies found in conventional accelerators, but will also provide a short-pulse electron beam suitable for use as an x-ray laser, a tunable x-ray source, and a multiple gigaelectronvolt tabletop accelerator. Our tabletop accelerator will leverage and extend the unique expertise and capabilities of LLNL and establish the Laboratory as a frontrunner in a new field that includes world-class laboratories.

Mission Relevance

The multiple gigaelectronvolt beams of femtosecond-duration electron bunches that this project will enable will be suitable for free-electron lasers producing high-energy x rays, tunable x-ray radiation through Thomson upshift, and tabletop accelerators—all applications that support high-energy-density physics investigations, biological studies to improve human health, and weapons studies.

FY09 Accomplishments and Results

In FY09 we (1) implemented a new electron injection mechanism, (2) accelerated electrons to 1.7 GeV over 1.5 cm, obtained after measuring a self-injection threshold that has limited acceleration to less than 1 GeV; and (3) used Thomson scattering to make initial measurements of the magnetically controlled plasma waveguide, which are the first imaging Thomson-scattering results to resolve scattering from the electron plasma wave and form the basis for our FY10 work to explore the ability of the magnetic field to shape the plasma channel.

Proposed Work for FY10

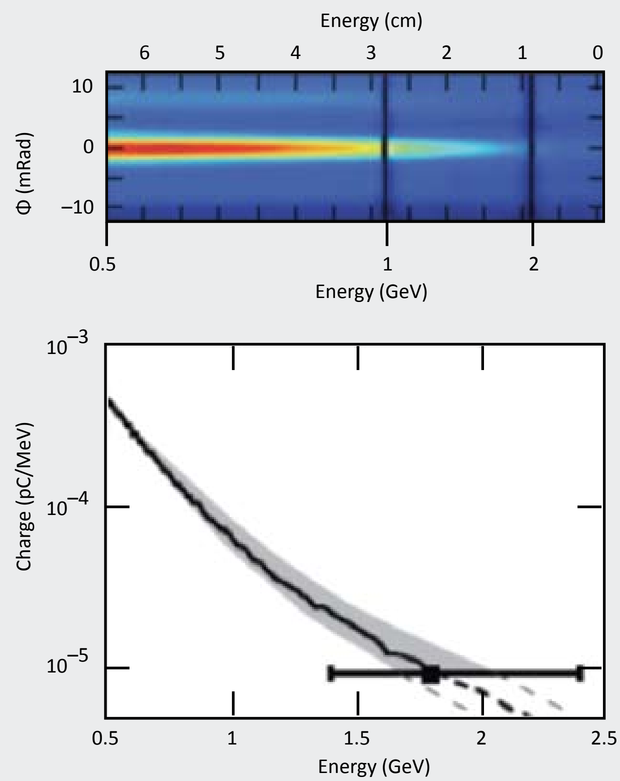
Our objective in FY10 is to demonstrate a magnetically controlled waveguide and to guide a relativistically intense laser beam over 5 cm. These results will be the longest low-density channels produced to date and will lead directly to electron acceleration of greater than 3 GeV. The design of these experiments is a direct result of hydrodynamic modeling performed in FY09, which shows that a 3-T external magnetic field is sufficient to produce a low-density channel. Specifically, we will perform eight weeks of experiments on Livermore's Janus long-pulse laser system to optimize the channel shape. This optimized system will then be moved to the Callisto short-pulse laser system where a greater than 10-TW, 60-fs beam will be used to demonstrate guiding. Successful completion of these objectives will be highly visible within the community, and we intend to publish the results in a high-profile journal.

Publications

Froula, D. H., et al., 2009. "Magnetically controlled plasma waveguide for laser wakefield acceleration." *Plasma Phys. Contr. Fusion* **51**, 024009. LLNL-JRNL-403962.

Froula, D. H., et al., 2009. "Measurements of the critical power for self-injection of electrons in a laser wakefield accelerator." *Phys. Rev. Lett.* **103**(21), 215006. LLNL-PRES-410631.

Leurent, V., et al., 2008. "Study of x-ray radiation from a laser wakefield accelerator." *Advanced accelerator concepts: Proc. 13th Advanced Accelerator Concepts Workshop*, vol. 1086,



Electrons are accelerated to 1.7 GeV in a 1.5-cm-long plasma using the 200-TW Callisto laser system.

pp. 235–240. AIP Conference Proceedings, Melville, NY. LLNL-PROC-406432.

Pollock, B. B., et al., 2008. “Multicentimeter long high density magnetic plasmas for optical guiding.” *Rev. Sci. Instrum.* **79**, 10F550. LLNL-CONF-403602.

Pollock, B. B., et al., 2009. “Two-screen method for determining electron beam energy and deflection from laser wakefield acceleration.” *Proc. 23rd Particle Accelerator Conference*. LLNL-PRES-410652.

Ross, J. S., et al., 2009. *Thomson scattering measurements in the collective and non-collective regime in laser produced plasmas.* OMEGA Laser Facility Users Group 2009 Workshop, Rochester, NY, April 29–May 1, 2009. LLNL-POST-412466.

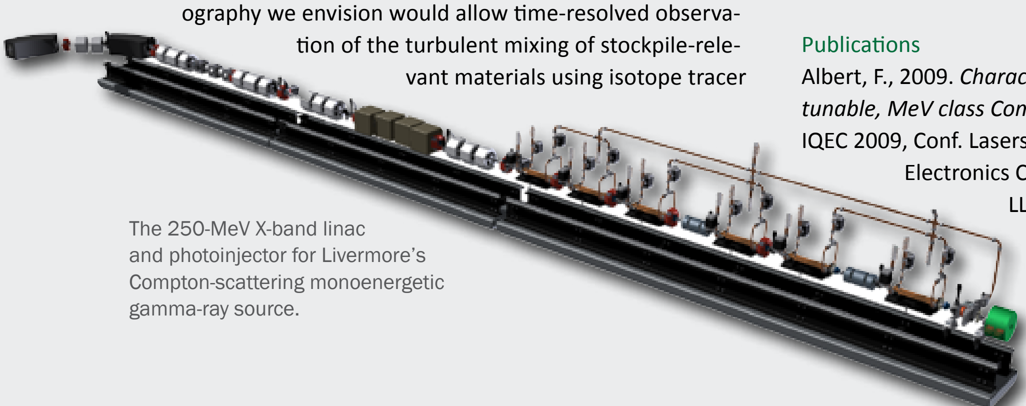
Visco, A., et al., 2009. “Temporal dispersion of a spectrometer.” *Rev. Sci. Instrum.* **79**, 10F545. LLNL-CONF-403770.

Precision Monoenergetic Gamma-Ray Science for NNSA Missions—Christopher Barty (09-SI-004)

Abstract

We intend to research compact, monoenergetic gamma-ray (MEGA-ray) science for four high-impact NNSA mission areas: (1) isotope-specific nuclear resonance fluorescence imaging of stockpile and ignition components, (2) isotopic assays of fission products and waste stream applications such as for the Global Nuclear Energy Partnership, (3) isotopic radiography and quantitative assays of the DOE complex’s legacy waste, and (4) isotope-specific flash radiography of multicomponent turbulent hydrodynamic experiments and ignited plasmas. Our goal is to establish and demonstrate the world’s first MEGA-ray system capable of meeting the needs of these new mission areas. This work will also provide unique abilities for the production and investigation of unique states of matter, photo–nuclear interactions, and advanced laser accelerators.

If successful, we will develop and demonstrate short-pulsed laser-based MEGA-ray sources for the static, isotope-specific imaging and assaying of highly enriched uranium, as well as for applications in stockpile stewardship, legacy waste, and dynamic nuclear resonance fluorescence imaging. The flash isotope radiography we envision would allow time-resolved observation of the turbulent mixing of stockpile-relevant materials using isotope tracer layers. With a modular compact design, the robust MEGA-ray sources we develop would also form the basis for portable isotope radiography tools for other national and homeland security applications.



The 250-MeV X-band linac and photoinjector for Livermore’s Compton-scattering monoenergetic gamma-ray source.

Mission Relevance

This project supports the Laboratory’s national security mission by developing a new and potentially revolutionary dynamic, isotope-specific radiography capability for stockpile stewardship and fundamental weapons physics, by increasing the proliferation resistance of the nuclear fuel cycle with precision isotopic monitoring, and by demonstrating the potential for MEGA-ray sources for highly enriched uranium detection at trade portals. The project also supports the environmental management mission by enabling quantitative assessment and reclassification of the DOE complex’s nuclear waste.

FY09 Accomplishments and Results

In FY09 we (1) designed the overall system including the high-brightness X-band linac and radiofrequency photoinjector, the fiber-based photocathode laser, the diode-pumped chirped-pulse amplification interaction laser, and the interaction region for gamma-ray production; (2) developed a new, fully three-dimensional nonlinear code to obtain high-precision description of long-pulse, weakly nonlinear Compton scattering that affects the gamma-ray brightness; (3) developed facility engineering and secured National Environmental Policy Act certification; and (4) performed simulations of flash isotopic radiography using Monte-Carlo codes, along with detector modeling. Highlights include high-resolution (0.18-mm-mrad) simulations of a 250-MeV, 0.25-nC electron bunch produced by a 5.59-cell radiofrequency gun coupled to six T-53 accelerator sections.

