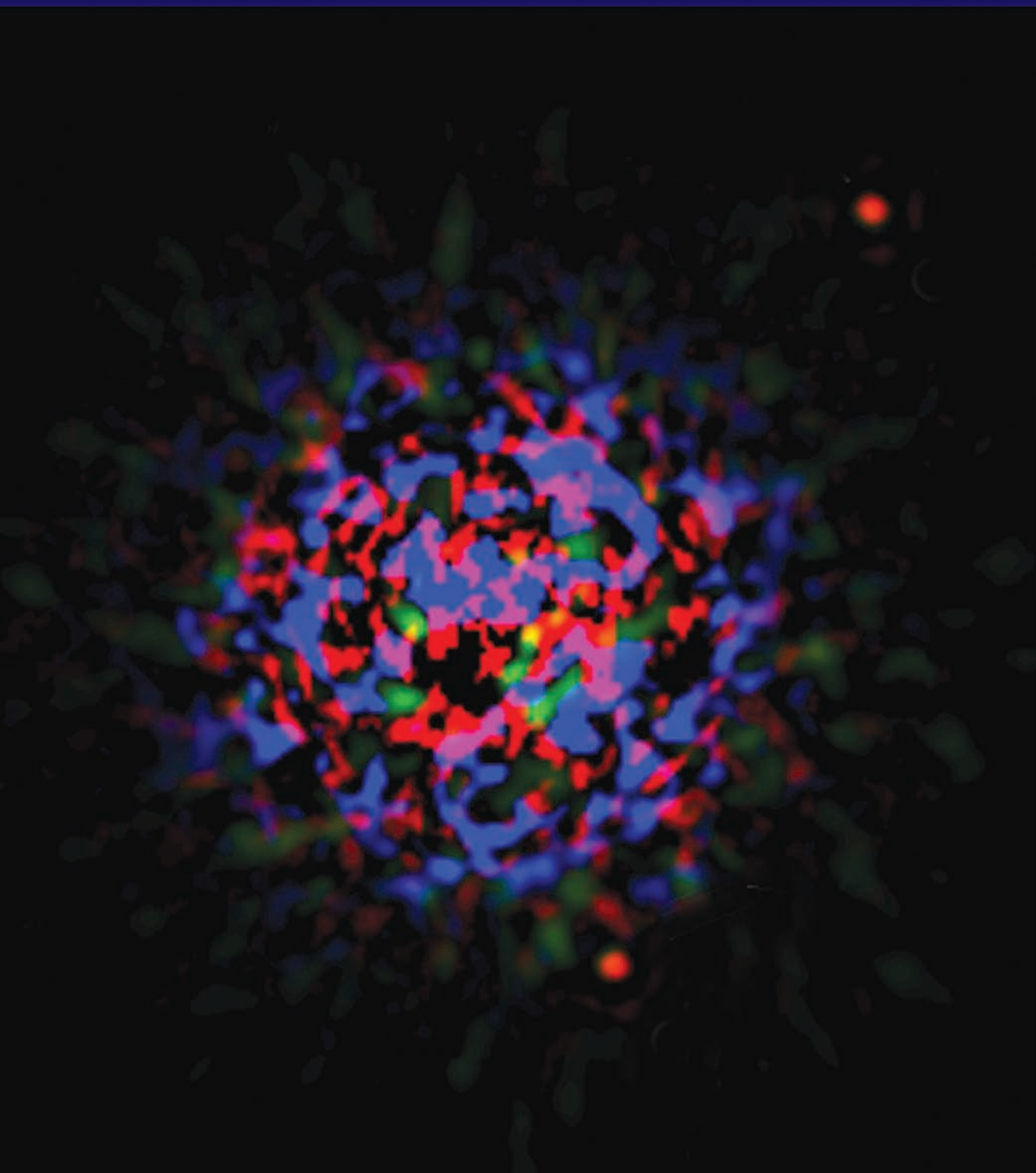# Laboratory Directed Research and Development

FY2008 Annual Report

Lawrence Livermore National Laboratory

About the Cover:

Using the Keck and Gemini land-based telescopes, astrophysicist Bruce Macintosh, along with colleagues from the NRC Herzberg Institute of Astrophysics in Canada, Lowell Observatory, and University of California at Los Angeles have discovered three new planets circling a star much like our own. This ground-breaking research was an outgrowth of Laboratory Directed Research and Development project 08-ERD-043, "Tracing the Shadows of Planetary Systems," which uses Livermore expertise in adaptive optics and image processing to observe the interplanetary dust that traces the formation and presence of planets and cometary belts in other solar systems. The team is comparing astronomical data with numerical scattering models and is developing an advanced adaptive optics controller that automatically identifies moving turbulent wind layers and pre-corrects for their motion in real time. *Science* magazine named Macintosh's research one of the top ten breakthroughs of 2008. The cover image shows the multiplanet solar system that orbits a dusty young star named HR8799 (the large multicolored sphere), which is about 140 light years away and about 1.5 times the size of our sun. Two of the three newly discovered planets are visible as small red spheres orbiting the star.

Disclaimer

Acknowledgments

The Laboratory Directed Research and Development Program extends its sincere appreciation to the principal investigators of fiscal year 2008 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.

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 that 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 $91.5 million for fiscal year 2008 sponsored 176 projects. These projects were selected through an extensive peer-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.

George Miller, Director

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 our ever-evolving national security mission.

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Laboratory Directed Research and Development

Overview

About the *FY2008 Laboratory Directed Research and Development Annual Report*

The Laboratory Directed Research and Development (LDRD) annual report for fiscal year 2008 (FY08) 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 FY08, and a list of publications that resulted from the research in FY08.

Summaries are organized in sections by research category (in alphabetical order). Within each research category, the projects are listed in order of their LDRD project category: Strategic Initiative (SI), Exploratory Research (ER), Laboratory-Wide Competition (LW), and Feasibility Study (FS). Within each project category, the individual project summaries appear in order of their project tracking code, a unique 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:

08-ERD-100

Fiscal year (FY08)

Project category

Serial number of this proposal in FY08
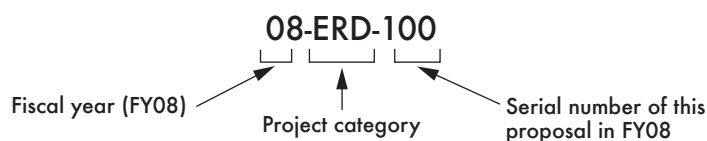
Program Overview—Innovation for Our Nation

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 to meet other important national security needs—homeland defense, counterterrorism, cybersecurity, and countering the spread of nuclear weapons, for example—that evolve in response to emerging threats. For broader national needs, the Laboratory executes programs in energy security and climate change, environmental assessment and management, 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 Department of Energy (DOE) Order 413.2B and other relevant DOE orders and guidelines.

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

Strategic Context for the LDRD Portfolio

The FY08 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 FY08, the top-level LDRD strategic planning process was guided by the *2006 U.S. Department of Energy Strategic Plan*[2] and by the Laboratory's long-range plan that will define the scientific and technical strategy for the coming decade. Further strategic context is given 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 FY08, 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.

The Laboratory's long-range strategic science and technology (S&T) plan continues to guide the LDRD portfolio planning process. Broadly inclusive, the Laboratory's S&T plan is intended to elicit the most far-reaching and innovative ideas for the future shape of science and technology at LLNL. The five thematic areas of the S&T plan are as follows:

- Weapons science.

- Threat prevention and response.

- Energy and environment.

- Photon science and applications.

- Enabling science and engineering.

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 a DOE 2007 report to

[2] *2006 U.S. Department of Energy Strategic Plan.* <http://www.energy.gov/about/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).

Congress: "The DOE LDRD program offers a flexible mechanism by which the multi-program national laboratories maintain their vitality and, in the process, prepare themselves to help address the Nation's future scientific and engineering challenges. . . .The flexibility inherent in the LDRD program is essential to maintaining the vitality of the laboratories that carry out the Department's missions and national needs."[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 the 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 focuses on innovative R&D activities that are likely to enable new directions for existing programs, help develop new programmatic areas within LLNL's mission responsibilities, or enhance the Laboratory's science and technology base. Projects in this category are usually larger and more technically challenging than projects funded in other categories. An SI project must be aligned with the strategic R&D priorities of at least one of the five thematic areas of LLNL's long-range strategic S&T plan.

Exploratory Research

The ER category is designed to help fulfill the strategic R&D needs of a Laboratory directorate (ERD) or institute (ERI). In this category, researchers submit proposals to their directorates and institutes, where the proposals are screened and subsequently forwarded to the ER selection committee for review. In FY08, LLNL's S&T plan continued to guide directorates in evaluating the ERD and ERI proposals.

Laboratory-Wide Competition

Projects in the LW category emphasize innovative research concepts and ideas and undergo limited management filtering. The LW competition is open to all LLNL staff in programmatic, scientific, engineering, and technical support areas. Researchers submit their project proposals directly to the review committee.

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.

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[4] *Department of Energy (DOE) FY 2007 Report to Congress—Laboratory Directed Research and Development at the DOE National Laboratories.* <http://www.cfo.doe.gov/CF1-2/Final%20FY%202007%20LDRD%20Report.pdf> (retrieved February 27, 2008).

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.

- Mathematics and Computing Sciences.

- Nuclear Science and Engineering.

- Physics.

The LDRD 2008 Portfolio—Innovation for Our Nation

Portfolio Overview

The FY08 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 selection process and received ongoing management oversight.

In FY08 the LDRD Program funded 176 projects with a total budget of $91.5 million. The distribution of funding among the LDRD project categories is shown in the pie chart on page 7.

Strategic Initiative

In FY08, the LDRD Program funded ten SI projects. Although the SI category represented only about 6% of the total number of LDRD projects for FY08, it accounted for 30% of the budget. SI projects ranged in funding from $1.5 to $7.1M.
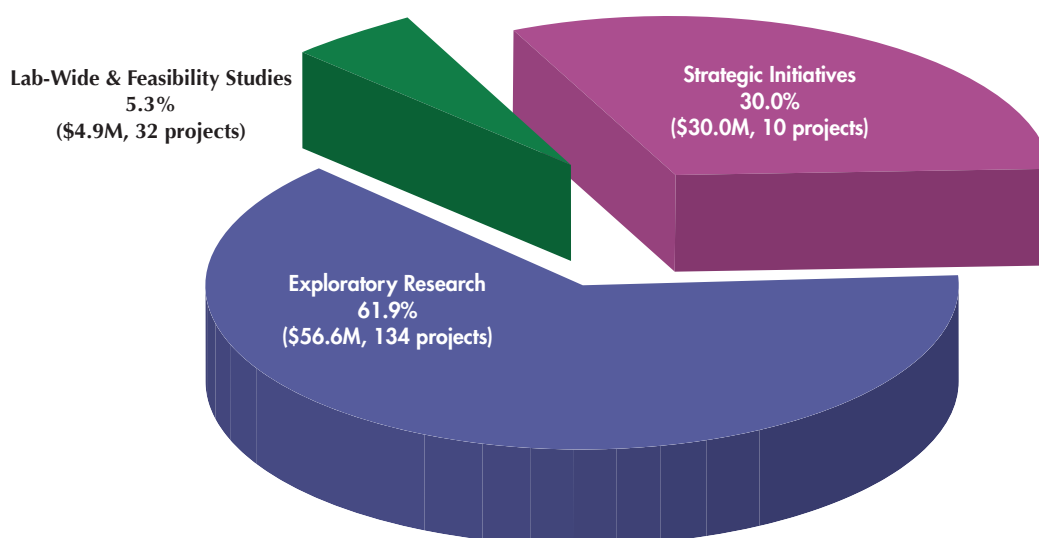
Distribution of funding among the LDRD project categories. Total funding for FY08 was $91.5M.

Exploratory Research

The LDRD Program funded 134 ER projects for FY08. The largest project category, ERs accounted for 76% of the number of LDRD projects and 62% of the budget for the fiscal year. Projects in this year's ER category ranged in budget from $25K to $2.1M.

Laboratory-Wide Competition

In FY08, 17 LW projects were funded, which represent about 10% of the LDRD projects for the year and 4% of the budget. LW projects are limited to $300K/year funding. The LW projects ranged in funding level from $175 to $233K.

Feasibility Study

The LDRD Program funded 15 FS projects in FY08, which represent about 8% of the LDRD projects for the year and less than 1% of the budget. FS projects are limited to $125K and a 12-month duration.

The top chart on page 8 shows the funding distribution by dollar amount for the 176 FY08 projects—66% of the projects were in the $101 to $500K range, with 10% falling below $100K. Projects in the $501K to $1M funding range accounted for 14% of the total, and another 9% of the projects received more than $1M. The average funding level for the 176 projects was $518K.

The percentage of LDRD funding and number of projects in each research category for FY08 is shown in the bottom chart on page 8.
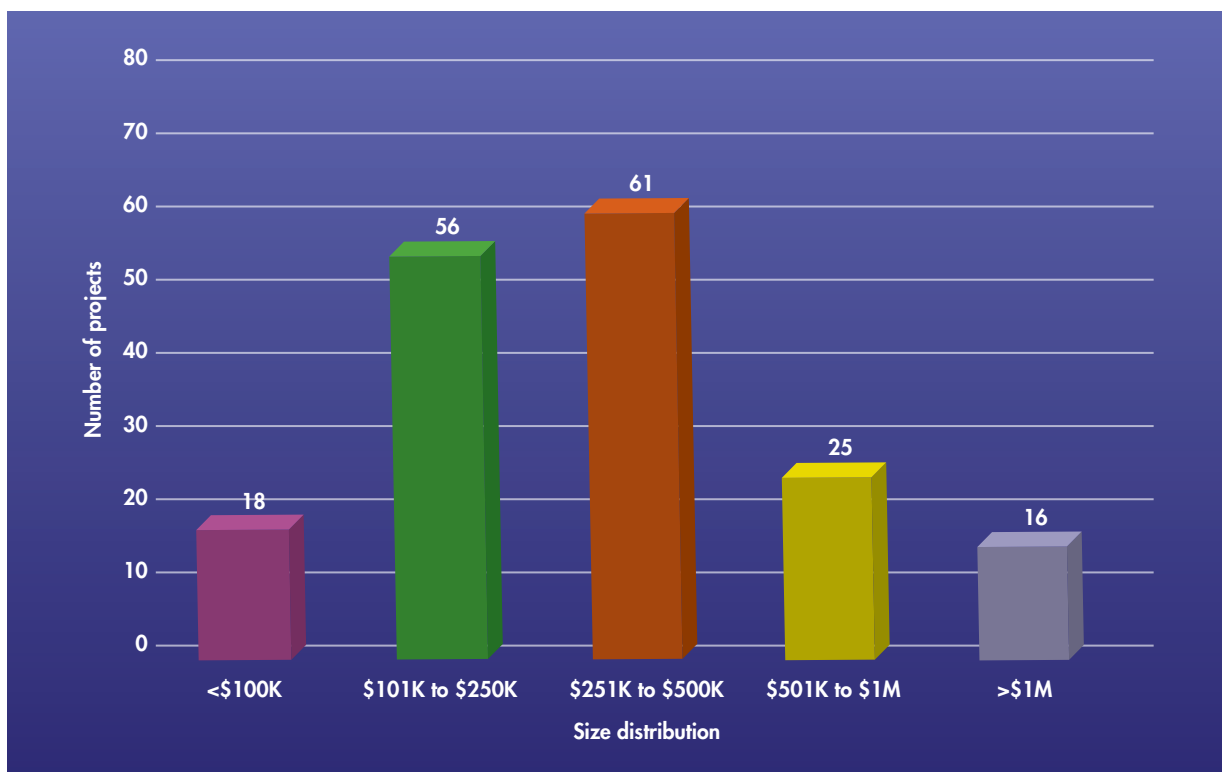
Number of projects and levels of funding. The average funding level for an LDRD project in FY08 was $518K.
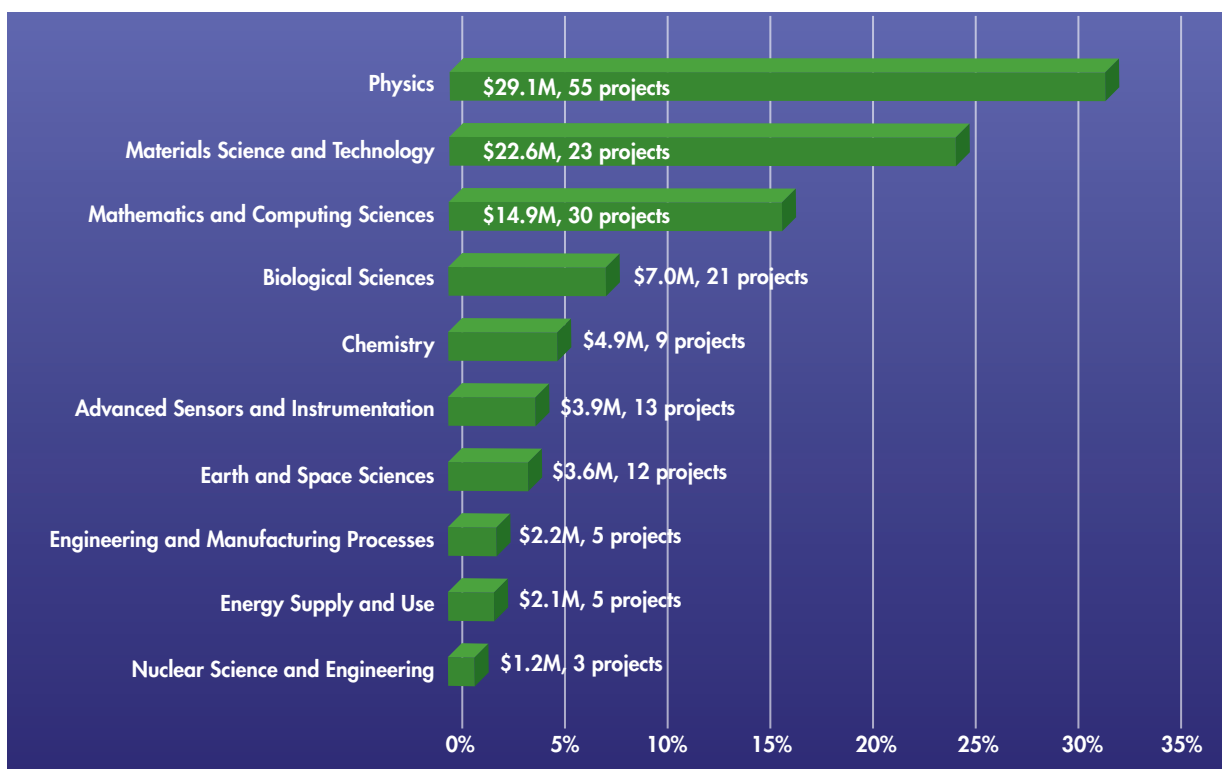
Percentage of LDRD funding and number of projects in each research category in FY08.

Highlights of 2008 LDRD Accomplishments

In FY08, 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 S&T Plan as well as for critical national needs.

WEAPONS SCIENCE

"Molecular Dynamics Simulations of Hot, Radiative Plasmas" (07-ERD-044)

Frank Graziani, Principal Investigator

Understanding the complex processes present in hot, dense radiative plasmas—mixtures of fast-moving gas and subatomic particles in nuclear decay—is vital to problems as varied as nuclear fusion energy and the physics of stars. The study of high-energy-density plasmas requires an understanding of matter at extreme conditions with pressures in excess of 1 megabar. This LDRD project targets hot, dense radiative plasmas incorporating intense levels of nuclear reactions. These plasmas have temperatures of a few hundred electronvolts to tens of kiloelectronvolts and densities of tens to hundreds of grams per cubic centimeters. The high temperature and density of these plasmas means there is a complex interplay of atomic, radiative, and thermonuclear processes that needs to be accurately described.

Developing an understanding of hot, dense radiative plasmas means understanding the physics of high-atomic-number ions in various states of ionization, with light ions undergoing thermonuclear reactions, electrons in various degrees of degeneracy, nonthermal charged particles depositing energy and momentum, and radiation fields undergoing scattering, absorption, and emission. The processes interact with each other in highly nonlinear ways. Therefore, uncertainties in the physics can lead to exponential amplification of a modeling error in a code simulation. Because of the complexity of the plasma state and the desire to make large multiphysics simulations manageable, computational physicists at DOE laboratories have been forced to make a number of simplifying assumptions in modeling these plasmas in the Advanced Scientific Computing radiation-hydrodynamic codes. Because of the lack of relevant experimental data, code models are based on theoretical treatments of energy exchange, ion stopping, and radiation that assume an ideal plasma. The theories often ignore strong scattering, bound states, dielectric properties of the plasma, and radiation, or treat it in an oversimplified fashion.

LDRD researchers have devised a computational ability to model the interactions of number of bodies in a many-component plasma, including both bremsstrahlung (the sudden retardation of a charged particle in an intense electric field) and inverse bremsstrahlung processes. The code is built upon a successful massively parallel computer platform that has been used for simulations of material phase transitions
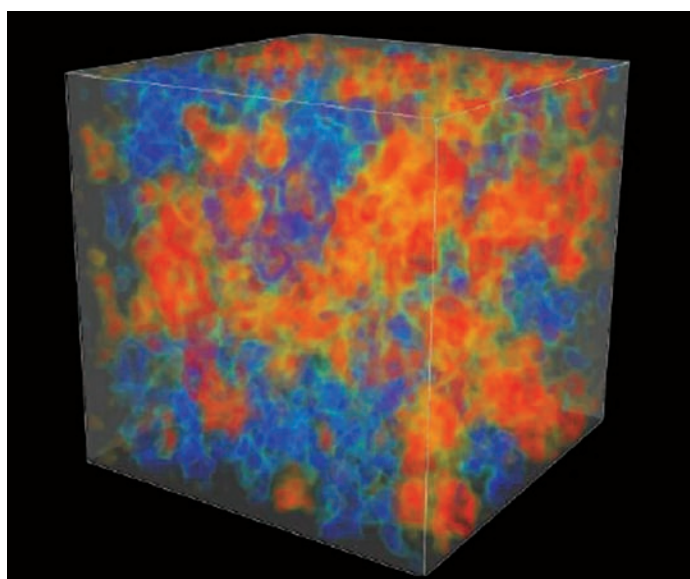
The potential energy and particle fluctuations are shown in a plasma simulation with a temperature of several kiloelectronvolts.

and formation of Kelvin–Helmholtz flow instabilities. The effort consisted of two parts. One focused on building a massively parallel solver to handle the charged-particle interactions. The other was to develop and implement algorithms for the treatment of radiation. The modeling of radiation must incorporate detailed balance in such a way that the radiation field relaxes to an equilibrium blackbody spectrum.

The initial applications of the plasma code were to the problem of electron-ion energy exchange (without radiation) in a plasma out of equilibrium. The LDRD team used the plasma molecular dynamics capability to predict the results of an upcoming electron-ion coupling experiment to be performed at Los Alamos National Laboratory. The results demonstrate that given adequate resolution, the experiment should be able to distinguish between various theoretical models. Including radiation in the molecular dynamics code has been the major focus of this project. The modeling code tags close collisions between electrons and ions, calculates the probability of a radiative event, and determines if that event is emission or absorption. To verify the results, the team examined radiation produced by a neutral hydrogen plasma held at 3 kiloelectrovolts—the molecular dynamics code relaxed to a blackbody spectrum.

Recent advances in a molecular dynamics code have enabled the LDRD researchers to run simulations of up to 125 million plasma particles on up to 131,072 tasks, using advanced computer platforms. The standard approach for simulating hot radiative plasmas on highly parallel computers examines contributions of radiation emitted from charged particles that are close to each other in the plasma (short-range) and those that are relatively far apart (long-range). The short-range charged pairs are "easy" to parallelize because communication between computer nodes modeling these pairs is local—that is, the nodes are physically close to each other. Long-range methods are hard to parallelize because of the amount of global computer communication involved. The team devised a solution that divides tasks unevenly, exploits computer concurrency, and avoids global communication.

The LDRD team is currently engaged in understanding energy exchange processes in nonequilibrium plasmas that consist of binary ionic mixtures. The team has added atomic physics processes so they can model partially ionized, high-atomic-number additives in the hydrogen plasma. The validated, state-of-the-art simulation capability for hot radiative plasmas that this project is developing extends LLNL's world leadership in high-energy-density physics to include not only experiments but also computational modeling. It establishes LLNL as the world center for high-energy-density physics. In addition, project results directly address the issue of predictive capability, which is at the core of the Stockpile Stewardship Program that ensures reliability of the country's nuclear arsenal.

PHOTON SCIENCE AND APPLICATIONS

"Serrated Light Illumination for Deflection-Encoded Recording (SLIDER)" (07-ERD-017)

John Heebner, Principal Investigator

High-speed photography was born in a 19th-century demonstration to the Royal Society in London, when photographer and inventor Henry F. Talbot set a newspaper page on a drum turning at high speed. Illuminating the page briefly with a spark, Talbot photographed a small area of the fast-moving print. On development of the negative, the print could be read clearly, the motion of the subject having been effectively frozen. Since then, researchers have successfully applied the technique to visualization and analysis of a variety of real-world events that take place too fast for the eye to see, from projectiles in flight to ballistic impacts. This LDRD project team is demonstrating an optical-based streak camera, which measures the variation in a pulse of light's intensity with time. These traditionally electron-based recording

instruments are a staple of experimental facilities to allow accurate measurements of high-speed, short-lived events from images.

Single-shot recording instrumentation is critical to performing experiments in high-energy-density physics, the study of the physics of matter and radiation under extreme conditions of temperature and pressure. Unfortunately, traditional instruments have undergone only minor incremental improvements in dynamic range and bandwidth in recent years. This instrumentation is largely based upon oscilloscopes and conventional, electron-based streak cameras. Because these technologies rely on electrons, they are fundamentally limited to trading off dynamic range for temporal resolution and do not scale well into the regime of one trillionth of a second (picosecond). Ultrafast methods attack the problem indirectly through spectral methods but are spectrally limited and thus more optimally suited for resolutions on the scale of quadrillionths of a second (femtoseconds) with very short record lengths.

With this LDRD project, researchers have demonstrated a novel method for high-fidelity recording in excess of 8 bits in the picosecond regime, which currently does not have any strong technology base. The technique leverages a wide body of research in ultrafast all-optical phenomena in semiconductors and mates it with well-established high-dynamic-range camera technology. It is expected that this capability will find wide applicability in supporting a variety of Laboratory missions with particular emphasis on upcoming defense, nuclear technology, and advanced laser experiments aimed at high dynamic-range characterization of nuclear fusion burn histories and ultrafast optical pulse contrast for the Advanced Radiographic Capability laser.

The novel serrated light illumination for deflection-encoded recording (SLIDER) concept is based on the lateral deflection of a signal-carrying optical beam propagating in the plane of a slab waveguide. The deflection is controlled by a well-timed activation of a sequential array of virtual prisms, which are invisible to the signal beam until an intense pump pulse is applied perpendicular to the slab geometry through a
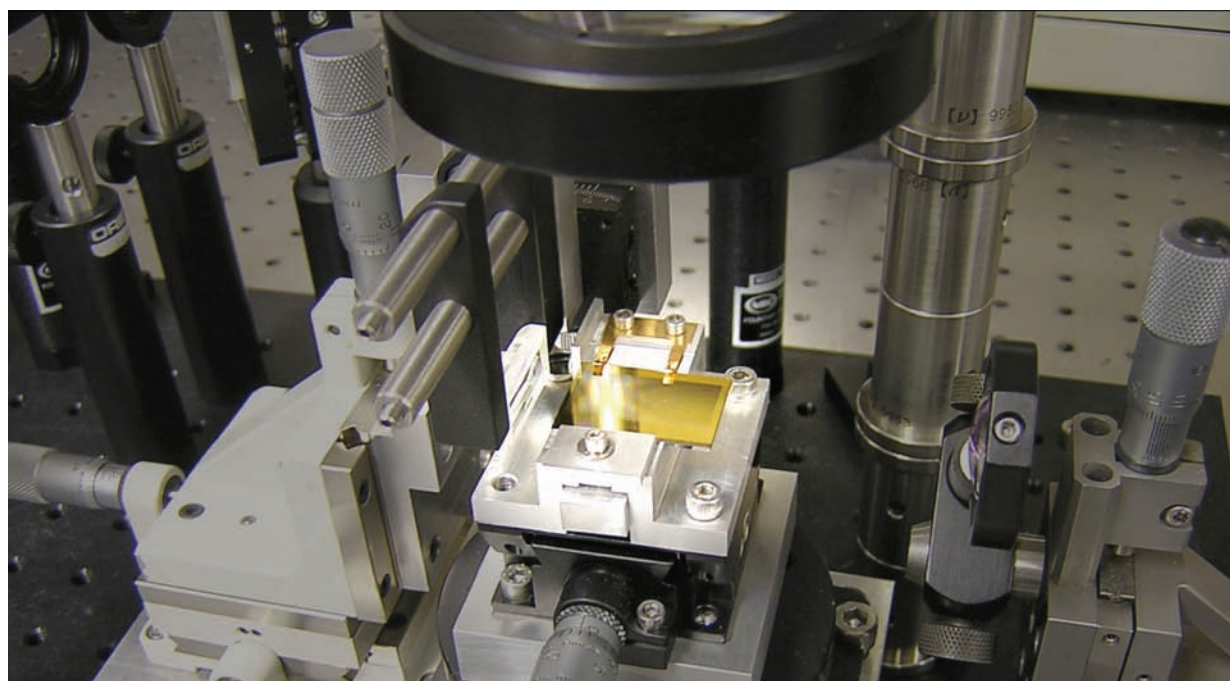
Ultrafast recording testbed constructed to validate the SLIDER concept with the waveguide-based deflector shown in the center.

serrated mask. The patterned illumination generates electron-hole pairs modifying the refractive index on a sub-picosecond timescale. The prisms are responsible for sweeping the beam angularly as a function of the time-of-flight (delay) across the device length. The angularly encoded output beam may then be mapped onto a camera through the use of lenses. The camera need not possess a fast response because each pixel is presented with a gated (deflection-sampled) time slice. This allows use of a high-dynamic-range camera for subsequent recording.

Single-shot measurement on a fast scale is crucial to experiments that support stockpile stewardship and high-energy-density physics by improving our ability to understand weapons physics and materials under extreme conditions of temperature, pressure, and strain rate. Fundamental questions in weapons design and high-energy-density 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.

In 2008, researchers conducted a detailed characterization of SLIDER performance by validating a detailed model with experimental data and using it to optimize design parameters. A resolution of 2.5 picoseconds and dynamic range of 3000:1 have already been achieved, and there is promise for pushing these performance parameters still further. In addition, the LDRD team has established a design concept for an integrated transient x-ray recording system mating SLIDER with an x-ray–optical encoder for use in experimentation at Livermore's National Ignition Facility.

"Active Detection and Imaging of Nuclear Materials with High-Brightness Gamma Rays" (06-SI-002)

Chris Barty, Principal Investigator

This LDRD Strategic Initiative leverages LLNL's world-leading capabilities in laser science, x-ray source development, and nuclear science to address the challenge of detecting concealed, highly enriched uranium, a countermeasure against nuclear proliferation and nuclear terrorism. The team is developing a novel tunable, ultrahigh-brightness, gamma-ray capability to enable a promising new class of active nuclear interrogation. Specifically, they have demonstrated the ability to generate a directed, tunable energy, monoenergetic gamma-ray beam. When the energy is tuned to the nuclear resonance fluorescence of uranium-235, it may provide an effective means of detecting concealed highly enriched uranium. The capabilities developed as part of this proposal also impact a wide range of applications important to nuclear stockpile science and technology, high-energy-density science and technology, and biological, chemical, and materials science and technology.

The research will lay the groundwork for an entirely new field of scientific pursuit, nuclear photoscience, in which one exploits and investigates the interaction of megaelectronvolt photons of unprecedented brightness with the nucleus. The isotopic selectivity of the proposed detection scheme is accomplished by monitoring high-energy gamma-ray excitation of nuclear resonance fluorescence in target nuclei. The possibility of using an isotope's unique nuclear resonance fluorescence fingerprint to actively detect small quantities of highly enriched uranium has been recognized as having tremendous potential for application to the problem of interrogating cargo containers, for example. The implementation of this technology depends critically on the quality of the gamma-ray illumination source. The broadband, continuum output of conventional machines using braking radiation is ill-matched to the narrow excitation width typical of nuclear resonance fluorescence transitions. In contrast, gamma-rays generated by decreasing-energy scattering of laser photons off a bright, relativistic, electron beam are quasi-monochromatic, tunable, highly collimated, and have been shown to scale in spectral brightness as the square of the gamma-ray energy.

A head-on view of the photon beam generated by the relatively compact Thomson-radiated extreme x-ray (T-REX) source at 478 kiloelectronvolts (top right). Spectral plot to the left shows the energy distribution for four different electron-beam energies, demonstrating proof of principle for the T-REX concept.
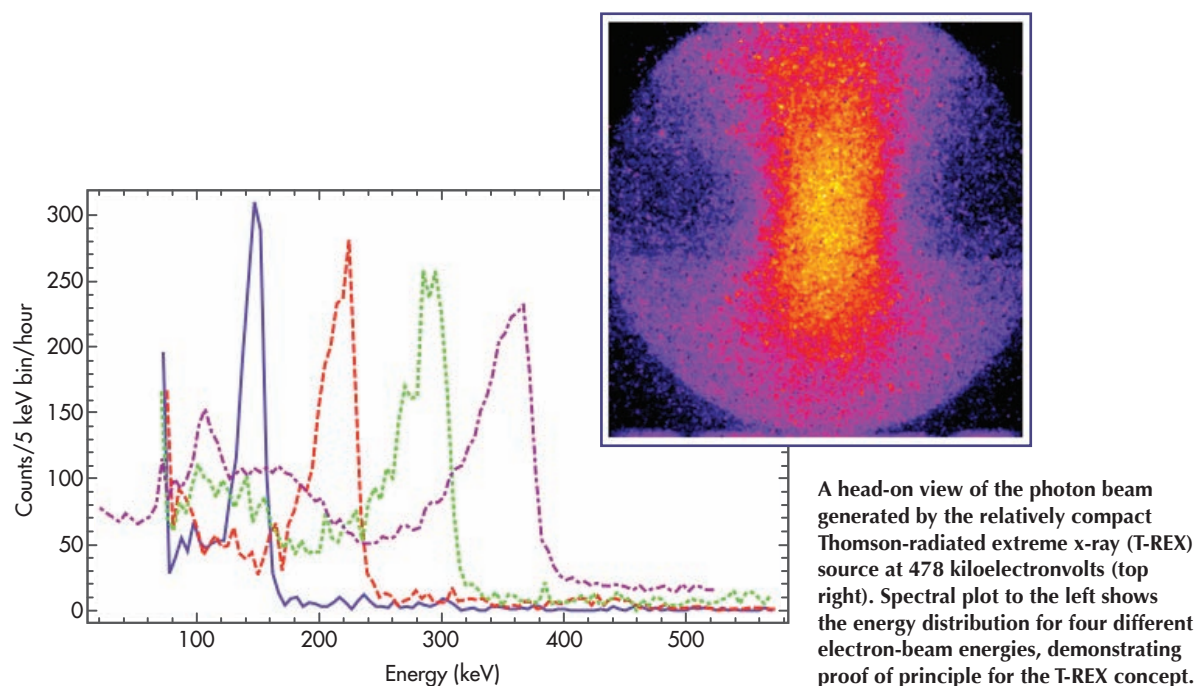
Using LLNL technology and expertise, the team is creating a relatively compact Thomson-radiated extreme x-ray (T-REX) source that would produce tunable pulses of narrow-bandwidth megaelectronvolt photons with a peak brightness more than 15 orders of magnitude beyond that currently available from the world's best synchrotrons. Studies indicate that nuclear resonance fluorescence–based detection systems using high-brightness gamma-ray sources of this type would be capable of rapidly finding illicit nuclear materials in sea-going cargo containers with quantifiable and uniquely low false positive and false negative rates. Because T-REX gamma-ray sources produce beam-like outputs, it is possible to not only detect the presence of specific isotopes, but also to image their distribution. The team has dubbed this novel imaging and detection capability, fluorescence imaging in the nuclear domain with extreme radiation, or FINDER.