Proposed Work for FY10

In FY10 we will (1) establish a test lab for X-band radiofrequency measurements and component characterization, as well as for magnet and electron-beam lattice subsystems; (2) integrate and test low-level radiofrequency and synchronization and construct the X-band radiofrequency gun, SLED-II compression line, and high-power X-band distribution system; (3) set up laser transport beam lines and define diagnostics, control points, and feedback loops; and (4) design the final stages of the interaction-region optics and diagnostics using upgraded models for electron-beam transport and laser focusing.

Publications

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Anderson, S. G., et al., 2009. *Observation of nonlinear space-charge induced phase space wave-breaking and emittance growth in a high-brightness photoinjector.* PAC09, Particle Accelerator Conf., Vancouver, Canada, May 4–8, 2009. LLNL-ABS-409323.

Barty, C. P. J., 2009. *Mono-energetic gamma-ray (MEGA-ray) sources and nuclear applications.* LEI 2009, Light at Extreme Intensities, Brasov, Romania, Oct. 16–21, 2009. LLNL-ABS-418058.

Chu, T. S., et al., 2009. *Precision 0.5 GW X-band RF system for advanced Compton scattering source.* 12th Ann. Directed Energy Symp., San Antonio, TX, Nov. 2–6, 2009. LLNL-PRES-419532.

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Gibson, D. J., et al., 2009. *Commissioning a tunable MeV-level Compton-scattering-based gamma-ray source.* LLNL-JRNL-414643.

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Physics and Chemistry of the Interiors of Large Planets: A New Generation of Condensed Matter—Gilbert Collins (09-SI-005)

Abstract

We propose to employ Livermore's advanced laser facilities and high-explosive pulse-power capabilities to systematically characterize condensed matter at extreme conditions to the gigabar pressure range and over tenfold compression. This research focuses on establishing a new generation of experiments accessing the unexplored regime of ultrahigh compression, with applications that range from understanding the origin and evolution of planets to testing and significantly extending fundamental theories of condensed matter. Our effort will form a community of the world's leading scientists in condensed matter and planetary science, which will sustain this new field of extreme condensed matter.

We expect to characterize iron and silica polymorphs from 10 to 100 Mbar to focus on conditions relevant to core conditions of the "super-Earth" planets now being discovered outside of our solar system. We will also determine the experimental constraints on planetary models using the planetary fluids hydrogen, helium, and mixtures studied with pre-compressed shocks and ramp loading. We will explore ultrahigh-pressure solid states to discover if a Wigner crystal state exists and attempt to determine if hydrogen becomes a superconductor or superfluid under these conditions. Finally, we expect to obtain the first information on chemistry at extreme (multigigabar) conditions, including the potential for "kilovolt chemistry."

Mission Relevance

To successfully maintain an aging stockpile, the nation needs new predictive capabilities. Of particular importance to the Stockpile Stewardship Program is the development of advanced capabilities to predict physical properties of matter under the extremely broad range of dynamic conditions. Of specific importance are equation-of-state and constitutive models. Our project will fully develop required experimental capabilities as well as provide important data on metals and hydrogenic liquids in support of the Laboratory's mission in national security.

FY09 Accomplishments and Results

We (1) measured the melt curve of diamond up to 11 Mbar—the highest pressure ever achieved in a solid in the laboratory; (2) developed a diffraction technique and used it to show that iron is hexagonally closely packed up to 5 Mbar; (3) developed an extended x-ray absorption fine structure technique and used it to measure the temperature of iron ramp-compressed up to 3 Mbar; (4) designed 30-Mbar ramp-compression experiments to be carried out at the National Ignition Facility (NIF) in FY10; (5) discovered that aluminum is very strong when compressed on nanosecond time scales; (6) studied the shock compression of deuterium; and (7) held a workshop on use of the NIF for University of California at Berkeley scholars and a plenary session at an American Association for the Advancement of Science meeting.

Proposed Work for FY10

In FY10 we propose to (1) test experimental approaches for studying ramp-compressed iron and ultradense hydrogen at University of Rochester's OMEGA laser; (2) collect diffraction and x-ray absorption data for solids at pressures 10 times higher than previously explored to determine their structure and short- and long-range order; (3) collect hydrogen equation-of-state and transport data for the most extreme densities yet studied at the LIL laser facility in France; (4) begin NIF experiments on properties of extreme states of matter, including electron–ion coupling in dense fuel, stopping powers in degenerate hydrogen, and thermal conduction in dense hydrogen; and (5) begin identifying advanced burning plasma and fusion concepts.

A time-integrated photograph of an OMEGA laser shot being used to measure high-pressure diamond melt. The diamond target is at center-right. The bright white light is ablated plasma, and the radial yellow lines are tracks.

Publications

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Hicks, D. G., et al., 2009. "Laser-driven single-shock compression of fluid deuterium from 45 to 220 GPa." *Phys. Rev. B* **79**, 14112. LLNL-JRNL-402514.

From Super-Earths to Nucleosynthesis: Probing Extreme High-Energy-Density States of Matter with X Rays—Bruce Remington (09-SI-010)

Abstract

We propose to develop advanced x-ray diagnostic systems to investigate two types of extreme high-energy-density states: materials at ultrahigh pressures (>10 Mbar), such as those found at the cores of newly discovered "super-Earth" exoplanets, as well as plasma physics conditions at ultrahigh densities (>100 g/cm^3) of nuclear burn in stars and supernovae. We will develop three types of diagnostic capabilities: (1) a lattice diagnostic, (2) an ultrafast x-ray diagnostic for investigating nuclear burn, and (3) a multiframe, single line-of-sight imager. We will also validate these capabilities through experiments at laser and calibration facilities. This project will enable precision science to be conducted on matter under the most extreme conditions of density and temperature accessible, which is important to both basic and applied science.

We will develop advanced x-ray diagnostic systems to probe extreme high-energy-density states of matter relevant to the science of super-Earths and nucleosynthesis, with the goal of enabling materials science at ultrahigh pressures and studies of burning plasmas at ultrahigh densities. These new capabilities will make it possible to probe super-Earth core conditions with a dynamic lattice-level diffraction diagnostic at 100-times higher pressures and 4-times higher x-ray energies than is currently possible. It will also enable the probe of nucleosynthesis plasma conditions by dynamic characterization of hot, dense burning plasmas at 100-times higher densities and with 100,000-times higher yield than is currently possible.

Mission Relevance

By developing the capabilities to measure material phase and lattice response at ultrahigh pressures and conditions in burning plasmas at ultrahigh densities, which are relevant to stockpile stewardship and high-energy-density science, this project supports the Laboratory's national security mission.

FY09 Accomplishments and Results

In FY09 we (1) experimentally demonstrated nanosecond single-shot white-light Laue diffraction at less than 10-keV x-ray energies in static single crystals of silicon and tantalum; (2) constructed diagnostics for testing to extend this to greater than 10-keV x-ray energies; (3) identified candidate tracer dopant, spectral emission lines in burning plasmas for measuring ion temperatures; (4) identified a promising bent-crystal technique for imaging burning plasmas; (5) identified promising semiconductor materials for use as an ultrafast x-ray detector for burning plasmas and assembled an optical system for testing this diffractive imaging concept; and (6) initiated design of a 64 × 64–pixel prototype multiframe single line-of-sight camera and investigated an optimal x-ray-to-optical converter (photodiode vs. scintillator) for this camera.

Proposed Work for FY10

In FY09 we will (1) conclude optimization of the high-energy, x-ray diffraction technique and demonstrate it in driven samples, as well as test the concept to dynamically measure dislocation density in shocked materials; (2) identify candidate spectral features to measure electron temperatures and density in burning plasma and develop experiments to validate this technique; (3) acquire higher-quality semiconductor materials, optimize the sensitivity for our ultrafast x-ray diagnostic, and develop a prototype system for proof-of-principle experimental tests of ultrafast imaging; and (4) develop a 64 × 64–pixel sensor and readout electronics for the multiframe camera and select the optimal x-ray-to-optical converter suitable for use on burning plasma and high-energy x-ray diffraction.

Publications

Remington, B. A., 2009. *Progress towards materials science above 1000 GPa (10 Mbar) on the NIF laser.* 9th Intl. Conf. Mechanical and Physical Behaviour of Materials under Dynamic Loading, Brussels, Belgium, Sept. 7–11, 2009. LLNL-CONF-411555.