The potential of this technology to offer a markedly superior solution to the pressing national problem of detecting clandestine nuclear material, including enriched uranium, has been recognized by the U.S. Department of Homeland Security, and international interest in T-REX sources and their potential applications has grown dramatically. A joint U.S.–Japan workshop on nuclear photoscience identified possible fundamental nuclear science questions that could be investigated with ultrahigh-brightness, polarized gamma-rays. An agreement to cooperatively evaluate high-average-power versions of the T-REX photogun technology on the new, high-repetition, energy recovery linac at the Daresbury Laboratory in Great Britain has also been discussed.

This research has initiated collaborations with the Massachusetts Institute of Technology, Passport Systems, and Pacific Northwest National Laboratory to identify a strong nuclear resonance fluorescence transition in uranium-235 upon which a highly enriched uranium FINDER and T-REX detection system can be based. A collaboration with the University of California at Los Angeles resulted in a new state-of-the-art photoinjector design. In 2008, the T-REX system achieved first light and high-energy x rays and gamma rays were generated at 776 kiloelectronvolts and at approximately 500 kiloelectronvolts, which in this spectral regime is believed to be the highest peak-brightness photon source in the world. In addition, near-record emittance and charge electron bunches were also created. A new technique for detection and use

of T-REX–like sources was invented and a record of invention was filed. Modeling efforts identified four high-profile potential NNSA relevant applications of T-REX isotope imaging. The NNSA, SLAC National Accelerator Laboratory, and Department of Homeland Security will collaborate to create a compact mono-energetic gamma-ray capability in the 1- to 3-megaelectronvolt range for isotope imaging applications.

The LDRD team anticipates that the Department of Defense, as well as industry, will express interest in this work for nondestructive evaluation applications. With outside collaborators, the team will pursue the application of T-REX technology to next-generation light sources and of T-REX high-intensity megaelectronvolt photon beams to fundamental nuclear science measurements. This work will place LLNL firmly in a world-leading position with respect to gamma-ray source capability and the development of novel nuclear photoscience applications.

THREAT PREVENTION AND RESPONSE

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

Paul Hoeprich, Principal Investigator

The cell membrane, or phospholipid bilayer, is the interface between the cellular machinery inside the cell and the fluid outside. As such, a large variety of protein receptors and identification proteins, such as antigens, are present on the membrane's surface. Membrane-associated proteins and protein complexes account for 30% or more of the cellular proteins in all living things, and are involved in an array of cellular processes required for organisms to survive, including energy production, communication between cells, and drug interactions. Membrane proteins are the mediators for what passes through every cell in the human body. Virtually all extra-cellular assaults, including infection by biological disease agents, are mediated through cell surface membrane proteins. With this project, LDRD researchers are investigating methods to produce and characterize membrane-associated proteins relevant to biodefense, human health and bioenergy research, and environmental biology.

Membrane proteins are challenging to study because of their insolubility and tendency to bunch together in a mass when removed from their protein lipid bilayer environment. A change in environment will alter the structure of a membrane protein to such an extent that it becomes nonfunctioning. To date, no general method exists for producing or isolating membrane proteins. Thus, very few membrane protein structures have been determined, and characterizing their functions and interactions is difficult. Of the more than 45,000 protein structures known today, less than 1% are membrane proteins. To capture these proteins, LDRD researchers are constructing atomic-scale biochemical assemblies in the laboratory that contain both proteins and lipids—nanolipoprotein (NLP) particles—and using them as substitutes for cell membranes. NLPs mimic the membrane protein's natural cellular environment. Because they are smaller and more stable in aqueous environments than the hydrophobic cell membranes, they offer an excellent platform for studying the structure and function of membrane proteins. The research team is developing robust NLP particle preparation and characterization methods as a platform for characterizing functional membrane proteins and is devising a technology that will routinely enable study of cell membrane proteins.

Because NLPs are similar to the lipoprotein particles that move through the bloodstream, NLP particles may serve as carriers of immunogenic proteins as potential vaccine-based countermeasures to disease. They may also serve as vehicles for delivery of therapeutic agents, as well as provide the opportunity to better understand the science of pathogenicity. NLP particles will enable capture of cell surface protein features associated with known biothreat organisms and potentially could aid in detection of emerging biothreats.

The LDRD team has organized the problem of membrane protein production into five well-defined pieces: target selection, in vitro translation, nanodisc assembly, affinity tag production, and characterization. Specific tasks include producing membrane proteins by cell-free methods and capturing these proteins in nanoscale membrane-type structures, or NLP particles. Researchers then optimize NLP production by creating semi-synthetic lipoprotein molecules and characterizing their constructs. Development of these capabilities are being demonstrated on a set of target proteins of relevance to the nation's Chemical and Biological National Security Program and to DOE's Genomics:GTL program.

Using high-resolution techniques such as atomic force microscopy, ion mobility spectroscopy, and electron microscopy, the team has imaged thousands of the NLPs they assembled in the laboratory. They found that stable NLPs exist in four sizes—at 14.5, 19, 23.5, and 28 nanometers in diameter. This surprising observation—that the size of NLPs could be "quantized"—may mean that these objects could follow rules more closely associated with physics and physical chemistry. The different imaging methods gave remarkably similar results about structure, which provided a starting point for simulations run on Laboratory supercomputers to model the structure of NLPs at the atomic scale and examine protein behavior in detail.
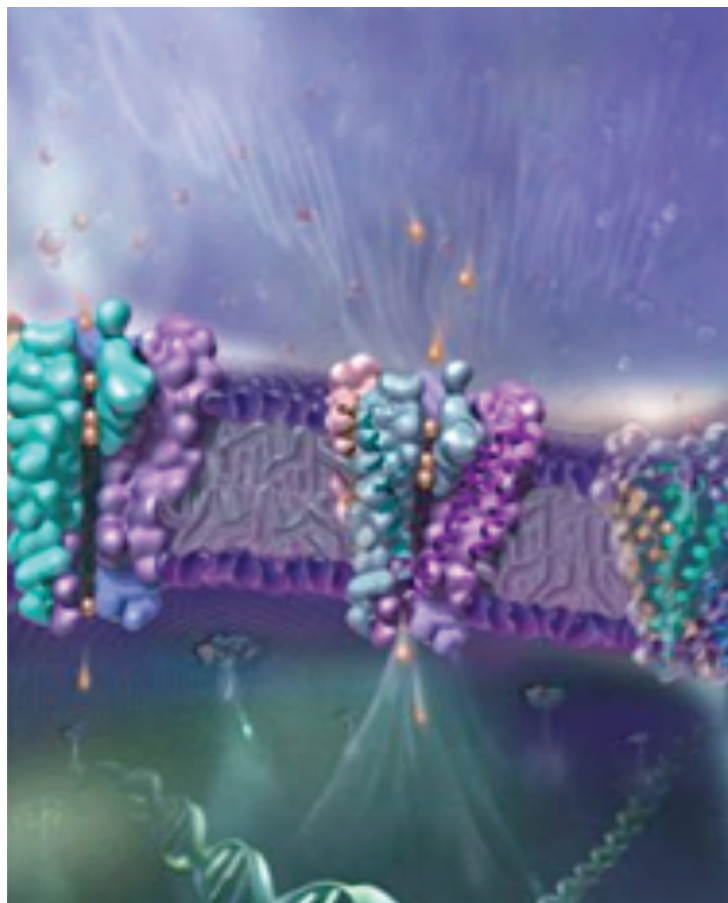
Artist conception of a section of a cell membrane wall and inner protoplasm. Functional proteins of the membrane are shown as globular clusters, with branch-like nanolipid constructs located between them.

The team has recently successfully constructed cell-free preparations of NLPs with various membrane proteins, including those from guanine nucleotide-binding proteins: *Yersinia pestis*, which is responsible for the bubonic plague, and functional hydrogenase from *Pyrococcus furiosus*, the fast-growing single-cell organism originally isolated from geothermally heated marine sediments. They also synthesized a helical portion of a semisynthetic protein that binds to lipids and prepared NLPs containing nickel-chelated lipids, conjugated a tagged envelope protein from the West Nile virus, and immunized mice with the construct. The result was a significant protection against a live viral infection. Finally, the researchers created a new NLP structure for a vaccine containing monophosphorylated lipid A, a known potent vaccine enhancer to improve immune response. Future efforts will center on cell-free protein synthesis for preparing NLP constructs of various target membrane proteins that are responsible for moving disease organisms across healthy cell membranes. In addition, the team will develop NLP-based vaccine countermeasures to pathogen and biological threats.

At the completion of this LDRD project, general technological approaches that contribute to understanding how biological membranes mediate the myriad of chemical reactions and events associated with cellular function will be available. The DOE's Genomics:GTL program, for example, seeks to develop a detailed understanding of the molecular machinery present in environmentally relevant microbes, decipher how they network within the cell, and determine how this leads to the production of functional communities of microorganisms. This knowledge will support DOE initiatives in microbial energy production,

environmental remediation, and carbon sequestration. A better understanding of membrane proteins will help scientists evaluate cellular response to chemical and biological warfare agents. In a similar vein, functional protein complexes could also act as field sensors to detect biotransformation of contaminants in underground water reservoirs. For healthcare, this technology may enable the design of new drugs for combating disease. The investigators envision future partnerships and collaborations with academic institutions and industry as well as the DOE, the Department of Homeland Security, and the National Institutes of Health in furthering the potential of producing proteins and membrane-associated complexes and synthesizing unique molecular affinity tags for each.

ENERGY AND CLIMATE

"Fossil-Fuel Emission Verification Capability" (07-ERD-064)

Tom Guilderson, Principal Investigator

Scientists have determined that the world is heating up even faster than predicted only a few years ago, and that the consequences will be catastrophic if emissions of carbon dioxide (CO_2) and other greenhouse gases that are trapping heat in our atmosphere are not reduced. 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 the Laboratory strongly qualified to supply independent verification of CO_2 emissions from fossil fuels.
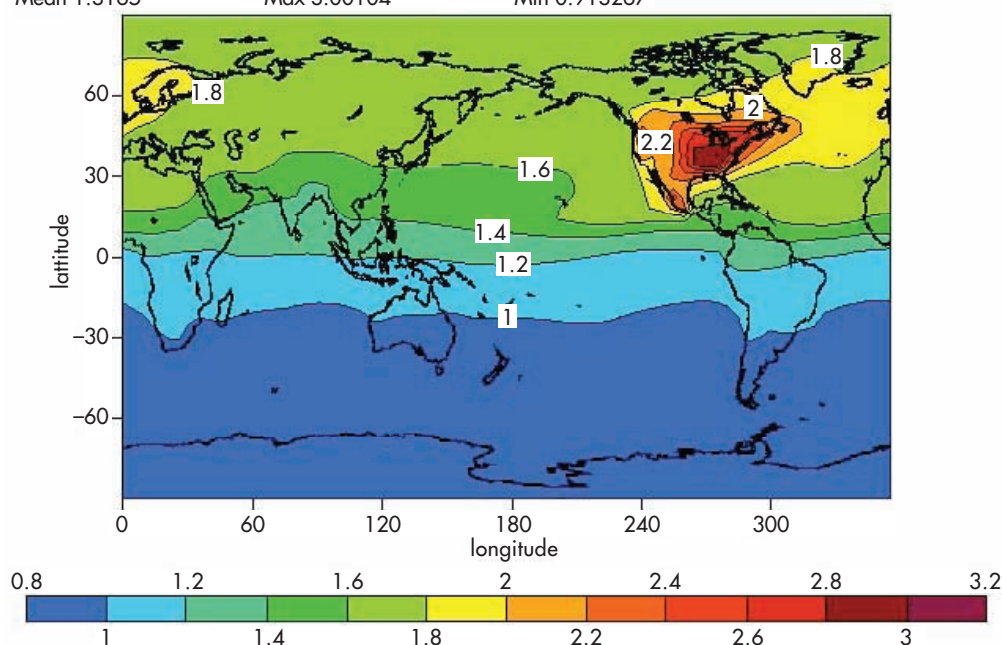
Atmospheric Tracer Transport Model Intercomparison results showing the fossil fuel signature for North America in 1995 relative to the global mean atmospheric carbon dioxide concentration integrated into the atmospheric column.

California's landmark bill AB 32 establishes a first-in-the-world comprehensive program of regulatory and market mechanisms to achieve real, quantifiable, cost-effective reductions of greenhouse gases. Using market-based incentives, California proposes to reduce carbon emissions to 1990 levels by the year 2020, a 25% reduction. And by 2050, emissions will be reduced emissions to 80% below 1990 levels. With the passage of AB 32 and the required verification of CO_2 emissions and mitigation strategies, federal agencies are looking at California as a model for a national program that will be forthcoming under legislation being considered in Washington.

This LDRD project will provide the basis for a measurement program that will be intimately coupled with advanced atmospheric transport and inversion computer models to provide a transparent and independent capability for verification of fossil-fuel CO_2 emissions in California. Researchers will establish the fossil-fuel emission variability for a metropolitan region in California and create a computer simulation–based framework for locating and tracking fossil-fuel emissions for California and document the needs for an independent emissions estimate using conventional CO_2 concentrations and carbon isotopes. Completion of these tasks will provide the basis for a fossil-fuel emission verification program for California and establish Lawrence Livermore as a key resource for implementing national carbon emission verification programs. In addition, these results will have similar analogies with other inert trace greenhouse gases.

Issues to be addressed include solving the inversion problem, where the values of model parameters must be obtained from the observed data—in this case, numerically estimating the emission magnitude and distribution of chemical species given measurements of chemical concentrations. Initial tasks included adaptation of an event reconstruction algorithm to applications involving multiple distributed sources and performing an intercomparison of the algorithms using synthetic data for 11 California air basins. The team has assessed global sources of CO_2 and stratospheric carbon-14 using global and regional air-quality forecasting models and initiated continuous CO_2 measurements at a Sacramento sampling tower and coordinated Los Angeles sampling with the California Air Resources Board.

The team has redesigned the air sample handling system to allow for better overall quality of the measurements and has met with managers of the California Air Resources Board to discuss the scientific basis of implementation of the verification needs of the board required under AB 32. The Weather Research and Forecast model coupled with chemistry code (WRF-Chem), available meteorological data, and an estimate of fossil-fuel carbon dioxide emissions derived from California Air Resources Board carbon monoxide emissions measurements have been utilized to explore a hypothetical sampling network design. The defining meteorological data from one week in January 2006 provided the horizontal air movement component for the simulation. The inversion solution is close to the input emission field with 10 to 12 idealized sensor locations and an approximately 3-hour sampling frequency. Federal Aviation Administration hazard designations (transmitters and towers) were considered as a potential network of measurement stations, but did not perform as well as idealized locations. A pilot observation program was therefore initiated at Walnut Grove in California's Central Valley in collaboration with Lawrence Berkeley National Laboratory and the National Oceanic and Atmospheric Administration, Earth System Research Laboratory. Discrete flask samples and subsequent analyses indicated about 8 to 30 parts per million of CO_2 above background levels in these air samples was derived from fossil-fuel use.

Additional efforts will center on further inversion methodology under different emission scenarios and weather patterns. In particular, although state-of-the-art atmospheric models can now be run with a resolution of several kilometers with reasonable fidelity, the nonlinear interactions of some atmospheric chemicals, the chaotic nature of the atmospheric equations, and sub-gridscale errors will require robust scientific advances in the inversion scheme. Researchers will compare ensemble-averaged emissions estimates versus a more limited real-time capability.

ENABLING SCIENCE AND TECHNOLOGY

"Nanomaterials for Fusion Application Targets" (08-SI-004)

Alex Hamza, Principal Investigator

Less than 20 years ago, nanomaterials—substances on the scale of one-billionth of a meter—were a curiosity. Today, their diverse technological applications seem to be endless. Materials reduced to the nanoscale show very different physical, chemical, and mechanical properties compared to those they exhibit on a macroscale. For example, nanoparticles have electronic structures that lie between that of bulk materials and atomic or molecular structures. Nanomaterials have real potential for impact in applications such as alternative energy conversion and energy harvesting. The development of new nanomaterials will also lead to new mass-produced consumer products in cosmetics, cars, building components, clothes, health, and new smart electronic devices. Novel assembly and manipulation of nanostructured materials in confined geometries with tailored composition and function will have applications in catalysis, sensing, hydrogen storage, advanced nuclear materials, corrosion-resistant coatings, and photonics.

The design of new nanomaterials with novel properties and functionalities requires atomic-level control of the material's structure. The fabrication of functional nanomaterials can be achieved by conventional top-down methods such as lithography or bottom-up approaches such as self-assembly. The latter approach can be very cost-effective for the fabrication of macroscopic three-dimensional nanostructures. However, self-assembly is scientifically very challenging because it requires detailed understanding of materials interactions at the atomic level. The goal of this LDRD project is twofold. The research team is advancing the scientific field of functional nanomaterials by combining the best of directed self-assembly with automated lithography and assembly to develop nanomaterials for fusion-energy applications for advanced laser systems. Second, they are applying this scientific knowledge to fabricate complex laser-fusion target structures by high-throughput techniques such as automated assembly and templating. Success will lay the scientific foundation for efficient production of laser fusion targets with unprecedented complexity.

A successful experiment at fusion-class laser facilities such as the National Ignition Facility creates a unique laboratory environment previously only available in a nuclear test. First among the unique characteristics is an inertially confined burning hydrogen plasma. Second is the bright neutron source that such a plasma
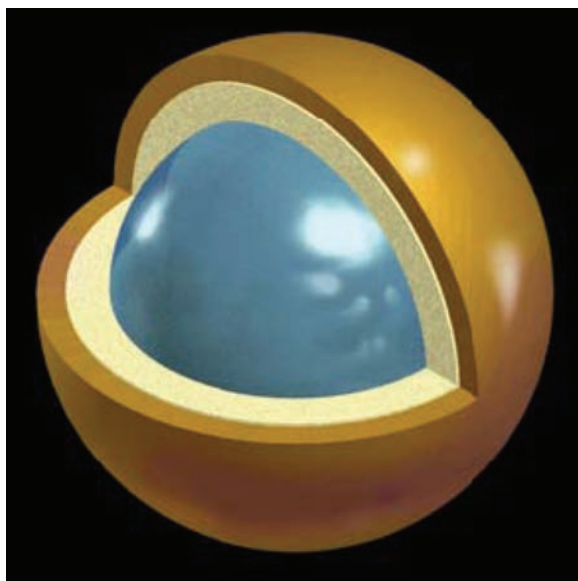
A conceptual high-energy-density physics target about 2 millimeters in diameter for use at Livermore's National Ignition Facility. Deuterium gas is encapsulated in high-atomic-number doped foam and deuterium ice and encased in an outer beryllium–copper shell.

will create. The challenge is to create laser targets that take advantage of this environment. To carry out experiments in this environment, researchers must place nanostructured materials with controlled composition and precise geometry in cubic millimeter spaces inside an inertial-confinement fusion capsule. Inertial fusion ignition will enable important laboratory and national missions, as well as new science. A series of such experiments is proposed for the National Ignition Facility, and NNSA's top scientific priority is significant advancement in the understanding of boost physics within the next five years. Thus, among the first proposed experiments is a suite of boost physics experiments. These are designed to investigate the mix in burning plasmas. Complex targets for study of the mix in burning hydrogen plasmas, nuclear physics in high-neutron-brightness environments, and fast-ignition inertial-confinement fusion require precisely placing nanoporous materials with small amounts of additional incorporated elements to alter the material's properties (a process known as doping), inside the target capsule.

Traditionally, target capsules are made by assembling prefabricated and machined components of the structure. This approach limits the complexity of the structures that can be achieved. With self-assembly techniques, complex targets could be built either from the inside out or outside in. In the latter case, the ablator shell with a fill hole would serve as both a template and a container in which materials could be grown or modified. LDRD researchers will use this "chemistry in a capsule" approach to generate complex nanostructures within the ablator shell by in situ self-assembly of functional building blocks. For example, a uniform and conforming film of a porous material lining the inside of the shell could be prepared by spin coating and subsequent curing by light, heat, or chemical initiation. Once formed, the properties of a nanoporous capsule liner could be further fine-tuned by atomic layer deposition. Possible applications include doping with mid-to-high-atomic-number elements as well as surface engineering of the wetting behavior. In principle, this self-assembly technique could be applied to any nanostructure formation.

In just the first year of this project, the LDRD team has made significant progress in all these areas. They have successfully demonstrated the feasibility of the chemistry in a capsule approach by loading a diamond laser target with the nanomaterial precursor solution and forming nanoporous foam inside the capsule. Team members installed an atomic-layer-deposition system and demonstrated that the technique can be applied to deposit mid-to-high-atomic-number elements on the nanoporous foam liner inside the capsule. They also demonstrated that the capsule liner can be rendered inactive and then reactivated for atomic layer deposition. This discovery opens the door to generating nanoporous foams with three-dimensional doping patterns by area-selective atomic layer deposition. The effects and requirements of this tailored doping on yield and symmetry of foam-filled capsules was assessed by hydrodynamic simulations. X-ray scattering was used to study the effects of wetting organic aerogels with liquid hydrogen on the foam morphology. These experiments demonstrated that even low-density aerogels can survive liquid hydrogen wetting and de-wetting cycles. Finally, an in situ film-stress-monitoring capability was developed to study the microstructure-stress correlation in thick metal films grown by magnetron sputtering. The team was able to control the texture—and thus the stress of thick beryllium films—by applying a bias to the substrate, thereby changing the initial stress state from tensile to compressive. Besides this impressive progress, they also developed novel nanomaterials for energy storage and conversion applications and studied their unique properties.

Future LDRD efforts will include casting of thin films of aerogels in target capsules by growing cross-linkable polymer brushes, for example. Using in situ x-ray techniques, the team will study the effect of aerogel morphology on wetting with liquid hydrogen. They will develop novel atomic-layer-deposition precursor chemistries for doping with high-atomic-number materials. Area-selective doping will be attempted through spatially selective modifications of the substrate's surface chemistry. In addition, new functionalities will be added to their nanomanipulator to measure thickness profiles from three-dimensional targets and to apply picoliter amounts of liquids. Researchers will continue work on stress control in metal deposition and develop predictive multiscale tools.

The successful conclusion of this LDRD project will enable the fabrication of complex targets for experiments to understand boost physics, investigate the dynamics of nuclear excited states, and pursue

inertial-confinement fusion fast ignition. It will also create new materials for catalysis, hydrogen storage, and self-healing nuclear reactor materials. A very important long-term benefit of this effort will be the establishment of an outstanding Laboratory team for the design and assembly of tailored nanomaterials and nanostructures.

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

J. Chance Carter, Principal Investigator

Hidden bombs or improvised explosive devices (IEDs) have caused over 60% of all American combat casualties in Iraq and 50% of combat casualties in Afghanistan. Videos of exploding U.S. vehicles and dead Americans are used by insurgents to win new supporters. The bombs have been hidden behind signs and guardrails, under roadside debris, or even inside animal carcasses, and deadly encounters with IEDs are amplified by ambushes of follow-on forces coming to the aid of those suffering an IED attack. The threat also includes vehicle-borne IEDs, where insurgents drive cars laden with explosives directly into a targeted group of service members. U.S. forces counter the devices with intelligence sources and by disrupting portions of the radio spectrum that insurgents use to trigger IEDs. However, insurgents quickly adapt to countermeasures, and new, more sophisticated devices are increasingly being used in both Iraq and Afghanistan. It is believed that mines and IEDs will continue to be weapons of choice for insurgents there, and there is concern that they will become widely used by terrorists worldwide. As a result, there is an immediate need to develop technologies for the standoff detection of high explosives.

Current, high-explosives detection methods span from simple colorimetric screening to more sophisticated speciation with advanced spectroscopic measurements. These techniques generally require contact or proximal sampling, which can be extremely hazardous. The idea of standoff resonance Raman detection of high-explosive materials is novel and has not been demonstrated. Raman spectroscopy is a light-scattering technique that uses a laser to measure the vibrational spectrum of a sample. The Raman spectrum is similar to an infrared spectrum and is very good for identifying molecules in mixtures. A Raman spectrum is a plot of scattered light intensity versus vibrational energy. The sample is illuminated with a monochromatic laser to acquire a Raman spectrum, and backscattered light is collected and analyzed using a spectrometer. Resonance Raman spectroscopy provides significantly stronger Raman signals than normal Raman and resonance enhancements over a thousandfold have been demonstrated for select high-explosive materials. In resonance Raman spectroscopy, the laser is tuned to match the wavelength of a strong electronic absorbance in the molecule. The advantage of Raman or resonance Raman for remote detection is that no direct contact with the sample is required. In principle, the Raman spectrum can be acquired for any compound within the line of sight of the instrument as long as enough scattered photons can be collected from the remote sample.

The objective of this LDRD project is to understand the fundamental resonance, Raman spectroscopic properties of high-explosive materials, with the ultimate goal of determining the feasibility of a technology to remotely detect IEDs. The team is determining the optimal conditions for resonance Raman of high-explosive materials, developing a method for determining enhancements relative to normal Raman technology, and determining resonance Raman sensitivity, selectivity, and response time for high-explosive materials. Additionally, they plan to evaluate signatures from laser-induced sample degradation, understand the timescale and pathway of sample degradation, and address background interference issues. This research aids the Laboratory's national security mission by developing the basis for a new standoff high-explosives-detection technology—an important capability needed to detect and mitigate the effects of IEDs

Munitions rigged for an improvised explosive device found in Baghdad, Iraq.

and other terrorist-related threats. Furthermore, this technology also has potential applications in standoff aging and degradation studies of nuclear and conventional weapons, which supports LLNL stockpile stewardship efforts.

The team has successfully developed an in-house benchtop ultraviolet micro-Raman system, devised an internal standard measurement method to quantify ultraviolet resonance Raman enhancements, and measured the normal Raman versus resonance Raman spectra of high-explosives materials. As an example, they were able to experimentally quantify the resonance Raman enhancement for TNT explosive using 229- and 244-nanometer excitation—preliminary results indicate an enhancement by several orders of magnitude. The researchers also studied the resonance Raman enhancement effect as a function of laser power to study sample degradation and conducted 532-nanometer excitation studies of TNT both in terms of potential resonance Raman enhancement and sample degradation. In addition, they successfully developed a pulsed-laser-based standoff system for high-explosives standoff measurements—measurements at standoff distances of tens of meters is the current focus of this ongoing LDRD effort.

Future work will include multiwavelength standoff resonance Raman studies in which the team will conduct multiwavelength measurements and compare optimal conditions, spectral differences, sensitivity, selectivity, and response time. Furthermore, researchers intend to characterize the fluorescence and absorption properties of degraded explosives at different irradiances and evaluate resonance Raman measurements in terms of laser power, pulse width, and raster scan rate and determine signal-to-noise ratios and detection limits. The successful completion of this LDRD project will form the science base for a whole new standoff detection technology. The Department of Defense has established—along with various national laboratories, the DOE, contractors, and academia—the Joint IED Defeat Organization to investigate effective countermeasures. It is expected that the Joint IED Defeat Organization, along with other federal agencies such as the Federal Bureau of Investigation, Central Intelligence Agency, and the Defense Advanced Research Projects Agency will be interested in further research into this standoff explosives detection capability developed by LDRD.

"Storage-Intensive Supercomputing" (07-ERD-063)

Maya Gokhale, Principal Investigator

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. Scientists at Livermore are using codes and supercomputers to delve into regimes of physics heretofore impossible to reach. A major component of DOE's science-based Stockpile Stewardship Program, computational modeling and simulation capabilities performed on supercomputers are used to assess the safety, security, and reliability of our nuclear stockpile. Effectively analyzing datasets generated by these massive simulations is difficult on present-day supercomputing architectures, which are optimized for raw compute cycles. Similarly, analyzing large social networks for evidence of terrorist interactions is ill-suited to compute-intensive supercomputers.

Data-intensive problems challenge conventional computing architectures with demanding central processor unit, memory, and input and output requirements. Without fast access to stored data, the supercomputing systems are little more than hard-to-program data-generation engines that create massive quantities of intractable, raw data. A software and hardware infrastructure to support simulation and analysis applications transforms the terascale supercomputer platform into a real tool. The infrastructure includes improved systems software, input and output applications, message-passing libraries, storage systems, performance tools, debuggers, visualization clusters, and data reduction and rendering procedures, or algorithms—all focused on making the machines and codes run more efficiently.

This LDRD project addresses efficient computation of data-intensive problems in national security and basic science by advancing storage-intensive supercomputing capabilities. Storage-intensive architectures offer an advantage over computation-intensive architectures by optimizing access to large sets of data. Problems that benefit from storage-intensive architectures include analysis of stockpile stewardship simulations, of large-scale graphs used to identify terrorist networks, of massive astronomy datasets, and of fusion-class laser optics imagery to assess damage. The team is developing new algorithms and applications to solve large-scale data analytics problems on supercomputer architectures. Research deliverables include system architecture demonstrations of data-oriented supercomputing clusters, parallel programming libraries for data-intensive parallel application, and software tools to measure performance of central processing unit access to data files. They are exploring new programming models, tools, and libraries to address the difficulty in developing software applications for storage-intensive architectures, with a goal of demonstrating architectures and associated software tools that achieve a tenfold speedup in performance on national security applications at reasonable cost in acquisition and programming effort. The team is partnering with industry collaborators in developing these new system architectures for storage-intensive supercomputing. With a rapid computer time-to-solution, Laboratory scientists can perform a new run every day, make numerous investigations, and explore multiple alternatives to solve data-intensive problems in nonproliferation and homeland security, defense applications, and analysis of scientific simulation data.

In the last year, LDRD researchers evaluated the open-source Google Parallel File System framework (named "Hadoop") to process large semantic graphs on storage-intensive computer cluster architectures. The team investigated some of the largest nonvolatile memory systems that have been built and pinpointed key issues in the system software that limit performance. A benchmark generator was developed that mimics the input and output activity of storage-intensive supercomputer applications with an error of less than 10%, along with a suite of small benchmarks that have been used to study input and output performance of novel storage systems. In addition, the team developed a flexible, hierarchical checkpoint
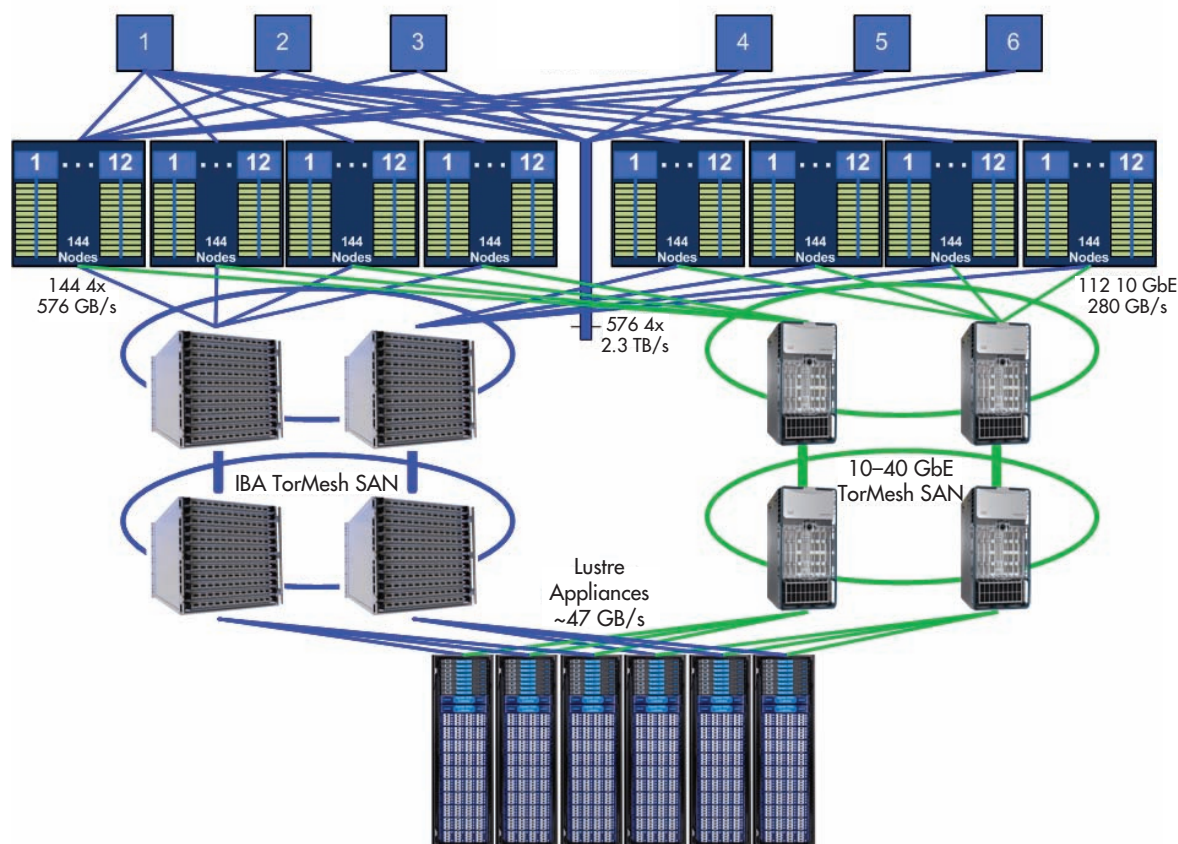
The Hyperion supercomputer at Lawrence Livermore. The first-phase machine, running at 46 trillion floating point operations per second, offers a novel open research platform for evaluating advanced computer architectures. Hyperion includes a high-performance storage testbed that will be used for storage-intensive supercomputing architecture studies.

file system to optimize transmission of simulation checkpoint data to the file system. Recognizing that data-intensive applications often also encounter compute bottlenecks, they mapped two data and compute-intensive applications onto a new single-chip device containing 336 individual processors and demonstrated a performance increase of 58 times over a typical computer workstation.

In the coming year, the project team will continue to collaborate with industrial partners to develop storage-intensive supercomputer system architectures that are flexible, scalable, robust, and cost effective, as well as address the difficulty of programming scalable applications software with file systems and programming models focused on data-intensive problems. Software tools will be created to measure performance, and new approaches will be developed for mapping algorithms and applications onto supercomputing architectures.

Successful storage-intensive supercomputing research establishes LLNL leadership in supercomputing architectures for data-intensive problems and enables new sponsors, increased funding from current sponsors for programs, and enhanced stature in the computer science research community. Collaborations across Laboratory programs, with industrial leaders such as IBM, and with academic institutions are a cornerstone of supercomputing research at Livermore. In addition, this LDRD project has attracted interest from the Defense Advanced Research Projects Agency to support study the storage-intensive computing systems for Department of Defense problems.

"Development of Integrated Microanalysis of Nanomaterials" (06-ERI-001)

John Bradley, Principal Investigator

Comets—small extraterrestrial bodies of ice, dust, and small rocky particles—are considered the oldest, most primitive bodies in the solar system. They were thought to be composed of preserved interstellar particles from 4.6 billion years ago, when the Sun and the planets began to form from a primordial disk of dust and gas. The nonvolatile mineral components of comets are probably natural nanomaterials that include preserved interstellar dust as well as the first solids condensed in the solar system. Thus, comet samples may be considered as forensic "time capsules" from the presolar molecular cloud and the earliest stages of solar system formation.