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The Microphysics of Burning, Hot Dense Radiative Plasmas—Frank Graziani (09-SI-011)

Abstract

We intend to develop a detailed microphysical understanding of the physics of burning, hot dense radiative plasmas by building a validated, state-of-the-art *N*-body simulation capability. The extreme conditions of these plasmas mean that experimental data for validation are difficult to obtain. What is needed for this data-starved environment is a quantitative way of telling whether or not the physics used to describe burning, hot dense radiative plasmas is correct. We will address this critical need by building a world-class massively parallel *N*-body simulation capability in

conjunction with experimental validation experiments. The microphysics of burning, hot dense radiative plasmas will be simulated without the assumptions that underlie current models used to calculate inertial-confinement fusion or astrophysical problems.

We expect to (1) develop an *N*-body simulation capability using molecular dynamics to investigate the properties of hot dense matter undergoing thermonuclear burn; (2) employ the new simulation capability to test microphysical foundations of widely accepted theoretical models; and (3) validate the new simulation capability using the ultrashort pulse lasers Titan at Livermore, the OMEGA laser at the University of Rochester, and the Linac Coherent Light Source at Stanford.

Mission Relevance

The results obtained with this project directly address the issue of predictive capability, which is at the core of the Stockpile Stewardship Program. Furthermore, the validated simulation capability for burning, hot dense radiative plasmas that we will develop extends LLNL's world leadership in high-energy-density physics to include not only experimental expertise but computational modeling as well. It will help establish LLNL as the world center for high-energy-density-physics in support of the Laboratory's mission in fundamental science breakthroughs.

FY09 Accomplishments and Results

We made significant changes in parallelization to our molecular dynamics simulation code. The new heterogeneous approach we adopted allowed the code to achieve 324.8 teraflops per second while running a 2.4-billion-particle simulation of a proton beam interacting with hot dense hydrogen plasma. This effort was acknowledged with a finalist finish in the Gordon Bell competition for high-performance computing. We also achieved over 80% parallel efficiency across 278,528 processors, resulting in the fastest-ever time to solution for the Coulomb problem—5 billion particle updates per second, more than 25 times faster than the prior state of the art. This new capability was used to investigate the ion-stopping problem in dense plasmas and to simulate laboratory experiments we will conduct in FY10.

Proposed Work for FY10

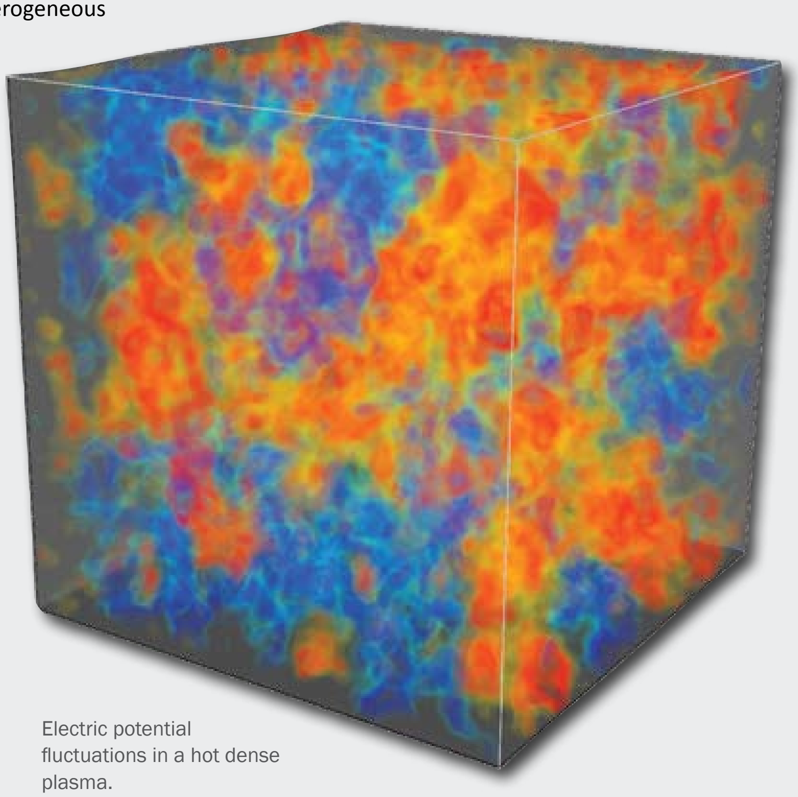
In FY10 we will (1) introduce light-isotope fusion reactions, implement wave-packet molecular dynamics, and enhance atomic physics capability by implementing three-body and radiative recombination; (2) explore modifications of wave-packet molecular dynamics with radiation; (3) explore modifications of the radiation algorithm in dense plasmas; (4) perform ion-stopping simulations in a one- and two-component plasma and determine energy splits, explore multiscale and implicit methods, and perform temperature equilibration runs in the presence of partially ionized atoms; (5) develop visualization tools; (6) perform ion-stopping-power experiments on the Titan laser; and (7) design and perform validation experiments at the Linac Coherent Light Source.

Publications

Benedict, L. X., et al., 2009. "Molecular dynamics simulations of electron-ion temperature equilibration in an SF6 plasma." *Phys. Rev. Lett.* **102**, 205004. LLNL-JRNL-412459.

Glosli, J. N., et al., 2009. "Molecular dynamics simulations of temperature equilibration in dense hydrogen." *Phys. Rev. E* **78**, 025401. LLNL-JRNL-401466.

More, R., et al., 2009. "Radiation in particle simulation." *High Energ. Density Phys.* **6**, 29. LLNL-PROC-413971.



Electric potential fluctuations in a hot dense plasma.

Improved Spectral Line-Shape Models for Opacity Calculations—Carlos Iglesias (09-ERD-004)

Abstract

Rosseland mean opacities are important for energy-transport simulations used in the design and analysis of laboratory applications such as inertial-confinement fusion. However, theoretical Rosseland mean opacities vary by as much as a factor of two because of uncertainties in models of spectral line shapes. Our main goal is to improve spectral line-shape models in the opacity codes by applying line-broadening theory to complex electronic configurations that have been heretofore neglected by the scientific community but are essential for opacity calculations. The results will be extended to the super-configuration array concept, which is vital for calculations involving myriad configurations. Finally, we will synthesize this gained knowledge into a suite of routines for incorporation into opacity codes.

The project will produce improved opacity codes by addressing three uncertain aspects of line-shape models: line-width calculation using approximate formulas, far-wing behavior, and line broadening in complex multi-electron ions. We will produce fast computer subroutines that parameterize these complex processes and incorporate the subroutines into opacity codes. These achievements will result in improved theoretical opacities, which will in turn resolve uncertainties in many laboratory applications that depend on the accurate simulation of energy-transport mechanisms.

Mission Relevance

This project supports the Laboratory's missions in national and energy security by addressing an important knowledge gap in advanced physical models for predictive capabilities for weapons science, nuclear physics, astrophysics, and high-energy-density science.

FY09 Accomplishments and Results

Opacity calculations require line shapes for many-electron ions. We investigated the role of excited spectator-electron effects on line shapes involving transitions of tightly bound electrons. We resolved, using the interference terms of Stark line broadening, the apparent contradiction of large line widths from excited spectators and the vanishing of their contribution in the limit of decoupling to the active electron. These interference terms are usually small for diagnostic lines but can dominate the line profile when excited electrons are present.

Proposed Work for FY10

In FY10 we will (1) develop a fast algorithm that contains the essential features of line broadening to improve the line-shape model in the opacity calculation; (2) compare computationally fast, but necessarily approximate schemes, to the more accurate but slow TOTAL code; (3) incorporate the fast modules into opacity models; (4) study the far-line wing; and (5) use Livermore experimental results independent of our effort to test theoretical calculations.

First-Principles Planetary Science—Kyle Caspersen (09-ERD-012)

Abstract

The objective of this project is to provide a first-principles understanding of the interiors of the four gas giants in our solar system—Jupiter, Saturn, Uranus, and Neptune. The lack of experimental data on the interior of these four planets leads to uncertainty and unanswered questions about their formation, current structure, and how they will evolve. We will address these questions using the predictive capability of first-principles calculations. In particular, we will calculate planetary lines of constant entropy (isentropes) to predict the pressures and temperatures in these gas giants and transport properties along the isentropes to provide insight into planetary dynamics.

In this proposal we will construct thermodynamically consistent, first-principles planetary isentropes that are free from most current assumptions. We will also calculate transport properties along these isentropes. This will be the first time that planetary isentropes and their corresponding transport properties have been calculated with completely first-principles calculations. The unequaled precision and predictive power of these calculations will allow us to address fundamental questions in the field of planetary science and will also directly benefit many ongoing efforts at LLNL, including equation-of-state table development, the generation of mixing and plasma models, and dynamic compression experiments.

Mission Relevance

This project supports LLNL's national security mission by developing predictive modes for examining the properties of materials under extreme conditions. Such techniques, if successful, will have direct application to equation-of-state models for materials of interest for stockpile stewardship and other Laboratory missions.

FY09 Accomplishments and Results

In FY09 we calculated isentropes for both Jupiter and Saturn and a whole family of isentropes for large hydrogen–helium worlds. We focused on transport properties for the ice giants—specifically, electrical and thermal conductivities. In addition, we used the isentropic data to provide a first-principles answer to an open question in planetary science—the temperature anomaly between Jupiter and Saturn.