Cometary material was captured in 2004, when the National Aeronautics and Space Administration's Stardust spacecraft flew through the cloud of particles surrounding the nucleus of comet Wild as it neared the orbit of Mars. As Stardust approached the 4.5-kilometer-diameter comet, the spacecraft briefly extended a collector filled with lightweight aerogel glass foam to capture thousands of tiny particles. On January 15, 2006, the spacecraft ejected its sample-return capsule onto the Utah desert southwest of Salt Lake City.
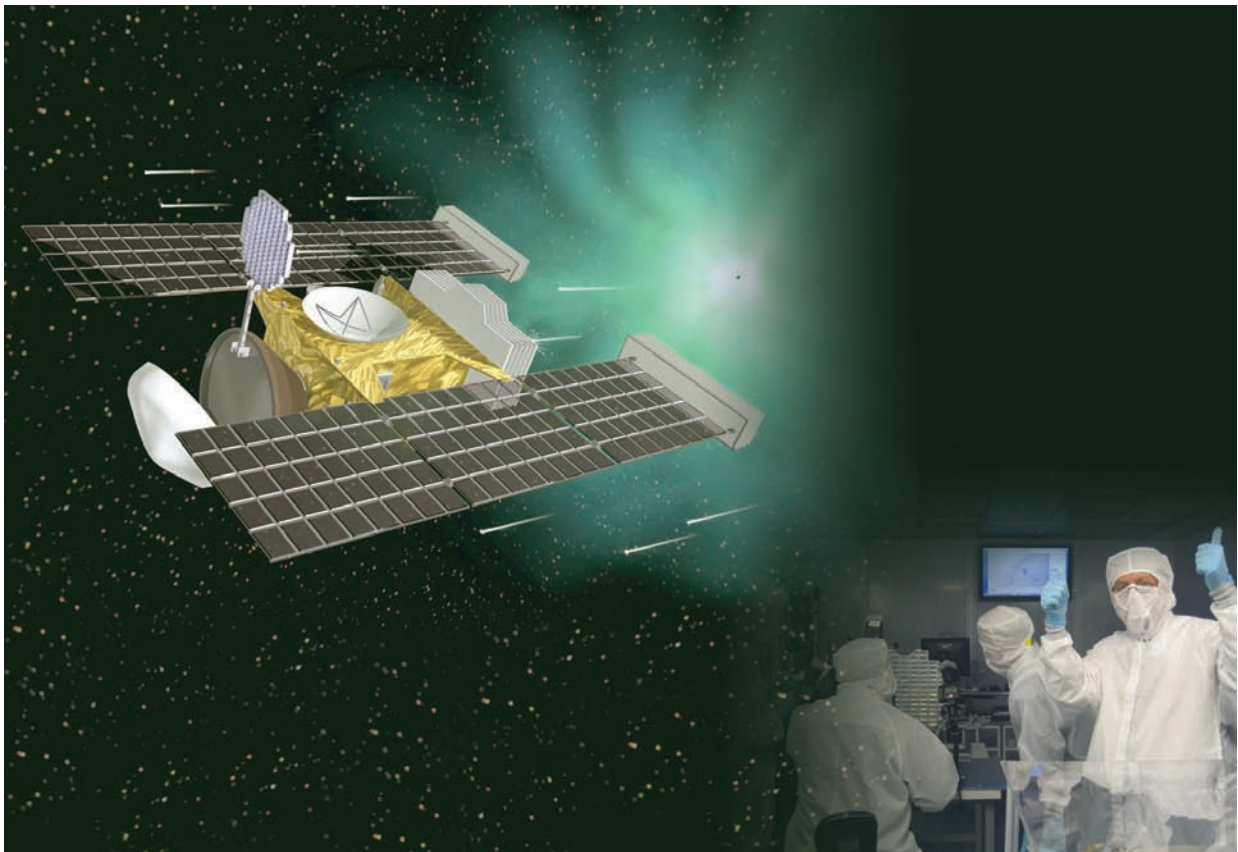
An artist's conception shows the Stardust spacecraft approaching Comet Wild 2. The spacecraft's cometary particle collector, filled with lightweight aerogel glass foam, is shown extended. The spacecraft is flanked by two solar panels. (Image courtesy of the National Aeronautics and Space Administration.) In the lower right photo, John Bradley gives the thumbs-up sign after scientists opened the Stardust sample return capsule in the clean room facility at the agency's Johnson Space Center.

LDRD researchers are part of a collaborative team investigating the mineralogical, chemical, and isotopic compositions of natural cometary nanomaterials from the Stardust mission using the outstanding array of signature analytical facilities at Livermore. The studies are providing new insight into cosmically primitive materials that will enable a better understanding of the earliest stages of disk accretion around stars. The skills and analysis techniques developed for the characterization of these natural nanomaterials are synergistic with several Livermore programmatic needs in the emerging fields of nanomaterials, nanotechnology, and forensics. The Stardust samples are also ideal training materials for a new generation of young scientists using state-of-the-art analytical instruments at the Laboratory.

The LDRD team is developing an integrated microanalysis capability utilizing advances in detection and imaging capabilities using electron microscopy and ion microprobe techniques with the state-of-the-art instrumentation at Lawrence Livermore to enable a new level of analytical techniques for nanoscale materials characterization that are directly applicable to the Laboratory's missions in stockpile stewardship and homeland security. For example, the techniques used to investigate Stardust samples can be used to interrogate interdicted materials as part of nuclear forensic efforts to counter nuclear proliferation and terrorism. The project also underscores the Laboratory's commitment to achieving breakthroughs in fundamental science and applied technology.

Cometary particulates scattered along impact tracks in aerogel and lining the microcrater walls in the aluminum foils of Stardust's collector were subjected to a multitechnique preliminary examination with synchrotron-based x-ray diffraction; nanometer-scale, secondary-ion mass spectrometry; and electron microscopy; and the initial findings were reported in *Science*. Surprising early observations revealed the scarcity of presolar material, the tiny interstellar grains produced around other stars that existed before the Sun and solar system formed. Furthermore, the identification of refractory (stable at high-temperature) mineral grains suggests a much more complex radial mixing of materials in the solar accretion disk than had previously been appreciated.

In 2008, the team conducted light gas-gun shots of mineral grains into aerogel as well as atomic-scale scanning transmission electron microscope studies of Stardust comet grains to determine the degree of alteration experienced by the materials during capture, the mineralogy of Wild-2 dust, the isotopic compositions of Stardust grains, and the bulk and trace element compositions. Researchers found that capture damage to the Stardust samples was significant but that important scientific information can still be found at the atomic scale. The Comet Wild 2 sample did not contain what was expected in a comet. The sample appeared to contain inner solar system materials similar to those found in meteorites (most meteorites are from the asteroid belt in the inner solar system). This totally unexpected finding, after roughly two years of careful examination of the returned sample, essentially redefined the direction of comet science and the thought that formation of the solar system was rather quiet and orderly—the process now appears to have been much more dynamic and violent. A paper describing this surprising finding appeared in *Science* in 2008.

The next step in this work is to fully integrate the state-of-the-art analytical instruments: the focused ion beam, field-emission scanning electron microscope, nanometer-scale secondary-ion mass spectrometer, and super-resolution scanning transmission electron microscope. This will enable precious samples, whether Stardust or one-of-a-kind nuclear forensics samples, to be analyzed with multiple analytical techniques, thereby maximizing the science yield. These activities have enhanced the international reputation of LLNL in materials science and space sciences and resulted in a high-profile, multidisciplinary project that was attractive to a broad range of researchers and highly successful in recruiting young talented scientists. In addition, it lead to numerous collaborations with academic institutions as well as federal agencies, and the results were reported in high-profile scientific journals.

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 FY08, LDRD costs at LLNL were $91.5M, which is 5.95% of the total Laboratory costs. The number of patents resulting from LDRD-funded research since 2000 and the percentage of total patents that were derived from LDRD research and development is shown in the table below. The year for which a patent is listed is the year in which the patent was granted; LDRD investment in a technology is sometimes 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.

As with patents, records of invention submitted by LDRD researchers account for a significant percentage of the total for Laboratory research. Overall, LDRD records of invention for 2000 to 2008 account for approximately 44% of the 1,387 total. In 2008, there were 110 records submitted at Livermore, with 46 (42%) of those attributable to LDRD-supported projects.

Patents	2000	2001	2002	2003	2004	2005	2006	2007	2008
All LLNL patents	93	89	97	71	95	93	63	62	57
LDRD patents	35	42	27	29	55	51	29	32	23
LDRD patents as percentage of total	38%	47%	28%	41%	58%	55%	46%	52%	40%

Patents resulting from LDRD-funded research as a percentage of all LLNL patents from 2000 to 2008.

The role of LDRD in producing Laboratory copyrighted material has also been determined for 2000 to 2008. Overall, LDRD-supported projects account for over 20% of the 723 Livermore copyrights for the period. In 2008, there were 68 LLNL copyrights, with 17 (25%) that could be attributed to LDRD research.

Scientific Journals

Scientific journals further the progress of science by reporting new research, sometimes marking fundamental breakthroughs and serving as part of the permanent scientific record. Each year, Laboratory scientists and engineers publish more than 1,000 papers in a wide range of peer-reviewed journals. In FY08 there were 1,097 such articles, of which 211 (19%) resulted from LDRD projects. The number of journal

Journal articles	2004	2005	2006	2007	2008
All LLNL articles	1,158	1,296	1,237	1,162	1,097
LDRD articles	210	250	247	237	211
LDRD articles as percentage of total	18%	19%	20%	20%	19%

Journal papers resulting from LDRD-funded research as a percentage of all LLNL papers from 2004 to 2008.

articles resulting from LDRD-funded research since 2004 and the percentage of total articles that were derived from LDRD research and development is shown in the table above. In addition, several LDRD-supported projects were featured on journal covers or named as significant accomplishments for the year, as detailed in the Awards and Recognition section starting on page 28.

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 FY08 LDRD portfolio included 92 formal collaborations involving 78 LDRD projects (44% of the total projects funded). Collaborating institutions included the University of California (35% of total collaborations), other academic institutions (46%), DOE sites (14%), and other collaborators (e.g., other government agencies and industry, 5%). These statistics do not include the numerous informal collaborations that investigators 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 FY08, the LDRD Program supported nearly 80% of the Laboratory postdoctoral researchers—there were 119 postdoctoral researchers at the Laboratory, of which 89 were supported by LDRD projects.

Awards and Recognition

A primary goal of LDRD is to foster excellence in science and technology that will, among other things, 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 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 Association for the Advancement of Science Fellow. Tomás Díaz de la Rubia was selected a 2008 fellow of the American Association for the Advancement of Science. Díaz de la Rubia, was one of 34 fellows elected in the physics category for distinguished contributions to computational materials science and radiation damage in materials. Currently the Laboratory chief research and development officer, he also served as a principal investigator for numerous LDRD materials science projects including fundamental studies of particle–solid interactions (92-ER-002), mechanisms of electromigration in stressed aluminum–copper and copper films (94-ERD-019), surface morphology in silicon during ion-beam processing (96-ERD-009), and the effects of radiation on the mechanical properties and structural integrity of nuclear materials (98-ERD-090).

Tomás Díaz de la Rubia

American Physical Society Fellow. James De Yoreo was nominated by the Biophysical Physics Division of the American Physical Society "for his pioneering work using in situ force microscopy to understand the physical principles underlying biocrystallization, particularly the control of biomolecules and other modifiers on energy landscapes, step dynamics, and morphological evolution during crystal formation." De Yoreo served as a manager and reviewer for Livermore's LDRD Program for several years and was a principal investigator for numerous related projects such as investigations of molecular-scale growth dynamics during crystallization from solution (95-ERP-144), the origins of laser damage in potassium dideuterium phosphate crystals (97-ERD-098), the physical basis for materials synthesis using biomineralization (97-LW-069), and dip-pen nanolithography for controlled protein deposition (01-ERD-086).

American Physical Society Outstanding Referee. Peter Beiersdorfer was part of the inaugural group of outstanding referees of the American Physical Society journals, as selected by the society's editors. His latest LDRD project is concerned with an imaging x-ray line-shape diagnostic for burning plasmas (09-ERD-061). Previous projects included the study of uncharted frontiers in the spectroscopy of highly charged ions (97-ERD-103), soft x-ray emission from comets (00-ERD-037), and understanding nuclear magnetic fields (05-LW-006).

American Physical Society Fellow James De Yoreo (left), American Physical Society Outstanding Referee Peter Beiersdorfer (middle), and American Physical Society California Section Vice Chair Karl van Bibber (right).

American Physical Society California Section Vice Chair. Karl van Bibber, former LDRD investigator and a past deputy administrator of the LDRD program at Livermore, has been named as vice chair of the American Physical Society's California section. Van Bibber headed various LDRD projects including advanced accelerator and detector technology (94-DI-008), the dark-matter galactic-axion experiment (96-LW-061), intense laser–electron beam interactions (97-SI-001), and high-energy physics with a photon collider (00-SI-005).

Best Poster. A presentation by postdoctoral researcher Youn-hi Woo was selected for a best poster prize at the 2008 American Chemical Society Meeting in New Orleans. The poster, titled "Visualization of Pathogen Invasion Dynamics and Mechanisms at the Single Cell Level Using Ligand Coated Microspheres and a FRET Reporter," was related to an LDRD project on the biophysical characterization of pathogen invasion (06-ERD-013).

DOE Outstanding Mentor Award. In 2008, 11 scientists from Livermore received Outstanding Mentor Awards from DOE. They included LDRD researchers Dustin Froula, who is currently studying the concept of a plasma waveguide for electron acceleration (08-LW-070), and Michael Thelen, who is characterizing hypothetical proteins (05-ERD-064).

DOE Plasma Physics Junior Faculty Award.
Christoph Niemann, currently part of an LDRD team studying conductivity in warm dense matter (08-LW-004), was honored with a 2008 DOE Plasma Physics Junior Faculty Award. Niemann, a National Ignition Facility professor at the University of California at Los Angeles, is establishing a research group on high-energy-density physics and laser–plasma interactions. In close collaboration with LLNL scientists, the group will perform experiments at the lasers available at Livermore and will serve as a conduit for developing students and postdoctoral researchers for NNSA programs.

Federal Laboratory Consortium Award for Excellence in Technology Transfer. LDRD helped generate technology that was the basis for the commercial success of the dielectric wall accelerator, which won the Federal Laboratory Consortium award for technology transfer in 2008. George Caporaso was the principal investigator for three LDRD projects that helped develop this technology, including research into an ultrahigh-gradient dielectric wall accelerator (93-DI-044) and a compact accelerator for proton therapy (02-ERD-003 and 03-ERD-073).

Glenn T. Seaborg Award for Nuclear Chemistry.
Presented by the American Chemical Society, the 2009 Glenn T. Seaborg Award for Nuclear Chemistry was given to Kenton Moody, who has

Christoph Niemann

been deeply involved in LDRD-supported superheavy element research over many years. His latest LDRD research examines rapid radiochemical separations for investigating the chemistry of the heaviest elements (08-ERD-030). Previous work by Moody and his collaborators includes the development of new fragment separation technology for superheavy element research (04-ERD-085). This collaboration reported the discovery of elements 113, 114, 115, 116, and 118 (31 new isotopes in all).

Jim Candy

Helmholtz–Rayleigh Interdisciplinary Silver Medal. James Candy, chief scientist for the Engineering Directorate at Lawrence Livermore, has been awarded the prestigious 2008 Helmholtz–Rayleigh Interdisciplinary Silver Medal "for his contributions to signal processing and underwater acoustics" by the Acoustical Society of America, a society of the American Institute of Physics. The Silver Medal is presented to individuals for contributions to the advancement of science, engineering, or human welfare through the application of acoustic principles or through research accomplishments in acoustics. Candy was the principal or co-investigator for numerous related LDRD projects, including the study of techniques for enhancing laser ultrasonic nondestructive evaluation (97-ERD-083), the dynamic focusing of acoustic energy for nondestructive evaluation (99-LW-045), and determining a novel method for extracting signals from noisy broadband data using Poynting vector measurements (07-ERD-018).

I2CAM Travel Award. The Institute for Complex Adaptive Matter (ICAM-I2CAM) is a distributed experiment-based multi-institutional partnership whose purpose is to identify major new research themes in complex adaptive matter. LDRD researcher Jason Jeffries, investigating the double-C curve behavior in the plutonium–gallium time–temperature–transformation diagram (07-ERD-047), earned a 2008 I2CAM Travel Award.

Journal Covers. In FY08, several LDRD-supported projects were featured on the covers of peer-reviewed journals. The November 15, 2007 issue of *Analytical Chemistry* featured Chris Bailey's LDRD project on the viral discovery platform (08-SI-002). In November of 2008, the cover of *Science* showed the first images of a newly discovered multiplanet solar system that orbits a young star, a result of a Bruce Macintosh LDRD project that is tracing the shadows of planetary systems (08-ERD-043). The April 2008 cover of *Computer* centers on the issues of data-intensive storage, and features the research of Maya Gokhale on storage-intensive supercomputing (07-ERD-063).
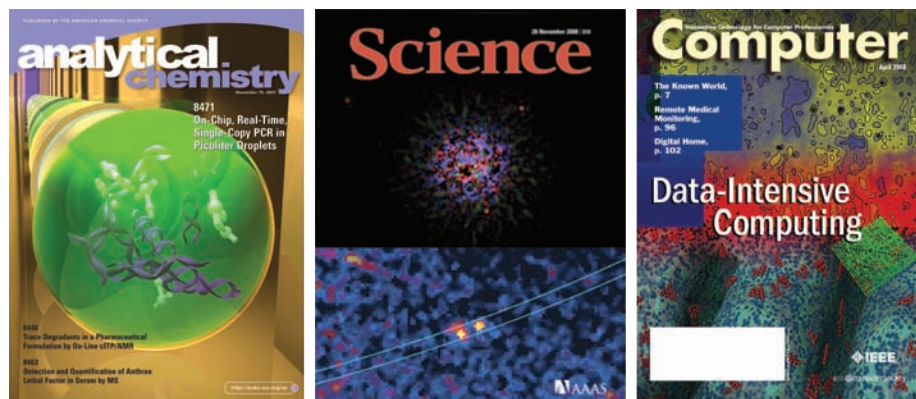
Journal covers of LDRD projects on the rapid identification and characterization of viruses in clinical samples (left), developing capabilities to observe the interplanetary dust that traces the formation and presence of planets and cometary belts in other solar systems (middle), and developing order-of-magnitude improvements in data-intensive supercomputer architectures for a broad range of data-intensive problems (right).

Macelwane Award. The American Geophysical Union presents the Macelwane Award for contributions to the geophysical sciences by an outstanding young scientist. Livermore LDRD collaborator James Badro was one of three winners for 2008. His current research focuses on the chemistry of core formation (06-ERI-002).

Mineralogical Society of America Award. James Badro was presented the Mineralogical Society of America Award in 2008, which recognizes early-career scientists who have made outstanding published contributions in a relevant research area. In addition to his research on the chemistry of core formation (06-ERI-002), Badro was also a member of the LDRD team that studied the mapping of phonons at high pressure for phase transformation and stability (04-ERD-106).

Nano 50 Awards. The top 50 technologies, products, and innovators that significantly impact nanotechnology are honored by the publishers of *Nanotech Briefs*. All six of the winners from Livermore were enabled by LDRD investments.

- Livermore researchers, in collaboration with industry and with initial support from LDRD, combined pulsed-laser technology with the electron optics of a standard transmission electron microscope to develop the dynamic transmission electron microscope, which won both Nano 50 and R&D 100 awards in 2008, and was initially supported by the LDRD project on time-resolved transitions via dynamic transmission electron microscopy (06-ERD-007).