Proposed Work for FY10

In FY10 we will (1) continue the calculation of relevant isentropes; (2) begin calculation of transport properties such as viscosity and diffusivity along the isentropes; (3) begin investigation of the kinetics of helium condensation; (4) expand the study of hydrogen mixtures beyond helium to other elements including other noble gases, as well as carbon and oxygen; and (5) hire a postdoctoral researcher.

Publications

Morales, M. A., et al., 2009. "Phase separation in hydrogen–helium mixtures at Mbar pressures." *Proc. Natl. Acad. Sci. USA* **106**, 1324. LLNL-JRNL-411757.

Imaging X-Ray Line Shape Diagnostic for Burning Plasmas—Peter Beiersdorfer (09-ERD-016)

Abstract

This project will investigate the suitability of neonlike tungsten as a tracer ion for measuring ion temperature and velocity in a hot, ignited plasma. Such measurements are crucial for achieving fusion ignition and burn. We will build a new type of imaging spectrometer, which will operate in a vacuum and use a spherically bent crystal in its Johann geometry. We will also test key aspects of a tungsten-based spectrometer, including throughput issues, window design, bake capability, and power dissipation of the detector in a vacuum. We will utilize LLNL's Electron Beam Ion Trap facility, which is uniquely suited to produce the relevant radiation.

If successful, this project will produce novel atomic data and enable world-class science experiments, such as measurements of excitation rate coefficients, ultrafast radiative lifetimes, and dielectronic rate coefficients, which have never before been measured for such high-Z systems, but are needed to determine ion temperature and motion. We will also provide the scientific and technological basis for choosing a tungsten-based instrument design and create a prototype instrument for hot plasmas with which we will assess the technological hurdles of measuring radiation from an ignited plasma.

Mission Relevance

This project supports the Laboratory's missions in energy security by developing groundbreaking technologies for achieving fusion-driven energy sources. This project will also help attract top talent to the Laboratory in this topical, cutting-edge field.

FY09 Accomplishments and Results

In FY09 we (1) successfully generated survey spectra for different charge balances recorded with our x-ray microcalorimeter; (2) used these spectra to investigate the spectral landscape surrounding the 2p–3s and 2p–3d transitions at 8.4 and 9.0 keV, respectively, and have identified additional candidate lines for diagnostics of burning plasmas; (3) made ionization equilibrium calculations for comparison with several of our measurements; and (4) designed a novel high-resolution imaging spectrometer optimized for measuring tungsten L-shell lines, which employs a spherical crystal and a high count-rate x-ray detector.

Proposed Work for FY10

In FY10 we will (1) finish design and construction of our high-resolution imaging spectrometer, which we are optimizing for measuring tungsten L-shell lines; (2) test both quartz and germanium crystals at Bragg angles near 45° and determine the spectral resolution in measurements on the Electron Beam Ion Trap source; (3) test throughput of the new instrument in comparison with concurrent microcalorimeter measurements, and also assess its imaging capabilities; and (4) use the new spectrometer to make high-resolution measurements of the relevant tungsten lines, including dielectronic satellite features and inner-shell satellite lines to assess blends that may affect the shapes of relevant diagnostic lines.

Publications

Clementson, J., et al., 2010. "Spectroscopy of M-shell x-ray transitions in Zn-like through Co-like W." *Phys. Scr.* **81**, 015301. LLNL-JRNL-414669

Podpaly, Y., et al., 2009. "High-resolution spectroscopy of $2s_{1/2}$–$2p_{3/2}$ transitions in W^{65+} through W^{71+}." *Phys. Rev. A.* **80**(5), 052504. LLNL-JRNL-416158.

Safronova, U. I., A. S. Safronova, and P. Beiersdorfer, 2009. "Excitation energies, radiative and autoionization rates, dielectronic satellite lines, and dielectronic recombination rates for excited states of Mg-like W from Na-like W." *J. Physics B: At. Mol. Opt. Phys.* **42**, 165010. LLNL-JRNL-413406.

Safronova, U. I., A. S. Safronova, and P. Beiersdorfer, 2009. "Excitation energies, radiative and autoionization rates, dielectronic satellite lines, and dielectronic recombination rates for excited states of Na-like W from Ne-like W." *At. Data Nucl. Data Tab.* **95**(6), 751. LLNL-JRNL-407732.

Trabert, E., in press. "In pursuit of high precision atomic lifetime measurements of multiply charged ions." *J. Physics B: At. Mol. Opt. Phys.* LLNL-JRNL- 413576.

Ultrafast Nanoscale Dynamic Imaging Using X-Ray Free-Electron Lasers—Stefan Hau-Riege (09-ERD-023)

Abstract

Fourth-generation x-ray light sources, such as x-ray free electron lasers (XFELs), offer to revolutionize x-ray science by delivering ultrashort (20–200 fs) pulses of unprecedented brightness (~1012 photons/pulse). This project takes advantage of the unprecedented capability of XFELs to probe the dynamic properties of materials under extreme conditions using the newly available ultrafast, ultrabright x-ray pulses from XFEL sources. We will first perform experiments to establish techniques and will then perform optical pump-probe and XFEL dynamic imaging at the near-atomic scale at the Linac Coherent Light Source (LCLS), when the Stanford facility comes online in 2010.

We propose to study foam-shock dynamics and two-phase ablation with optical pump–XFEL probe experiments and examine the equation of state of high-energy-density matter with XFEL pump-probe hydrodynamics experiments. In addition, we expect to perform dynamic imaging experiments at LCLS that will reveal solid-shock dynamics at near-atomic scale. The successful completion of this project will establish Livermore's leadership in these high-energy-density experiments using XFELs and enable numerous future discoveries in the field. Programs in stockpile stewardship and inertial-confinement fusion are dependent on high-quality data describing the properties and processes of high-energy-density matter, and results from these experiments will contribute valuable data and new techniques to these programs.

Mission Relevance

By exploiting an entirely new generation of x-ray sources, this project supports the Stockpile Stewardship Program, which is highly dependent on high-quality data describing the properties and processes of high-energy-density matter. National security and weapons science are served through the proposed study of dynamic systems with broad application to the investigation of material dynamics under extreme conditions. Novel imaging techniques are also at the cutting edge of photon science applications, which will be developed at LCLS.

FY09 Accomplishments and Results

In FY09 we (1) measured the expansion dynamics of aluminum spheres on silicon nitride membrane structures—with and without a tamper—at the FLASH soft x-ray free-electron laser in Hamburg, Germany, with a wavelength of 13 nm; (2) compared the experimental results with hydrodynamic computer simulation using the LLNL equation-of-state library, observing good agreement; and (3) performed experiments on solid and gas targets with the LCLS hard-XFEL to understand the interaction of materials to this extreme radiation.

Proposed Work for FY10

In FY10 we will perform experiments at the LCLS that focus on time-resolved imaging of the microstructure of high-energy-density materials. Specifically, we will (1) diffract the LCLS beam off a material at several tens of electronvolts to observe the onset of Bragg spot fading, resulting in the maximum fluence to probe crystalline materials without perturbation, and obtain information about the onset of nonthermal melting—for the wavelength range between 0.6 and 1.6 nm, we will choose a material with a large unit cell size, such as graphite; (2) perform the first time-resolved LCLS diffraction experiments on driven samples using a long-pulse optical laser to induce large-amplitude waves or shocks in a film; and (3) compare the results with molecular dynamics simulations.

Publications

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Scrape-Off Layer Flow Studies in Tokamaks—Thomas Rognlien (09-ERD-025)

Abstract

The purpose of this project is to develop new techniques to measure boundary-plasma flows in tokamaks and assess and implement new physics and computational methods in the UEDGE code to understand and predict the flows, which are presently unexplained. Boundary flows play a critical role in tritium accumulation via co-deposition in devices using carbon, such as the International Thermonuclear Experimental Reactor, which will operate with a strict tritium-inventory limit. We will design an optical imaging system based on a Fourier transform spectrometer that permits measurements in high-power plasmas to be tested in the DIII-D tokamak at General Atomics in San Diego. To make reliable predictions of the boundary flows with UEDGE, we will implement and validate new algorithms and physics—for example, kinetic effects distilled from our kinetic TEMPEST code.

We expect to deliver a prototype optical system on the DIII-D tokamak that can reliably measure plasma flows in at least one poloidal segment of the scrape-off layer, the outer layer of a tokamak plasma that is affected (scraped off) by a divertor or limiter. In addition, other suitable diagnostic techniques may be identified. The upgraded version of UEDGE will be implemented, and comprehensive validation will be performed to determine physics of the measured flows that can be applied to optimize device operation and future design. Synergy of experimental, theoretical, and simulation work will lead to major advancement of boundary plasma physics, positioning LLNL for an anticipated new device design. Results will be published in journals relevant to magnetic-confinement fusion.

Mission Relevance

Development of a new diagnostic system and its use to validate advanced simulations of the boundary plasma in magnetically confined fusion devices supports the Laboratory's mission in energy security through development of fusion energy in tokamaks. The project will help to establish fusion as an abundant, reliable, and clean energy source. In addition, our research supports the Laboratory's emerging science and technology plan of research in high-energy-density and burning plasmas, as well as efforts in high-fidelity simulations.

FY09 Accomplishments and Results

We (1) installed a Fourier transform spectrometer on the DIII-D tokamak in collaboration with the Australian National University and used it to generate initial data on edge plasma flow, (2) recruited a postdoctoral researcher with strong numerical skills to aid in upgrading UEDGE, (3) developed and tested a new algorithm that extends the range of converged simulations in the strong-flow regime, and (4) began generating estimates of kinetic corrections.

Proposed Work for FY10

In FY10 we will (1) focus on further developing the experimental technique for flow measurement, including a prototype on the DIII-D tokamak; (2) make improvements to the UEDGE fluid model; and (3) compare our calculations with the experimental results.

Publications

Nam, S. K., and T. D. Rognlien, 2009. *Comparison of cross-magnetic-field drift algorithms in UEDGE.* 51st Ann. Mtg. Division of Plasma Phys., Atlanta, GA, Nov. 2–6, 2009. LLNL-ABS-414790.

Understanding the Initiation of High-Voltage Vacuum Insulator Flashover—Timothy Houck (09-ERD-028)

Abstract

Advanced, high-performance pulsed-power systems are used in applications related to national security, including nuclear weapons science. The vacuum insulator is a critical component of such systems, limiting maximum achievable performance. If designed incorrectly, the component can lead to failure of the entire system. Although scientific knowledge developed from simple experiments provides an understanding of an insulator's performance, that knowledge is not readily translated into a tool for reliably predicting the performance of an operational system. In this project, we will develop a computer model of electrical breakdown at a dielectric–vacuum interface for use in designing vacuum insulators for advanced, high-performance pulsed-power systems. We will leverage LLNL's advances in computational resources, which provide a means to bridge the gap between knowledge and application.

If successful, we will produce an important computational tool for designing pulsed-power systems. We also expect to demonstrate computationally that a few basic physics phenomena are

responsible for the initiation of electrical breakdown across the dielectric–vacuum interface, known as vacuum insulator flashover. Varying the geometry, materials, and environment used in simulations will show how different initiation mechanisms evolve. This tool will make it possible to study complex insulator designs in realistic operational applications and predict performance. We will also deliver a proposed insulator design, including expected performance, for the next generation of coaxial flux-compression generators.

Mission Relevance

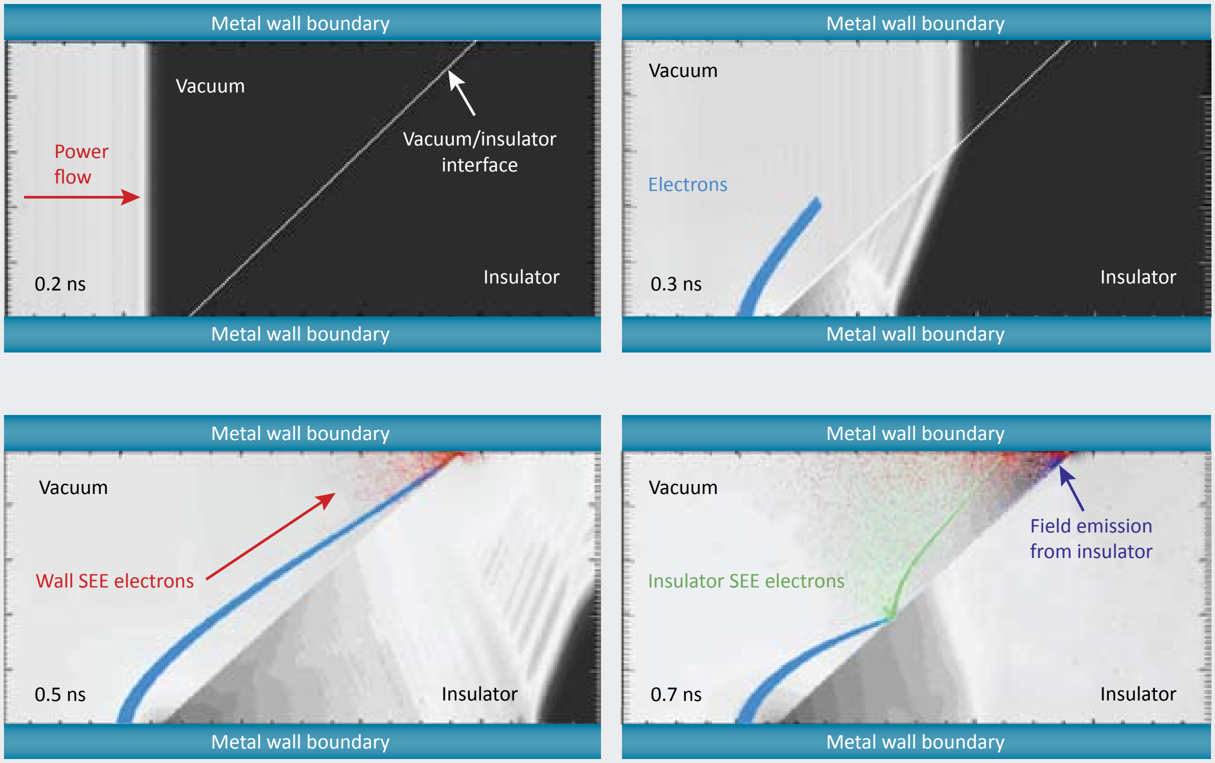
This project supports LLNL's national security mission by providing an important tool for developing capabilities in high-energy-density physics and nuclear weapons science. Our computational model will allow LLNL to become a world-class center for high-voltage vacuum insulator design and testing, thus helping LLNL attract top talent.

FY09 Accomplishments and Results

In FY09 we (1) selected the particle-in-cell code VORPAL and installed it on the Open Computing Facility at Livermore; (2) checked various algorithms such as electromagnetic energy propagation, field emission, secondary electron emission, and impact ionization; (3) modified the code's secondary electron emission model for our application—the secondary electron emission phenomenon deals with production of electrons when incident electrons impact a surface, and if more electrons emerge from the surface than impact, an avalanche of electrons can form and initiate flashover; and (4) completed a series of increasingly complex simulations, starting with a base design and an empty power flow channel, by adding dielectric interfaces (insulators), field emission, secondary emission from insulator and metal surfaces, and desorbed gas layers. The final complex design serves as the basis of ongoing studies this coming year.

Proposed Work for FY10

In FY10 we will continue more complex situations where two or more competing flashover mechanisms are present and/or mitigating techniques are employed. We anticipate discovering software incompatibilities between the various physics modules that were not obvious for the simpler designs considered in the previous year. A significant effort may be needed in correcting and validating the modules. Specifically, we will (1) continue to study complex designs and optimization studies, (2) design a novel insulator for ultralow-inductance power channels, and (3) study insulator designs that could have programmatic impacts.



Electromagnetic power (white area) flows from left passing through an angled insulator. Emitted electrons are swept by the electromagnetic field into the opposing wall and insulator, producing secondary electrons.

Publications

Perkins, M. P., et al., 2009. *Progress on simulating the initiation of vacuum insulator flashover.* 17th IEEE Intl. Pulsed Power Conf., Washington, DC, June 29–July 2, 2009. LLNL-PROC-414298.

Critical Enabling Issues for Burning-Plasma Diagnostics—Steven Allen (09-ERD-030)

Abstract

This project will study and define two diagnostic techniques for tokamak burning plasmas: a motional Stark effect (MSE) technique to measure current profile and an infrared-radiation fast-scanning technique to measure plasma wall temperature. For the MSE technique, we will address several important issues of MSE measurement: a polarization-preserving vacuum window, techniques to minimize stress birefringence caused by vacuum forces and temperature gradients, and whole-spectrum measurement of the Stark spectrum. For the infrared-radiation technique, we will investigate the feasibility of developing a fast, two-color scanning diagnostic for conducting measurements in burning plasma experiments such as the International Thermonuclear Experimental Reactor (ITER) in France.

In collaboration with the University of Arizona, we will pursue MSE polarization engineering and develop a polarization-preserving vacuum window. Measurements of the whole Stark spectrum will be used to compare an alternate measurement technique with MSE and to evaluate the effects of different plasma conditions on details of the spectrum. We will also develop a prototype, fast two-color infrared-radiation line scanner—two colors make the measurements less susceptible to changes in surface emissivity—for the measurement of tokamak wall temperatures.

Graduate student Josh King working inside the General Atomics DIII-D tokamak fusion reactor in San Diego on the calibration of the motional Stark effect diagnostic.

Mission Relevance

This project supports LLNL's mission in energy security by making important contributions to the study of the physics of magnetic-fusion burning plasmas, such as those in ITER, and by applying cutting-edge tools to the development of fusion energy as an abundant, reliable, and clean energy source.