- Paul Hoeprich and Matt Coleman were recognized for nanolopoprotein-particle formation based on an LDRD project on developing and integrating novel technologies for the production and characterization of membrane proteins (07-SI-003).
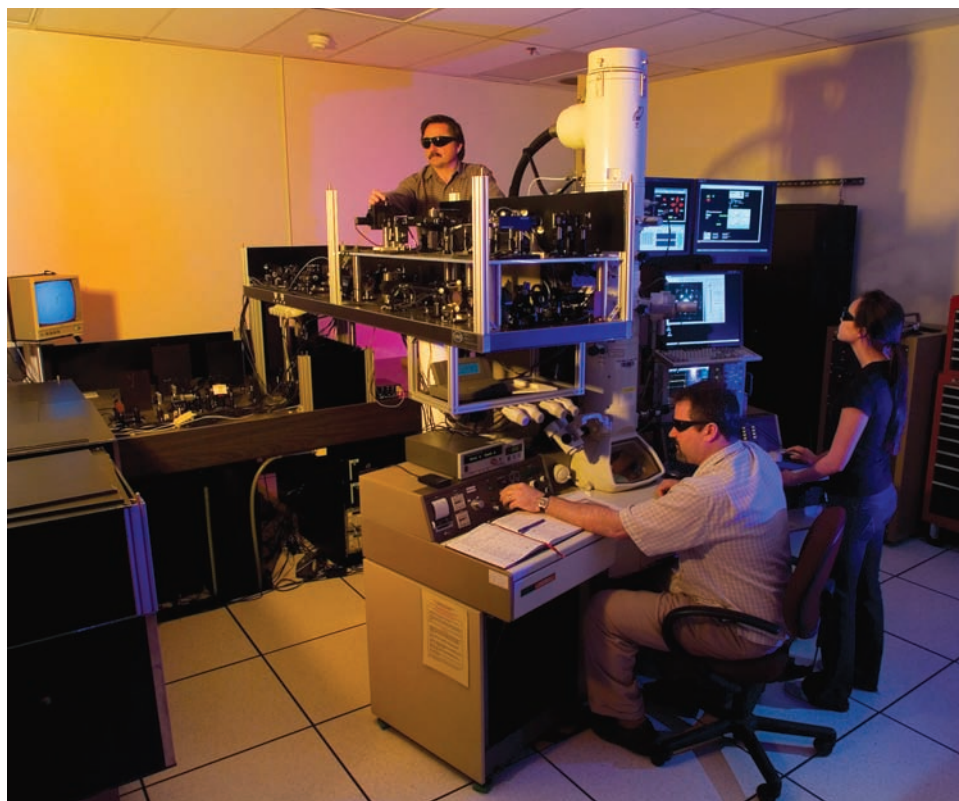
The dynamic transmission electron microscope captures single-molecule-scale images a million times faster than conventional instruments.

- Sonia Létant received an award for designing and fabricating functional nanopores. She developed a novel approach to address the challenge posed by the fabrication of artificial membranes. Her work in functional nanopores started with LDRD support for DNA detection through designed apertures (03-ERD-013), and she is currently part of an LDRD project examining the ultrafast laser synthesis of nanopore arrays in silicon (09-LW-016).

- Nerine Cherepy won for fabricating transparent ceramics from nanoparticles. The Laboratory's capability for fabricating transparent ceramics was enabled in part by LDRD investments in this area, including a project studying ceramic laser materials (05-ERD-037).

- Alex Gash's work, which involves the application of inorganic synthetic techniques to the formulation of energetic nanocomposites, was recognized in the technology category. He is part of the LDRD team for the transformational materials initiative (06-SI-005).

- Morris Wang won an award in the inventor's category for research on the mechanical behavior of bulk nanostructured materials and nanolaminates, semiconducting nanowires, mass transport behavior of nanotubes, and transmission electron microscopy. His current LDRD research focuses on nanomaterials for fusion application targets (08-SI-004).

National Academy of Sciences Member. In 2008, the National Academy of Science elected Claire Max a member. Max was the principal investigator for nine LDRD projects concerned with the development and demonstration of adaptive optics, for which she was recognized with this honor. Her LDRD studies included high-resolution astronomy (93-ERI-046), application of adaptive optics to astrophysical observations (94-DI-007), ultrahigh-contrast imaging (98-ERD-036), and examination of nearby active galactic nuclei (00-ERD-049). Max is now a member of the faculty at the University of California at Santa Cruz.

OASCR Visualization Award. Office of Advanced Scientific Computing Research (OASCR) awards are presented by the DOE Office of Science for research visualizations tools. A team led by Dave Eder received a 2008 OASCR visualization award at the annual Scientific Discovery through Advanced Computing (SciDAC) meeting in Seattle. Eder's team is working on issues related to electromagnetic pulses that result from extremely short but very high-energy laser bursts (06-ERD-055).

Two frames from the OASCR-winning simulation of electromagnetic pulses inside the Titan laser target chamber. The laser beams enter the chamber at the far right and hit the large curved object at the left, which represents a mirror that directs the laser beams onto the target. The upright stalks represent stands for diagnostic instruments and mirrors. The colored circles show the contours of the resulting electrical fields.

Presidential Early Career Awards for Scientists and Engineers (PECASE). This award is the highest honor bestowed by the U.S. government on outstanding scientists and engineers beginning their independent careers, and is intended to recognize and nurture young scientists and engineers who show exceptional potential for leadership at the frontiers of scientific knowledge. In FY08, LDRD established support for three new winners: Carlos Pantano (University of Illinois, Urbana Champaign), Jeff Kyser (Columbia University), and Shawn Newsam (University of California at Merced). They are affiliated with LDRD projects regarding mesoscale studies of hydrodynamic instability growth in the presence of electric and

From left: Carlos Pantano, Jeff Kyser, and Shawn Newsam.

magnetic fields (08-ERD-062), deformation of low-symmetry and multiphase materials (07-ERD-024), and hierarchical vehicle activity models for site security (08-ERD-067), respectively.

R&D 100 Awards. In 2008, LDRD-supported technologies won two of the three R&D 100 awards presented to the Laboratory by *R&D Magazine*.
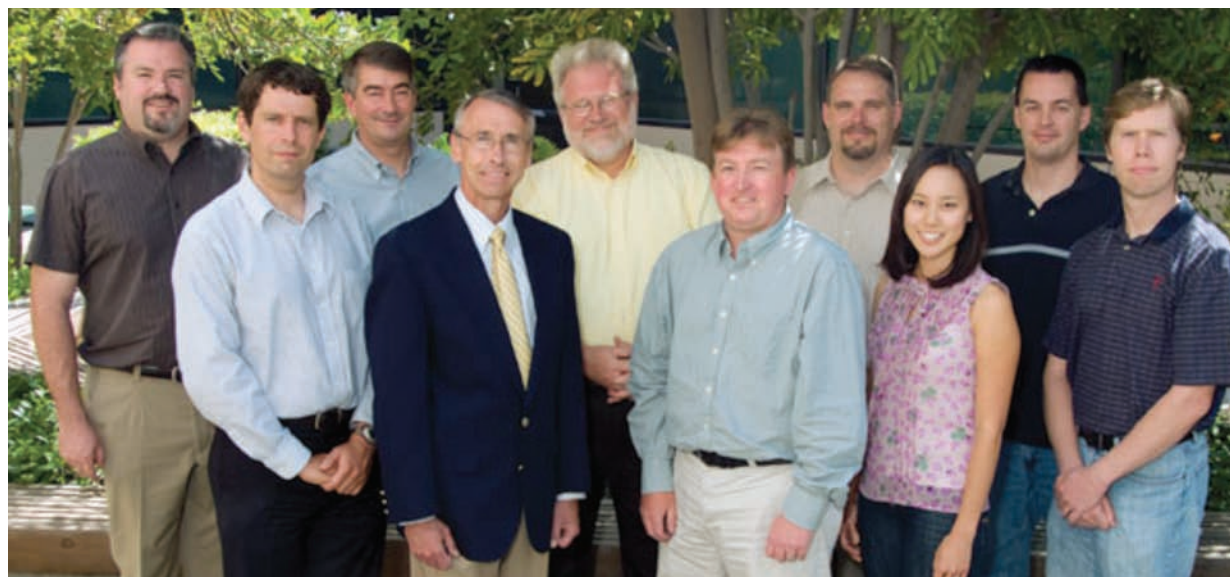
The dynamic transmission electron microscope development team (from left): Thomas LaGrange, Bryan Reed, Geoffrey Campbell, Wayne King, William DeHope, Nigel Browning, Richard Shuttlesworth, Judy Kim, Benjamin Pyke, and Michael Armstrong. Not pictured: Brent Stuart, Mitra Taheri, J. Bradley Pesavento, and Benjamin Torralva.

- **Taking Ultrafast Snapshots of Material Changes.** Working with researchers from JEOL USA, Inc., a Livermore team has developed the dynamic transmission electron microscope. The instrument captures images with better than 10-nanometer resolution in 15 nanoseconds, a million times faster than the typical 30-millisecond exposure time required by a conventional transmission electron microscope. Using the new microscope, scientists can see for the first time how materials behave under unusual conditions, such as an applied stress, extreme temperature change, and corrosive environment. This technology was supported in the early stages by an LDRD project on time-resolved phase transitions via dynamic transmission electron microscopy (06-ERD-007).

- **SecureBox: National Security through Secure Cargo.** SecureBox is a security mechanism developed at Lawrence Livermore to help monitor the over 11 million cargo-container shipments that arrive in the U.S. every year. The technology was an outgrowth of several projects that explored different detection and communication approaches to this problem (02-ERD-064, 03-ERD-025, and 07-ERD-019). SecureBox uses Livermore-developed ultrawideband radar and communication technology to accurately detect and report intrusions along any of a container's six walls, and works effectively even when a container is buried in a stack of other containers or located deep within the hold of a ship. The technology was licensed to Secure Box Corporation in 2007.

SecureBox is a wireless device that can be installed within the metal corrugation of a cargo container to detect intrusions.

***Science's* Top Ten Breakthroughs of 2008.** Bruce Macintosh's project on tracing the shadows of planetary systems (08-ERD-043), in collaboration with the NRC Herzberg Institute of Astrophysics in Canada, Lowell Observatory, and University of California at Los Angeles, reached the second spot on *Science* magazine's recognition of ten of the year's most significant scientific accomplishments. *Science*, published by the American Association for the Advancement of Science, looked for research that answers major questions about how the universe works and paves the way for future discoveries.

STEO Award. A 2008 Science, Technology, Engineering and Operations (STEO) award was presented by the Science and Technology Principal Directorate at Livermore to a group of theoretical and experimental scientists who were cited for "taking on the extraordinary challenge of advancing our understanding of the complex science of plutonium and for the discoveries. . .made over the last few years as evidenced by the outstanding number of high-impact publications in the peer review literature." LDRD researchers Michael Fluss and Scott McCall contributed to this effort with their study of the quantum properties of plutonium and plutonium compounds (07-ERD-048), along with Keri Jayne Blobaum's investigation of double-C curve behavior in the plutonium–gallium time–temperature–transformation diagram (07-ERD-047) and Patrick Allen's research on the thermodynamics and structure of plutonium alloys (01-ERD-030).

The team that helped expand the understanding of plutonium is shown along with Science and Technology Principal Directorate managers.

***The Scientist* Survey.** The Laboratory is ranked in the top 25 national institutes as one of the best places to work for postdoctoral candidates, according to an international poll conducted by *The Scientist* magazine. Livermore was ranked 24 for having strong benefits, pay, and compensation. The LDRD Program serves to recruit top researchers in science and technology through exciting projects at the forefront of science and technology. LDRD typically supports about 80% of the Laboratory postdoctoral researchers, more than any other program, and many go on to become full-time employees.

Hope Ishii (right) shows cometary and interplanetary dust samples from the Stardust mission to members of the media during a press event in 2006.

Young Trailblazers Award. Presented by *Science Spectrum* magazine, the 2008 award went to Hope Ishii, whose latest LDRD projects focus on the development of integrated microanalysis of nanomaterials (06-ERI-001) and analysis of geographic indicators for nuclear forensics (08-ERD-065). Previously, Ishii was part of the LDRD team that performed the first-ever study of cometary material collected by the Stardust space mission (03-ERI-007).
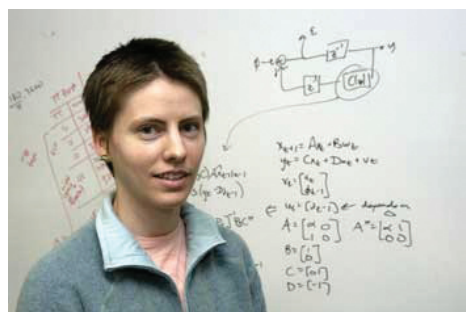
Lisa Poyneer

Zuhair A. Munir Award. The best Ph.D. thesis prize at the University of California at Davis for 2008 was awarded to Lisa Poyneer, who is a member of the LDRD team tracing the shadows of planetary systems (08-ERD-043). Innovations described in her dissertation include the spatially filtered wavefront sensor, which prevents aliasing, and a predictive wavefront controller, which uses Kalman filtering to keep up with the optical effects of the turbulent atmosphere.

Laboratory Directed Research and Development

Advanced Sensors
and Instrumentation

Leading the Quantum Limit Revolution

S. Darin Kinion   **05-ERD-073**

Abstract

The goal of this project is to utilize microstrip superconducting quantum interference device (SQUID) amplifiers to revolutionize experiments, ranging from quantum coherence to particle astrophysics, that require improved signal-to-noise ratio. The primary science deliverable will be a single electron transistor (SET) readout that is sensitive enough to enable single-spin detection in a solid-state system. We plan to develop robust packaging for the SQUID amplifier and then use the SQUID response to read out the signal from resonant-frequency SETs. These experiments will be performed in collaboration with resonant-frequency SET experts located at Yale University, the University of New South Wales, Australia, and the University of Maryland. Packaged ultralow noise SQUIDs will also permit prototyping experiments to determine the ultimate sensitivity of the Axion Dark Matter Experiment at LLNL.

The most important result will be the demonstration of the resonant-frequency SET readout by a microstrip SQUID amplifier that is sensitive enough to detect a single spin in a solid-state system. This will be a breakthrough for quantum computations and quantum information applications. We expect to demonstrate the quantum limit for charge amplification and position measurement in nanomechanical resonators. Based on our recent successful results, we also anticipate a demonstration of dramatically reduced noise performance in the Axion Dark Matter Experiment. Our results will be published in peer-reviewed journals, and university collaborations will attract top-echelon postdoctoral researchers to Lawrence Livermore.

Mission Relevance

This project will open the door to implementations of quantum computing and quantum information secure communication architectures that support national and homeland security missions. This work also will support the Laboratory's mission in discovery-class science, such as the Axion Dark Matter Experiment.

FY08 Accomplishments and Results

We achieved noise–temperature results with the SQUID amplifier that are the closest ever to the standard quantum limit and supplied the Axion Dark Matter Experiment with data from our amplifier. We also developed ideas for using the amplifier in a dispersive readout scheme to provide very fast, low-noise measurements. A paper describing the amplifier's performance was published in *Applied Physics Letters*. The success of this project has enabled both a definitive search for dark-matter axions and greatly improved the odds of building a practical quantum computer. The Intelligence Advanced Research Projects Activity agency is continuing efforts to develop the SQUID amplifier and apply it to the readout of superconducting quantum bits.

Publications

Kinion, D., and J. Clarke, 2008. "Microstrip superconducting quantum interference device radio-frequency amplifier: Scattering parameters and input coupling." *Appl. Phys. Lett.* **92**, 172503. UCRL-TR-226752.

Biophysical Characterization of Pathogen Invasion

Amy L. Hiddessen   06-ERD-013

Abstract

A fundamental understanding of pathogen infection and host response is needed to develop new treatments for infectious disease. To address this challenge, a comprehensive description of key processes is needed, including data on the spatiotemporal expression of molecular effectors and regulators of signaling cascades. Using a model pathogen system having well-characterized pathogen ligands and host receptors, we will, for the first time, quantitatively characterize the virulent ligand–host cell-receptor interaction and subsequent signal transduction using novel atomic force microscopy (AFM) that is combined with advanced optical methods. We also will develop a new capability for pathogen and host-cell characterization.

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.

FY08 Accomplishments and Results

We (1) attached ligands to beads and fixed the beads on AFM tips for successful delivery to cells; (2) visualized the real-time cellular actin response upon AFM ligand delivery and filed a

full patent application; (3) conjugated pH reporters to ligand-coated beads and completed novel real-time measurements of internalization (namely, measurements of time scales of epithelial cell phagosomal acidification) after concluding that measuring the spatiotemporal process of internalization of the beads alone was necessary before completing AFM-based measurement of internalization dependence on ligand density; and (4) completed cellular laser surgery measurements using a stand-alone setup.

Proposed Work for FY09

In FY09, we will (1) complete and document our development of a novel, combined chemical and physical tracking method for the real-time visualization of pathogen entry; (2) use our new method to measure the real-time, dynamic process of pathogen entry into a single host cell and to determine how the host response correlates to varying InlA bead concentration; (3) deliver pathogen mimics using an optical trap and use live cell reporters to measure host signaling response to mimics; (4) visualize the step-wise biophysical process of entry (hypothesized as binding, translocation, and internalization); and (5) attempt to characterize initial binding with force measurements using AFM or optical trapping methods.

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. Am. Soc. Cell Biology, Washington, D.C., Dec. 1–5, 2007. UCRL-ABS-236840.

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.

Thermal-Fluidic System for Manipulating Biomolecules and Viruses

Kevin D. Ness   06-ERD-040

Abstract

We propose to develop a reconfigurable fluidic system that will simultaneously separate, concentrate, and purify biomolecules and viruses. Many pathogen detection, mitigation, and protection applications require manipulation of biomolecules or viruses to accurately quantify the presence of a particular substance or synthesize and investigate the function of a molecule. We will achieve this manipulation in a single system by utilizing a novel microfluidic technology—temperature-gradient focusing—an equilibrium-gradient version of capillary electrophoresis that allows for the stationary fractionation and an approximate 10,000-fold increase in concentration of target analytes based on bulk electrophoretic mobility.

Beginning with the manually controlled, proof-of-principle temperature-gradient focusing system, we will develop a more robust system to concentrate and separate different virus strains as a final preparation for detection, and will demonstrate the capability to dramatically enhance

the efficiency of processes for in vitro transcription and translation protein expression through protein purification and separation. Expected results include a demonstrated improvement of our system separation resolution using different capture chip designs for fluorescent dyes, e-tags, and proteins. Successful demonstration of these capabilities will also establish the system's utility for other biological applications.