FY09 Accomplishments and Results

In FY09 we (1) installed, debugged, and improved a new fast MSE measurement technique including a digital lock-in detection, (2) obtained the first data from this system, (3) began measurements of the system's Mueller matrix, and (4) began measurements of the entire MSE spectrum.

Proposed Work for FY10

In FY09 we expect to (1) complete the signal-to-noise assessment of the new polarimeter system, and thereby determine if plasma magnetohydrodynamic signals can be observed; (2) assess the performance of the new digital lock-in signal detection and compare the signal-to-noise with an analog lock-in system; (3) make significant progress in the design of the new polarization-preserving vacuum window and identify prototypical positive and negative Verdet (Faraday rotation) glasses; (4) test our prototype, and if successful, perform testing on an existing tokamak system; and (5) begin conceptual design of the fast infrared-radiation imager.

Experimental Determination of Dense Plasma Effects on Bound States in Extreme States of Matter—

Ronnie Shepherd (09-ERD-032)

Abstract

We propose a series of experiments coupled with calculations and simulations to study the bound states of a well-characterized, dense plasma to determine the conditions in which the outer electrons are no longer bound to the ionic core in a dense plasma. The study will be performed by measuring K-shell absorption spectra while varying the electron density. The density will be varied by the short-pulse laser heating of aerogels and the shock heating of solids. In addition to absorption, we will also measure target temperature to eliminate the ionization from temperature. The measurements will test the effects of continuum lowering and pressure ionization in dense plasma—conditions that occur in stellar interiors and nuclear weapons explosions.

We expect to provide detailed data on the average occupation number for outer bound states in plasmas ranging from weak regimes to strong, coupling regimes. We expect these data to benchmark pressure ionization and continuum-lowering models. This groundbreaking work is expected to appear in high-profile journals and set a new standard in plasma physics experiments.

Mission Relevance

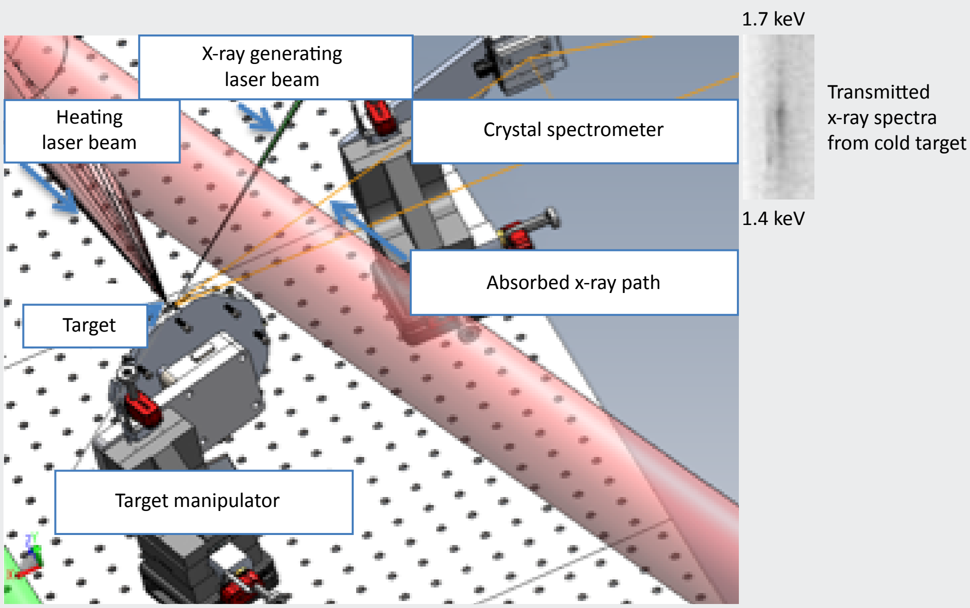
This project supports LLNL's national and energy security missions by improving advanced physical models and enabling critical calculations for weapons physics and inertial-confinement fusion.

FY09 Accomplishments and Results

In FY09 we (1) designed and built our aerogel targets—silicon dioxide aerogels of 10, 100, 250, and 500 mg/cm^3 were fabricated and attached to 400-Å silicon-nitride windows; (2) successfully completed the experimental layout for the x-ray absorption experiments and fabricated all the necessary equipment to perform the initial experiments—a preliminary set of experiments was performed using the design and target; and (3) successfully demonstrated the frequency domain interferometer diagnostic and alignment. Because of a shortened laser schedule at the Livermore Jupiter Laser Facility, we were not able to complete the experimental campaign to generate our first data set. We are planning to resume this experimental campaign next calendar year.

Proposed Work for FY10

In FY10 we will (1) complete and analyze data from the Jupiter experiment, model the data, and publish the results; (2) build and test our streaked x-ray pyrometer; (3) field this diagnostic on a series of experiments to measure temperature using x-ray emissivity; (4) perform preliminary experiments on shock-compressed materials at France's LULI and Livermore's Titan laser facilities to characterize preheat and thermodynamic conditions; and (5) perform, if time allows, our first x-ray absorption campaign on shock-compressed materials.



Experimental layout for our x-ray absorption experiment, along with x-ray absorption data for an unheated target.

Uses of Ignition at the National Ignition Facility—
L. John Perkins (09-ERD-036)

Abstract
This research seeks to address one of the most important scientific questions facing the Laboratory in the next decade: How will the achievement of ignition and thermonuclear yield at the National Ignition Facility (NIF) be utilized to provide unique weapons physics data for the Stockpile Stewardship Program? Accordingly, we propose to establish the technical basis of a new target concept with experimental packages that operate in the nuclear (high-energy-density) regime, unattainable on any other facility. Such targets could be fielded directly following the NIF ignition campaign. We will focus on data on two critical performance uncertainties that must be resolved in order for this platform to be used in stockpile stewardship.

We expect to produce a significant answer to the question of how NIF would be best utilized once ignition is achieved. The results from this study will position the Laboratory to take full advantage of NIF ignition with technically credible proposals for advanced, stockpile-relevant targets that make full use of high-energy densities stemming from ignition and thermonuclear burn.

Mission Relevance
This work supports the Laboratory's mission in national security by furthering the development of advanced experimental platforms for NIF, advanced physical models for predictive capability, and advanced weapons physics simulation capabilities, and by supporting high-energy-density burning plasma science and beyond-state-of-the-art diagnostics for stockpile science.

FY09 Accomplishments and Results
In FY09 we (1) scoped the design of three novel NIF target platforms of direct relevance to data needs for the Stockpile Stewardship Program; (2) demonstrated the unique potential for NIF targets that operate in the ignition and thermonuclear burn regime, unattainable on any other facility outside a nuclear test, with potential to provide data of direct relevance to weapons physics needs in the nuclear phase of operation; and (3) determined that the most promising of these designs offers simple target fabrication, modest laser performance requirements, good prospects of being fielded in the near term and, in particular, prospective data of direct relevance to the National Boost Initiative and to our primary design codes.

Proposed Work for FY10
In FY10 we propose to (1) select one of the three candidate target designs that we evaluated in FY09 and concentrate on this platform as a candidate for the first near-term NIF ignition and burn stockpile stewardship platform; (2) optimize the one-dimensional design and energetics and then proceed to two-dimensional symmetry and stability analysis together with specifications of NIF laser requirements including energy, power, timing, and final-focus geometry; and (3) assess the target's potential to provide specific principal data needs for primary design codes as well as NIF diagnostics requirements. We seek, therefore, to close the loop between primary data needs, NIF target design, and code validation.

Arc Initiation of High Explosives—James Mccarrick (09-ERD-042)

Abstract
Recent experiments have shown unique aspects of arc initiation in high explosives (HE), such as low thresholds that scale inversely with input power and that cannot be predicted or reproduced with existing computational models. These issues pose significant implications for the safety and surety of existing and future weapon systems. The objective of this project is to develop a fundamental understanding of the physical mechanism of arc initiation in HE. To this end, we will perform experiments required to support the physical model for specific HE. We will also develop a rigorous, nonempirical physical model appropriate to the unique combinations of plasma-energy transport and high-temperature HE kinetics. Time-resolved infrared spectroscopy and microcalorimetry will supply data to support the model. Our experiments involve novel applications of existing LLNL facilities and fabrication experience.

This project will result in a fundamental understanding of (1) the processes governing energy transport in confined high-power arcs, (2) the kinetics of HE in the unique limit of temperatures of the same order as activation energies, and (3) the transition process from a static volume of overdriven reactive material to a propagating detonation. This combination of knowledge will yield a physical model that will provide previously nonexistent predictive capability for safety analysis and future engineered applications. We expect publications in peer-reviewed journals and patent opportunities relating to the use of HE for mining operations.