Mission Relevance

The project will contribute to the Laboratory's national security and homeland security missions in biodefense by demonstrating the ability to pre-concentrate viruses for fast detection and identification, as well as the ability to enhance production speed and efficiency of synthetic reagents for the detection of threat toxins, bacteria, and viruses. Both applications support efforts that enhance the rapid detection of engineered or naturally emerging viruses, bacteria, or other toxins.

FY08 Accomplishments and Results

In FY08 we (1) developed a new thermal-fluidic system that reproducibly controls fluid flow, temperature gradients, and electric fields while allowing fluorescent optical access and adjustable temperature-gradient length in microfabricated glass chips; (2) successfully demonstrated, with this system, the capture and concentration of a small fluorescent dye molecule; (3) developed a three-dimensional numerical model that captures the relevant physics during the electrokinetic focusing process; and (4) solved the relevant field variables (temperature, velocity, and voltage) using finite-element modeling, then solved for the analyte concentration profiles using a Brownian dynamics simulation. These numerical results showed good agreement with experimental data.

Proposed Work for FY09

In FY09 we will perform biological tests with the automated scanning mode of the temperature-gradient focusing system we developed. The main experiments will be (1) viral concentration and separation using fluorescently labeled viruses spiked into clinical samples (nasopharyngeal swab and wash), (2) protein concentration and separation using in vitro transcription and translation samples, (3) demonstration of high-throughput and resolution separations, and (4) numerical simulations to quantitatively determine biological electrophoretic mobility of analytes captured with our temperature-gradient focusing system.

Serrated Light Illumination for Deflection-Encoded Recording (SLIDER)

John E. Heebner   07-ERD-017

Abstract

Fast, high-fidelity, single-shot diagnostics are critical to experiments in high-energy-density 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 (1–100 ps) in which a strong technology base does not exist. Our technique avoids the fidelity–resolution tradeoff by implementing a novel ultrafast optical deflection technique mated with well-established high-fidelity camera technology. After a proof-of-principle demonstration in FY07, we plan a full characterization along with a study of the feasibility of implementing SLIDER on a fusion-class laser the following year.

If successful, we will demonstrate an all-optical streak camera capable of picosecond temporal resolution with a dynamic range in excess of 8 bits and eventually scalable to much higher values. We place particular emphasis on the measurement of fusion burn histories and the characterization of ultrashort petawatt, advanced radiographic capability pulses with heretofore unrealized dynamic range. This work leverages the Laboratory'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 high-energy-density physics. Fundamental questions in weapons design and high-energy-density 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.

FY08 Accomplishments and Results

In FY08, we conducted a detailed characterization of SLIDER temporal resolution. Specifically, we (1) identified and mitigated key limitations to resolvable spot size using a refined device and setup, (2) validated a detailed model with experimental data and used it to optimize design parameters aimed at minimizing plasma absorption prior to next-round fabrication, and (3) established a design concept for an integrated transient x-ray recording system mating SLIDER with an x-ray–optical encoder for use in experimentation at the National Ignition Facility. We filed a patent based on the underlying concept.

Proposed Work for FY09

For FY09, we will continue to address the technological prerequisites for constructing a fielded instrument mating SLIDER with an x-ray–optical converter for recording x-ray transients. Specifically, we intend to (1) drive the resolution and dynamic range to reach targeted goals, (2) remap and extend the record length to an appropriate regime better targeting fusion burn history requirements, and (3) develop a back-end diagnostic for recording the x-ray-imprinted optical signals.

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.

Ultraviolet–Visible Resonance Raman Studies of High Explosives, Impurities, and Degradation Products for Enhanced Standoff Detection

Jerry C. Carter   **07-ERD-041**

Abstract

Improvised explosive devices 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 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 detection of improvised explosive devices. 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 timescales 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 improvised explosive devices 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.

FY08 Accomplishments and Results

In FY08 we (1) examined additional HE materials, including their normal and resonance Raman spectral signatures and resonance Raman enhancements; (2) completed TNT degradation studies as a function of laser power density; (3) completed standoff (normal) Raman measurements of select HE materials; and (4) modeled the total Raman signal for standoff sampling applications for highly absorbing molecules with varying-resonance Raman enhancements.

Proposed Work for FY09

In FY09, we will (1) conduct multiple-wavelength resonance Raman measurements and compare the results with optimal conditions, spectral differences, sensitivity, selectivity, and response time; (2) compare and contrast the sensitivity of imaging versus non-imaging approaches for HE detection, which represents a potential paradigm shift in standoff detection methodologies; (3) characterize the fluorescence and absorption properties of degraded HE materials at different irradiances utilizing Raman, fluorescence, and mass spectrometry; and (4) evaluate resonance Raman measurements in terms of laser power, pulse width, and raster scan rate and determine signal-to-noise ratios and detection limits.

Salicylic Acid Derivatives: A New Class of Scintillators for High-Energy Neutron Detection

Natalia P. 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 using organic scintillators. However, single-crystal stilbene, the most effective pulse-shape discrimination 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. The candidates most suited to high-energy neutron detection will be selected for growth of large crystals.

Our main deliverable will be identification and development of new, efficient, readily available, 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, efficient scintillator materials for the detection and monitoring of fissile materials, this project supports LLNL's national security and homeland security missions.

FY08 Accomplishments and Results

In FY08 we concentrated on growing new crystal materials based on scintillation efficiency. More than 100 organic compounds were grown to a centimeter-scale size and characterized for neutron–gamma pulse-shape discrimination. The results showed that in crystals larger than 1 mm, neutron–gamma separation does not depend on crystal sizes but instead is substantially influenced by impurities. About 12 new materials with a pulse-shape discrimination greater than stilbene have been identified. The highest pulse-shape discrimination found was in polyphenyl organic compounds, while condensed phenyl-ring organics showed lower levels—and one phenyl-ring material exhibited low or no pulse-shape discrimination at all. These results will be used for more detailed studies of mechanisms in organic materials in FY09.

Proposed Work for FY09

In FY09 we will focus on studies of the fundamental mechanisms of pulse-shape discrimination in organic materials. Specifically we will (1) grow and characterize 50 to 60 additional compounds; (2) conduct studies relating to the nature of particular materials such as molecular and crystallographic structure, the packing of phenyl rings, and hydrogen content; (3) identify the main factors influencing pulse-shape discrimination in organic compounds; and (4) create a database of scintillation, pulse-shape discrimination, and other physical properties of new organic crystals, which will further development of new theoretical models of pulse-shape discrimination processes in organic scintillators and selection of the best high-energy neutron-detector materials.

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.

Broadband Heterodyne Infrared Spectrometer: A Path to Quantum Noise-Limited Performance

Joseph W. 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. Our approach is unique in that a broadband source will be used in such a way that hundreds of individual spectral channels will simultaneously record a high-resolution infrared spectrum. This approach can potentially achieve quantum noise-limited performance with a room-temperature infrared spectrometer. Previously, requirements for cooling the spectrometer and detector limited the size, weight, and power—a significant impediment to implementation in a number of applications. Room-temperature operation has been a long-sought goal to minimize size, weight, and power, and this approach is the only one identified as 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 fabricated a breadboard-sized demonstration unit, established performance models and measures, and designed and characterized a compact field unit.

Mission Relevance

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

FY08 Accomplishments and Results

In FY08 we developed tools to model heterodyne spectrometer performance, and we used these tools to calculate signal and noise levels under uncooled operational conditions. We found that the very low impedance levels in the detection circuit necessary for high-frequency operation required a novel concept for a nanostructured radiofrequency-current amplifier. Our focus therefore shifted from the previously proposed spectrometer fabrication to pursuit of this cutting-edge detection concept. We successfully assembled key components of the amplifier at LLNL and used our model results to design a new detector system that is being fabricated by our partner at the Jet Propulsion Laboratory of the National Aeronautics and Space Administration. In addition, we researched detector material band structures as part of the detector system design effort.

Proposed Work for FY09

For FY09, we propose to develop a novel optical detection architecture based on our first-year modeling effort. We will also implement an experimental test bed that will establish feasibility of our room-temperature heterodyne infrared spectrometer.

Tracing the Shadows of Planetary Systems

Bruce A. Macintosh   08-ERD-043

Abstract

The study of other solar systems is driven by the intersection of advanced optical technology and fundamental unanswered questions such as how do solar systems form 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 in other solar systems. 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 the evolution of the system and its planets. We will develop an advanced AO controller that greatly extends the capabilities of the Gemini Planet Imager now under construction, automatically identifies moving turbulent wind layers, and pre-corrects 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 nonastronomical slant-path 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

Adaptive optics is a key competency at Lawrence Livermore for 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.

FY08 Accomplishments and Results

In FY08, we used the Keck, Gemini, and Hubble telescopes to study young dusty stars in the solar neighborhood. This led to an extremely exciting result—the direct imaging of an entire multiple-planet extrasolar system consisting of three massive planets orbiting a young massive star. This was the first such image ever taken and a tremendous milestone in the study of extrasolar systems, and was featured on the cover of the prestigious journal *Science*. We also began designing a polarimetric mode for Keck, used AO test data from Gemini and Keck to verify that our algorithm can automatically measure wind speeds of multiple independent atmospheric layers, and presented the results of our Gemini Planet Imager simulations to the American Astronomical Society, which also published the results in the *Astrophysical Journal*.

Proposed Work for FY09

In FY09 we will (1) match our Keck and Hubble data on circumstellar dust disks against radiative-transfer Monte Carlo scattering models, (2) design a plan for a large-scale 200-night exoplanet survey at the Gemini Observatory, (3) install a polarimeter on the Keck AO system and begin observations, (4) implement and test predictive control on the existing AO testbed, (5) use astronomical AO data to refine the predictive controller and study performance, (6) obtain spatially filtered measurements of fine-structure atmosphere from the Palomar well-corrected subaperture (and possibly the Lick Observatory's new microelectromechanical systems–based Visible Light Laser Guidestar Experiments system), and (7) evaluate if any existing AO system would allow the on-sky closed-loop testing of our predictive control capabilities.

Publications

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de Pater, I., M. Showalter, and B. Macintosh, 2008. "Keck observations of the 2002–2003 Jovian ring plane crossing." *Icarus* **195**, 348. UCRL-JRNL-237040.

Evans, J., et al., 2008. "Contrast analysis and stability on the ExAO testbed." *Proc. SPIE* **7015**, 7015K. UCRL-PROC-404640.

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Zuckerman, B., et al., 2008. "Gas and dust associated with the strange isolated star BP Piscium." *Astrophys. J.* **683**, 1085. UCRL-PROC-359554.

Point-of-Care Diagnostic for Foot-and-Mouth Disease Virus

Benjamin J. Hindson   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. In addition, we will produce 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. We also expect to produce peer-reviewed journal articles that will generate international recognition for LLNL.

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, cutting-edge scientific field.

FY08 Accomplishments and Results

In FY08, we (1) performed an isothermal assay with internal controls for detecting the bacteria *Staphylococcus aureus*, (2) tested lyophilizing reagents and successfully separated betaine from the master mix formulation; (3) devised a visible detection system based on a polychlorinated biphenyl board-mounted photodiode, which registers emission from a blue LED responsible for exciting a dye that intercalates DNA—as DNA amplifies, the dye intercalates the increasing amount of DNA and the signal intensity increases; and (4) obtained data from various picogreen dye concentrations in *S. aureus* sample mixtures.

Proposed Work for FY09
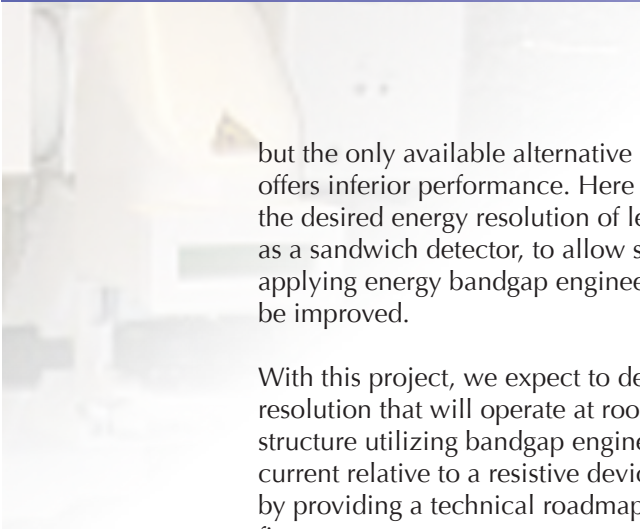
In FY09, we will (1) build a beta prototype that includes lateral flow detection and refinements based on lessons learned from the alpha prototype developed in FY08, (2) field-test and evaluate the device, (3) generate validation data on the beta prototype using real-world samples from the FMD World Reference Laboratory, and (4) begin to pursue commercialization of the alpha and beta prototype modules.

Cadmium–Zinc–Telluride Sandwich Detectors for Gamma Radiation

Rebecca J. 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 develop 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.

FY08 Accomplishments and Results

In FY08, we (1) determined the relationship between resolution, dark current, and Schottky barriers; (2) prepared amorphous material films, including electron beam-evaporated germanium and chemical vapor-deposited hydrogenated silicon; (3) characterized the films using current-voltage methods for resistivity, Rutherford backscattering for hydrogen content (for hydrogenated silicon), and substrate curvature measurements for stress evaluation; (4) fabricated prototype low-leakage gamma detectors utilizing an amorphous layer between the metal contact and the cadmium-telluride; and (5) measured an effective resistivity greater than 10^{11} ohm-cm at 100 V in the prototype detectors, demonstrating that this approach is a possible means for improving the energy resolution of CZT gamma detectors.

Proposed Work for FY09

In FY09, we propose to (1) benchmark our models with experimentally obtained data from FY08 and refine our models to account for any discrepancy, (2) design and fabricate CZT detectors with amorphous layers and carry out both electrical and radiation characterization, (3) use these structures to characterize the interface and energy barrier between the amorphous material and single-crystalline CZT, and (4) demonstrate an effective resistivity greater than 10^{11} ohm-cm at 200 V in our prototype detectors, providing a more stringent test of this approach for improving energy resolution.

Hybridization, Regeneration, and Selective Release on DNA Microarrays

N. Reginald Beer   **08-ERD-064**

Abstract

Use of DNA 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 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 hours) 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) the chemical and physical changes that occur during the processes of in vitro DNA hybridization; (2) the stabilities of different chemical couplings between DNA molecules and surfaces; (3) the controlling mechanisms between DNA in solution and DNA affixed to a solid support in hybridization experiments; (4) the influence of optical, thermal, and fluidic effects on the intrinsic binding or stringency for DNA targets on probes; and (5) the analysis of individual spots to eliminate the complex background signal.

Mission Relevance

This work supports the national security mission in 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 counterterrorism and force protection efforts.

FY08 Accomplishments and Results

In FY08, we (1) initiated development of a real-time image-processing system, (2) developed and tested a flow cell integrated with the imaging system, (3) identified the type of optical system that offers optimal transmission and absorption for selective release and designed the optical system and the chip registration for single-spot resolution, (4) developed and tested a carbon dioxide laser system, and (5) determined that absorption-temperature experiments have proven the ability to deposit energy in aqueous droplets with negligible thermal blooming.

Proposed Work for FY09

We will (1) develop an optical selective release, elution, and capture method for isolating and recovering oligonucleotides from the microarray surface; (2) conduct flow-cell experiments with chemical and thermal control and real-time hybridization imaging, varying probe and analyte concentrations, temperature and fluid-flow profiles, and fluorescence imaging; (3) develop analytical and finite-volume models of advection, diffusion, and reaction and correlate these models with experimental results; and (4) experimentally compare silate and phosphonate glass-coupling stability.

Modeling of Threats to U.S. Intelligence, Surveillance, and Reconnaissance Capabilities

Scot S. Olivier   08-FS-004

Abstract

The objective of this study is to determine the feasibility of implementing accurate, comprehensive computer models of the threats to space assets that are part of the national intelligence, surveillance, and reconnaissance (ISR) infrastructure. These models could be used to help design and evaluate strategies for combating threats. To assess model efficacy, we will develop conceptual designs based on our understanding of the underlying physics and technology of the threats. We will evaluate computational requirements, with the goal of demonstrating the feasibility of accurately simulating a broad range of threats to ISR space assets using realistic, modern computational capabilities.

The results of this work will include: (1) conceptual designs for computer models of threats to ISR space assets, (2) an evaluation of the necessary computational requirements, and (3) a determination of the possibility of implementing these models using modern computational capabilities. The design concepts will be based on our detailed understanding of the physics and technology underlying the threats to ISR space assets. Evaluation of the computational requirements will include considerations of the statistical analyses needed to evaluate the range of scenarios for certain classes of threats. Demonstrating model feasibility is a necessary first step in improving our ability to effectively counter threats to ISR capabilities.

Mission Relevance

This work leverages unique LLNL technical expertise in space science, cyber technology, multiscale modeling techniques, and supercomputing infrastructure in direct support of the Livermore mission in advanced defense capabilities. This work will develop key analytic modeling capabilities necessary to help meet current and emerging national security and defense needs for protecting the country's ISR capabilities.

FY08 Accomplishments and Results

In FY08 we successfully achieved the study's objectives. Specifically, we (1) developed a conceptual design for a computer modeling framework appropriate for encompassing simulations of threats to the country's ISR space assets, (2) assessed the computational requirements for using this modeling framework for specific scenarios, (3) determined the feasibility of implementing these simulations using modern computational capabilities, (4) developed a set of requirements for the computer models, (5) reviewed the current modeling tools within the defense and intelligence communities, and (6) assessed the possibilities for incorporating existing tools into our design concepts. We anticipate that substantial portions of this conceptual design work will be implemented in a follow-on project under Livermore's Strategic Mission Support, as well as work-for-others projects.

Publications

Olivier, S. S., 2008. *A simulation and modeling framework for space situational awareness.* 2008 Advanced Maui Optical and Space Surveillance Technologies Conf., Wailea, HI, Sept. 16–19, 2008. LLNL-CONF-407013.