Mission Relevance

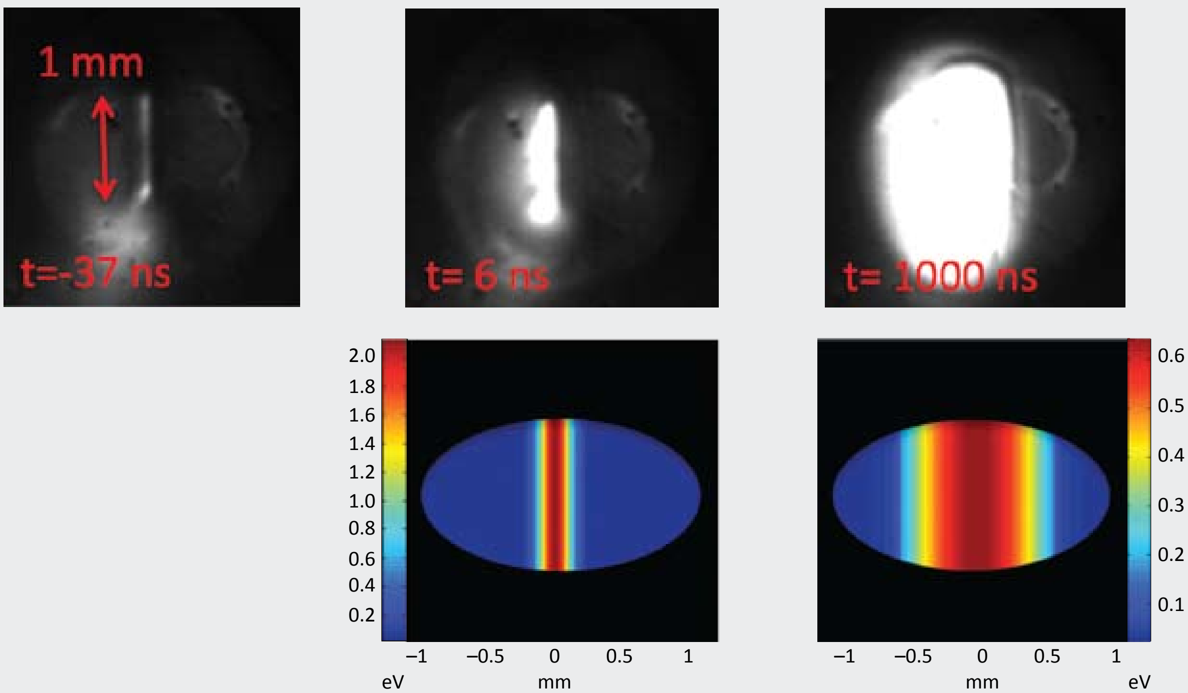
This work falls squarely in the weapons science theme of the Laboratory's institutional science and technology plan, by achieving better understanding of the safety of the existing stockpile and by improving basic HE science, which in turn enables improved safety and surety of the future designs that will ultimately be necessary for a more efficient weapon complex. In general, this work provides a strong head start for the Laboratory becoming an HE center of excellence as part of NNSA's "preferred alternative" complex transformation.

FY09 Accomplishments and Results

In FY09 we (1) completed an 8-MW explosive pulse generator that produces highly repeatable surface arcs along substrates with thin (~500-nm) films of inert or energetic materials; (2) quantitatively compared the Fourier transform infrared spectra of post-spark pentaerythritol tetranitrate explosive films with modeling, and showed ablation is a key energy-loss mechanism in lightly confined geometries; (3) determined that time-resolved emission spectra confirm peak temperatures in the electrovolt range, and showed a hot channel that persists much longer than the current pulse; and (4) worked to determine how time-resolved infrared spectra can be used to distinguish between several possible suppression mechanisms of product formation in chemical kinetics at these elevated temperatures.

Proposed Work for FY10

In FY10 we anticipate (1) performing an additional short time-resolved infrared campaign to fill in any gaps identified in FY09 results; (2) developing a validated high-temperature, fast-time-scale high-explosives kinetics model based on the data acquired in FY09; and (3) designing and performing an experiment to resolve the energy-transport mechanism between the arc and high explosives, most likely employing the microcalorimetric diagnostic originally proposed.



Gated images of a surface arc across an inert substrate, including early streamer formation, at times relative to the main current rise (top). One-dimensional simulation of the channel hydrodynamics (bottom).

An Atomic Inner-Shell X-Ray Laser Pumped by the Linac Coherent Light Source—Nina Rohringer (09-LW-044)

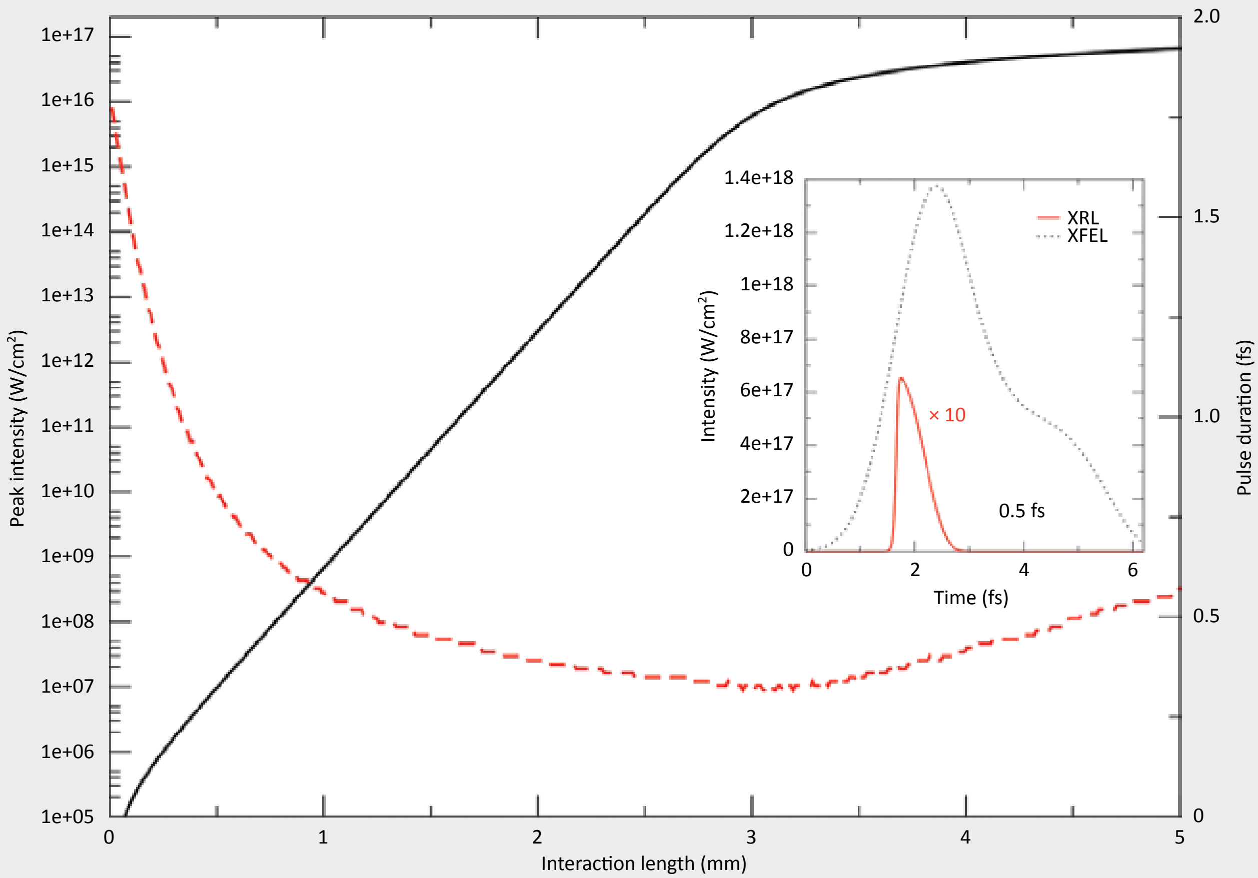
Abstract

We propose to develop a discretely tunable, greater than 100-fs x-ray laser with nanometer wavelengths and peak intensities reaching 1×10^{18} W/cm^2 by using the Linac Coherent Light Source (LCLS) at Stanford to pump an atomic inner-shell x-ray laser. In contrast to other proposals to slice LCLS pulses, our inexpensive method can be directly implemented on the LCLS's atomic, molecular, and optical science instrument. Methods such as x-ray photoelectron spectroscopy and x-ray diffraction would benefit from a time resolution of only a few femtoseconds. The new source would enable the study of nonlinear quantum optical effects in the x-ray regime for the first time, opening avenues to new basic science. We will first assess the optimal pumping regime by numerically simulating the time-dependent gain, then field a proof-of-principle experiment—lasing the 2p-to-1s transition in hydrogen-like neon.

We intend to achieve our target pulse duration, wavelength, and intensity by using heavier-gain materials and tuning the LCLS photon energy accordingly. These high-intensity, ultrashort pulses would improve the longitudinal coherence properties of the LCLS. Increased time resolution would enable pump-probe studies of chemical reactions of an ensemble of molecules or phase transitions in solids, while the longer coherence time and more stable shot-to-shot spectrum will make possible, for the first time ever, the direct study of nonlinear quantum optical effects in the x-ray regime.

Mission Relevance

The proposed work supports LLNL's mission in breakthrough science and advanced technology by developing a beyond-the-state-of-the-art instrumental capability studying ultrafast,



Output intensity and pulse duration of an x-ray free electron laser–pumped inner-shell transition of singly ionized neon as a function of interaction length. The inset shows the temporal profile of the x-ray laser.

nonlinear physics and the physics of high-intensity x-ray–atom interactions.

FY09 Accomplishments and Results

In FY09 we (1) developed a time-dependent computational model of the x-ray laser output, including propagation and absorption of an x-ray free electron laser pump pulse and the build-up, propagation, and amplification of the atomic inner-shell x-ray radiation; (2) analyzed different pumping regimes; and (3) initiated design on the gas cell and tested components for radiation damage during commissioning experiments at the LCLS.

Proposed Work for FY10

Small-signal gain calculations indicate that it will be possible to saturate several lasing transitions of different ionic species, resulting in temporally separated femtosecond x-ray pulses of different wavelengths. Therefore, in FY10 we will (1) develop self-consistent gain calculations to study this multicolor regime; (2) extend the one-dimensional gain model to two dimensions by ray-tracing methods, thereby theoretically predicting the intensity profile of the x-ray laser; and (3) perform experiments at LCLS to demonstrate lasing in hydrogen-like neon. To this end, an x-ray spectrometer appropriate for use at the atomic, molecular, and optical science instrument at LCLS will be developed, as recommended by the LCLS review team, in contrast to our original plan of using an electron time-of-flight spectrometer.

Publications

Rohringer, N., 2009. “An atomic inner-shell laser pumped with an x-ray free-electron laser.” *J. Phys.: Conf. Ser.* **194**, 012012. LLNL-CONF-415032.

Rohringer, N., 2009. *Ultrashort non-linear interactions of x-rays with atoms.* DAMOP 2009, 40th Ann. Mtg. Division of Atomic, Molecular, and Optical Physics, Charlottesville, VA, May 19–23, 2009. LLNL-ABS-410509.

Rohringer, N., and R. London, 2009. “Atomic inner-shell x-ray laser pumped by an x-ray free-electron laser.” *Phys. Rev. A* **80**, 013809. LLNL-JRNL-410667.

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Varma, H. R., et al., 2009. “Above-threshold ionization in the x-ray regime.” *Phys. Rev. A* **80**, 053424. LLNL-JRNL-413508.

Direct Search for Decay of the Thorium-229 Nuclear Isomer—Jason Burke (09-LW-061)

Abstract

The main objective of our proposal is measurement of the thorium-229 isomer half-life to determine the transition linewidth. Providing that the isomeric transition is not strongly internally converted, we will attempt to observe the ultraviolet light emitted by the nucleus directly using a ultraviolet grating spectrometer. Observation of this transition would allow direct excitation of the nucleus for applications such as nuclear clocks, precision tests of fundamental constants, and potentially, quantum computer bits.

We intend to measure the half-life of the thorium-229 isomer and will attempt to directly measure the wavelength of light emitted in the decay. Knowledge of these properties is required to enable direct manipulation of the nuclear state. We expect that laser manipulation of the thorium-229 nucleus could lead to unprecedented studies of the interplay between atomic and nuclear systems, provide a new frequency standard, be used as a quantum bit for quantum computing with extremely long decoherence times, and improve the search for time variation of fundamental physical constants by as many as six orders of magnitude.

Mission Relevance

Our research described here supports the Laboratory’s commitment to discovery-class science. Potential applications include the areas of photon science, high-performance computing, and global security. The low-lying nuclear level in thorium-229 has attracted the attention of scientists all over the world and has been the subject of much experimental and theoretical interest. A successful determination of the half-life, and therefore natural linewidth, of the thorium-229 isomer would position Livermore as an eminent facility for the pursuit of fundamental issues in nuclear physics.

FY09 Accomplishments and Results

In FY09 we (1) designed, constructed, and began using the vacuum system, detectors, and the catcher plate and shuttle system; (2) used uranium-233 and plutonium-239 thin sources to produce thin samples of the isotopes on catcher plates; (3) achieved the highest initial counting rates of any conversion electron experiment in the literature that was optimized for uranium-235m decay conversion electrons; and (4) performed several searches, covering the seconds-to-day half-life range, for the thorium-229m 7.6-eV isomer using both a multichannel plate detector, Einzel lens system, and several photomultiplier tubes covering different wavelength ranges.

Proposed Work for FY10

In FY10 we propose to observe and quantitatively characterize the half-life of thorium-229m. We will investigate the effects different materials have on the thorium-229 nucleus half-life. By varying the environment of valence electrons, we can potentially shut-off the internal conversion branch. This would enable us to observe the direct gamma decay of thorium-229m, the lowest known gamma ray, which would allow us to directly observe the gamma-ray decay and measure it using a ultraviolet spectrometer. Direct observation of the wavelength enables the use of lasers to directly excite the nuclear isomer.

Investigation of Short-Pulse Laser-Pumped Gamma-Ray Lasers—Ronnie Shepherd (09-LW-080)

Abstract

Since lasers were first developed, researchers have speculated about the possibility of lasing nuclear transitions. The promise of coherent, directional, and energetic photons would have applications in basic science, technology, medicine, and defense. The goal of this project is to create a gamma-ray laser pumped by one of two possible drive mechanisms—synchrotron radiation generated by short-pulse lasers, or hot electrons. We will determine the laser coupling efficiency to synchrotron radiation and hot electrons as a function of laser input energy. After determining the drive characteristics, we will choose from a list of possible inversion nuclei (both isomeric and non-isomeric) and attempt to measure gain.

If successful, this project will achieve the first-ever gamma-ray laser, which would have potential impact in both scientific and industrial applications. At the very least, we will produce an accurate study of the requirements for such a system to succeed.

Mission Relevance

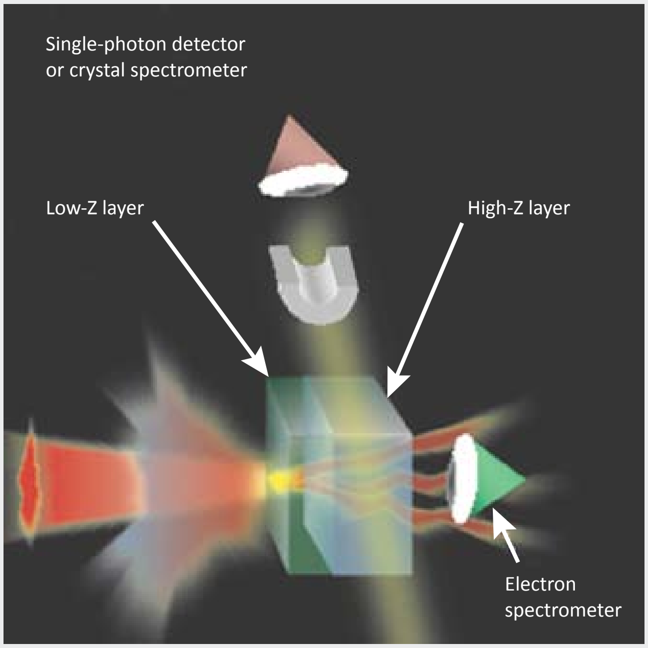
This technology could find eventual application to the national security mission by enabling the efficient delivery of large amounts of energy to a target. This project also supports LLNL's mission in breakthrough science and technology by pursuing new and unique applications of ultrashort-pulse laser technology, which if successful, will advance research in the areas of chemistry, materials science, and life sciences.

FY09 Accomplishments and Results

During our first year we have completed one of our two main goals: we selected electron-driven transition as the pump source. The hot-electron driver was chosen because of the time required to develop the synchrotron source and discovery of several reasonable nuclear candidates that could be pumped using hot electrons. Electron energy populations were studied at Livermore's Titan laser using several electron spectrometers. The data were reduced and the results suggest large populations of electrons with adequate energy to pump low-level (<200-keV) nuclear states. Additionally, we've established a collaboration with the University of Michigan to characterize the transmission grating spectrometer and ultrafast scintillator we've built for the project.

Proposed Work for FY10

For FY10 we will (1) generate the experimental targets, which are isotopes formed in a nuclear reactor; (2) perform a preliminary nuclear reaction test to study the efficiency of hot-electron coupling to the nuclear isotope; (3) perform gain-length studies on the isotopes to search for gamma-ray lasing; and (4) publish our results—we expect a publication on the detector, the physics of electron-pumping of nuclear excited states, and potentially on measured gain from nuclear excited states.



Proposed experimental setup for our gamma-ray laser experiment.

Systems engineer and LDRD investigator Richard Montesanti operates the precision robotic assembly machine. For more information about this *R&D Magazine* award-winning technology, see page 19.

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