A Micro-Optical-Mechanical Photoacoustic Spectrometer
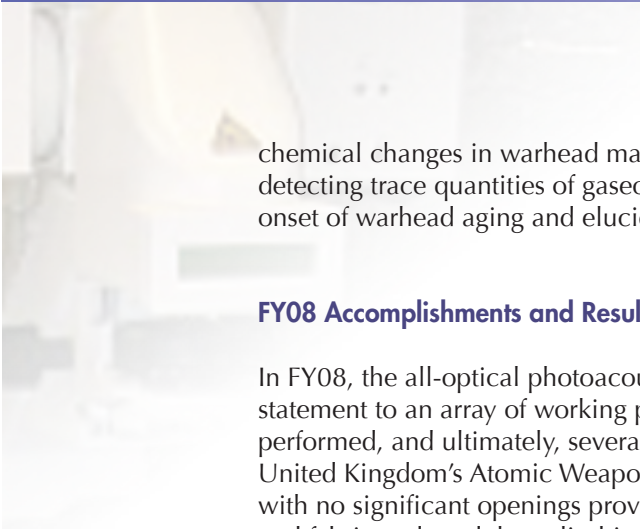
Jack Kotovsky   08-FS-010

Abstract

We will investigate the basic feasibility of a photoacoustic spectroscopy sensor for multispecies detection. State-of-the-art photoacoustic spectroscopy systems are based on electrical transducers and are tuned for single species. A multispecie, all-optical detection system would have multiple applications for advanced fusion-class lasers, explosives detection, and energetic materials research. In addition, the sensor addresses weapons program needs by enabling monitoring of chemical changes in an aging warhead as well as changes in polymeric and energetic materials as evidenced by the evolution or consumption of gaseous species. We intend to explore the feasibility of (1) an all-optical device for energetic environments, (2) a multispecie device for broad gas detection, and (3) a microscale device for deployment in confined spaces. The proposed effort would allow a reduction in size of the detection system from that of a shoebox to that of a pea, necessary for a variety of applications.

Mission Relevance

This work explores the generation of new photoacoustic techniques for multispecie detection in support of the Stockpile Stewardship Program. Specifically, the work allows LLNL to employ its unique microfabrication capabilities to develop technologies for monitoring physical and

chemical changes in warhead materials as they age. Establishing the feasibility of reliably detecting trace quantities of gaseous species indicative of chemical changes can help signal the onset of warhead aging and elucidate the mechanisms and kinetics of aging processes.

FY08 Accomplishments and Results

In FY08, the all-optical photoacoustic spectroscopy sensor system evolved from a problem statement to an array of working prototypes. The system was conceived, preliminary studies performed, and ultimately, several prototypes were built. Modeling work performed by the United Kingdom's Atomic Weapons Establishment suggests a cylindrical acoustic chamber with no significant openings provides excellent pressure response. Therefore, we designed and fabricated modular cylindrical prototypes to allow system characterization under varied chamber dimensions. Several chamber lengths and diameters were created, and a circular diaphragm detector was created that includes a multilayer material stack for stress tuning. Optical measurements show that we achieved an excellent optical return. Finally, the power and sensing systems were designed to be insensitive to position variation. The successful conclusion of this project demonstrated that a miniature photoacoustic spectrometer is possible that makes use of a micro-optical-mechanical detector, and numerous prototypes were fabricated, exceeding our original goals for the project. Our prototypes are currently in testing at the Atomic Weapons Establishment as part of an enhanced collaboration.

Laboratory Directed Research and Development

Biological Sciences

Characterizing Hypothetical Proteins

Michael P. Thelen   05-ERD-064

Abstract

Nearly half the proteins inferred from microbial genome sequences are unconfirmed and bear little resemblance to known proteins, yet many of these "hypothetical proteins" are important in nature. We propose to establish functions for a significant fraction of hypothetical proteins from an uncultivated microbial community by analyzing protein complexes and the sequences that encode them. We will determine protein distribution in a biofilm community by fractionation and proteome analysis, identify source organisms and genome context, and measure protein abundance. To characterize unknown proteins, we will analyze protein sequences to predict functions, isolate multiprotein complexes, and test predicted functions using parallel biochemical assays.

This research will advance the understanding of how microbes act in their natural environment, particularly the molecular mechanisms of iron oxidation, biofilm formation, and evolution of adaptive mechanisms such as acid tolerance. We will develop new analytical methods, find novel genes, and determine the function of previously unknown proteins, all of which will serve to accelerate environmental research and enhance the scientific basis for LLNL's current focus on a variety of microbes, such as for biosecurity. Important insights into protein function will result from the development of computational modeling tools. Furthermore, this project will establish unique expertise in the emerging area of proteogenomic analysis, and continue to build collaborations with researchers at the University of California at Berkeley.

Mission Relevance

This project supports the Laboratory's national security mission by developing metagenomic and proteomic approaches that can be extended to the discovery and identification of viral backgrounds that would interfere with both protein- and genome-based strategies for detecting engineered viral agents. This project will support LLNL's environmental management mission by developing new approaches to understanding natural microbial systems that influence metal-contaminated environments. It also supports the energy security mission because these microbial systems exacerbate environmental problems caused by mining principle energy sources (e.g., coal and uranium). This will provide an excellent starting point for future work in biosciences and environmental science, including potential support for DOE's Genomics:GTL program.

FY08 Accomplishments and Results

In FY08 we (1) completed the proteomic analysis of several thousand proteins extracted from a natural microbial community, examined their cellular locations, and identified sequence

homologies that imply function for about 75% of these; (2) determined protein interactions for several multiprotein complexes using chromatography and mass spectrometry techniques; (3) achieved direct testing of biochemical functions and interactions for several cases; and (4) completed our high-throughput computational analysis of 620 detected proteins of unknown function, with over 85% of these assigned a protein fold and superfamily. This project resulted in the first proteomic description of a microbial community and new methods for isolating, identifying, and predicting function for hundreds to thousands of proteins from a natural environmental setting. Further research in this area will be supported by the DOE's Genomics:GTL program to develop a comprehensive understanding of the interactions and functions of individual microbial species within complex communities.

Publications

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Wilmes, P., et al., 2008. "Natural acidophilic biofilm communities reflect distinct organismal and functional organization." *ISME J.* advance online publication, Oct. 9, 2008. LLNL-JRNL-409226.

Developing and Integrating Novel Technologies for the Production and Characterization of Membrane Proteins

Paul D. 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 and demonstrate unambiguous formation of membrane protein–NLP constructs.

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, human health research, bioenergy research, and environmental biology.

Mission Relevance

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

FY08 Accomplishments and Results

In FY08 we (1) made cell-free preparations of NLPs with several membrane proteins—including G-protein–coupled receptors, *Yersinia pestis* membrane proteins, and functional hydrogenase from *Pyrococcus furiosus*; (2) synthesized a helical portion of semisynthetic apolipoprotein apoE422K; (3) prepared NLPs containing nickel-chelated lipids, conjugated a tagged envelope protein from the West Nile virus, and immunized mice with the nickel–NLP–envelope protein construct, demonstrating significant protection (>70% chance of survival) against a live viral challenge; and (4) made a new NLP construct for a vaccine containing monophosphorylated lipid A, a known potent vaccine adjuvant.

Proposed Work for FY09

We will continue our efforts in cell-free protein synthesis for the preparation of NLP constructs of target membrane proteins such as the YopB, YopD, H5, GPR109B, and GABA receptors. In addition, we will develop NLP-based vaccine countermeasures.

Publications

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Development of Single-Cell Raman Spectroscopy for Cancer Screening and Therapy Monitoring

James W. Chan   06-ERD-051

Abstract

Current methods for cancer prognosis and monitoring patient response to therapy are nonspecific and invasive, making the development of better methods for early detection of cancer and its recurrence vital for improved survival rates. Our objective is to develop new techniques for early cancer detection and therapy monitoring using single-cell Raman spectroscopy. We hope to identify new Raman markers associated with cancer cells, cancer stem cells, drug-resistant cancer cells, and cancer cell response to treatment conditions (e.g., chemotherapy and radiation) that can be used to improve detection and therapy response. To understand the biology of these markers, we will acquire data on different leukemia cell types from clinical samples, apply algorithms for analysis, and correlate results to clinical parameters.

We expect to (1) develop laser-tweezers Raman spectroscopy to characterize unique spectral markers of single, living cancer cells; (2) acquire spectral markers associated with dynamic cell response to chemotherapy and radiation treatment; (3) determine this technique's accuracy and sensitivity; (4) achieve a fundamental understanding of the biological relevance of these spectral markers; and (5) develop an optical trapping, nonlinear coherent anti-Stokes Raman spectroscopy method that should significantly speed up single-cell analysis. The cancer signatures and their dynamic changes to stimuli, as well as the data algorithms and Raman technology developed, will lead to a novel clinical tool that will replace or complement existing technology to improve early detection and diagnosis.

Mission Relevance

This project supports the Laboratory's mission in bioscience to improve human health. By developing multiplexed assays and Raman-based optical techniques for cancer diagnostic applications, this project will enable more cost-effective, highly specific, early disease-detection technology and biomedical instrumentation. In addition, success in this work can impact homeland and national security by defining an approach to analyzing cell biochemistry that could result in high-throughput screening methods for identification of an exposed population following a biological event.

FY08 Accomplishments and Results

In FY08, we studied whether Raman spectroscopy can identify unique spectral markers for assessing cell response to chemical and radiation treatment. Specifically, we (1) exposed cells to radiation levels from 0 to 1 Gy and found that changes associated with DNA and protein modification could be observed; (2) exposed cells to doxorubicin, identifying unique spectra reflecting apoptosis and observing markers of drug concentrations within cells; (3) characterized the unique spectra of cancer stem cells and determined that cell fixation impairs the Raman identification of cancer cells; and (4) developed a prototype compact, bench-top microfluidic based Raman system. This project demonstrated that Raman spectroscopy can be a powerful clinical method for single-cell cancer diagnosis and therapy monitoring, providing unique capabilities not available from existing clinical methods such as flow cytometry. Multiple government agencies—including the National Institutes of Health and the Department of Defense—and various foundations supporting leukemia research have expressed interest in building on the foundations of this effort to study the biological relevance of these Raman markers and create a clinical Raman benchtop system.

Publications

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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 (also known as rabbit fever) in humans—highlights a need for continued research efforts to understand the interactions of this organism with host immune defenses. Very little is known about how this 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. Our goals are to uncover global host–response patterns that may be used for early detection of exposure to this potential biowarfare pathogen and to understand how *F. tularensis* evades innate immune defenses to cause disease. Proposed work will build on extensive genomic and virulence expertise at Lawrence Livermore.

If successful, this project will identify the 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. 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 security and homeland security missions in the area of biodefense.

FY08 Accomplishments and Results

In FY08 we analyzed ten fully virulent *F. tularensis* isolates during amoeba infections, conducting extensive electromagnetic analyses of the infected amoeba and determining that the bacteria survive inside vacuoles in amoeba cysts. We also identified two previously uncharacterized bacterial proteins that appear to play a role in both environmental persistence and pathogenesis.

Proposed Work for FY09

In FY09 we will define the interaction of the proteins identified in FY08 with host phagocytic cells by (1) purifying the bacterial proteins and then assessing their effects on human and mouse cells using protein cytokine arrays as a readout for host-cell activation, (2) generating antibodies

directed against these two proteins for use in host-cell trafficking studies, and (3) finalizing host microarray data including unique, fully virulent isolates obtained in collaboration with Brigham Young University.

Publications

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

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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 impacted 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 general principles of how individual microorganisms and communities of microorganisms manage both internal and external stochastic variations to avoid the multitude of 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 new, network-based antimicrobial approaches.

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.

FY08 Accomplishments and Results

We (1) completed the stochastic analysis of two small gene circuits (an autoregulatory and a two-gene toggle switch) and analyzed four extended gene circuits, (2) made progress on dynamic flux balance analysis and developed another flux balance method to combine messenger RNA (mRNA) with metabolic models, (3) added the production of virulence factors to our model and began expanding the level of detail, (4) finished validating the genome-level metabolic models using available mRNA and proteomics data and developed a new method to identify cryptic genes and pseudogenes, (5) completed three different genome-level *Y. pestis* biovar models and one model for *Y. pseudotuberculosis* and performed comparative analysis, and (6) completed robustness analysis of the models.

Proposed Work for FY09

In FY09, we propose to (1) complete testing and development of our dynamic flux balance approach; (2) analyze noise propagation and robustness in currently available whole-cell metabolic models and *Yersiniae* metabolic models; (3) perform evolutionary analysis of the transition of *Y. pseudotuberculosis* to *Y. pestis* and combine whole-cell metabolic models for *Y. pestis* with the regulatory module of the master regulator protein CsrA, which is involved in secondary metabolism, quorum sensing, and virulence; (4) complete analysis of metabolic robustness properties and identify potential network-based antimicrobial strategies; and (5) analyze experimental results to validate our lethality predictions.

Publications

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Development of Novel Antimicrobial Proteins and Peptides Based on Bacteriophage Endolysins

Paul J. 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 and segments of these genes 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 hope to produce antimicrobial proteins or peptides that can rapidly lyse (burst) *Bacillus anthracis*, which causes anthrax, and related pathogenic bacilli. In addition, we will produce antimicrobial proteins or peptides that can rapidly lyse *Yersinia* species, including *Y. pestis*, which causes plague. We also 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 security and homeland security missions.

FY08 Accomplishments and Results

In FY08 we identified new, more stable, efficient endolysins and measured their enzymatic properties, physiological range, and host range. Specifically, we (1) conducted endolysin N- and C-terminal fragment analyses, which revealed that the majority of the protein is required for activity; (2) identified a very diverse set of new endolysin genes in phage and prophage genomes; (3) characterized the endolysins rapidly using our flow cytometry–based assay; (4) performed computer alignment of multiple endolysin sequences and identified lytic and target recognition sequences, verifying that endolysins work in a two-step process of cell recognition followed by lysis; (5) tested four endolysins against *B. anthracis* and related microbes, finding endolysin Bczk2532 to be especially stable and potent; and (6) synthesized and began purifying four additional endolysins that attack *Y. pestis*.

Proposed Work for FY09

In FY09, we propose to (1) continue in vitro protein synthesis to produce each endolysin or endolysin fragment and test their specific activity, stability, and enzymatic characteristics; (2) continue to target specific portions of endolysin proteins based on computational studies to identify the minimum sequences required for lytic and cognitive functions, which will, in turn, generate additional gene constructs encoding pertinent portions of these proteins; (3) measure function and properties of peptides to determine their specificity and impact on bacterial targets; and (4) continue analysis of bacterial genome-sequence databases to identify phage and prophage endolysins that can be added to this study.

Development of Novel Transgenic Technologies to Study Genome Regulation and Architecture

Gabriela G. Loots   07-ERD-046

Abstract

We propose to develop novel transgenic technologies to identify and characterize the biological function of non-coding 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*. Transposon-mediated transgenesis in frogs enables foreign DNA to be 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 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 LLNL's mission in biotechnology 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 Laboratory outreach and recruitment through its potential to attract top-notch university collaborators, students, and postdoctoral researchers to the Laboratory.

FY08 Accomplishments and Results

We have (1) developed an in vivo transgenic method that utilizes a universal reporter based on the transposable element Tol2 and the Katushka red fluorescent protein; (2) evaluated its efficiency using a kidney enhancer as a positive control; (3) examined the function of 20 candidate enhancer elements—10 putative liver and 10 putative muscle enhancers; (4) determined loxP site pairs that promote in vivo integration in vitro, and built constructs to examine their function in vivo; and (5) generated transgenic tadpoles that we will raise to maturity to examine germ-line transmission—they will be genotyped to determine rate of transgenesis and mated to wild frogs to determine the rate of germ-line transmission.

Proposed Work for FY09

We will (1) continue to examine position effects and germ-line transmission in newly generated loxP and insulator transgenic lines, (2) optimize loxP-mediated transgenic in vivo integration in frogs, (3) use homologous recombination to engineer a bacterial artificial chromosome by inserting Katushka as a reporter into the transposable element Tol2, (4) test this method in transgenic frogs to determine if position effects are eliminated and different alleles of the same bacterial artificial chromosome can be analyzed for impact on Katushka expression, and (5) use microarray expression data in collaboration with the National Center for Biotechnology Information to generate ten predictions of tissue-specific enhancers and analyze their function in vivo in transgenic frogs.

Microarrays and NanoSIMS: Linking Microbial Identity and Function

Jennifer Pett-Ridge   07-ERD-053

Abstract

This project will develop a next-generation microarray for the 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 degrade contaminants.

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 be used to define the 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 the development of biofuels, fuel cell bioreactors, and secure energy sources; and supports the environmental management mission by furthering the remediation of contaminated sites and enabling modeling of microbial roles in carbon sequestration and global climate change.

FY08 Accomplishments and Results

We (1) completed our new alkyl phosphonate–indium tin oxide array and filed a record of invention; (2) used the array to hybridize with DNA and RNA, then measured minus-ten-times background intensity and plus-ten-times signal-to-noise ratios relative to traditional arrays and found that our new arrays may be repeatedly hybridized and stripped, allowing reuse and reduced costs; (3) made significant progress on NanoSIMS combined with stable isotope probing; (4) calibrated hybridization protocols for carbon-13 RNA from bacteria and improved RNA extraction and biotin end-labeling protocols; and (5) combined in situ phylogenetic and metabolic labeling to create a new technique—enhanced element labeling–catalyzed reporter deposition fluorescence in situ hybridization (EL-FISH)—and tested oral biofilms with the EL-FISH method, which will be featured on the cover of each issue of the 2009 volume of the *International Society for Microbial Ecology Journal*.

Proposed Work for FY09

In FY09, we will (1) move beyond pilot study tests and begin to analyze complex community rRNA–RNA hybrids to reduce the quantity of RNA necessary for identification; (2) continue our focus on rRNA extracts from the DOE Hanford site, where carbon-13 lactate has been added to contaminated soil to stimulate chromium reduction; (3) use NanoSIMS to resolve carbon-12 rRNA from carbon-13 rRNA probe spots and identify which organisms co-metabolized carbon-13 lactate; and (4) employ our new EL-FISH approach for linking phylogeny and metabolism in biofilms—specifically, human oral TM7 bacteria (associated with periodontal disease) labeled with nitrogen-15–labeled amino acids and carbon-13 oligosaccharides, and biofilms from medical implant devices.

Publications

Behrens, S., et al., 2008. "Linking microbial phylogeny to metabolic activity at the single-cell level by using enhanced element labeling-catalyzed reporter deposition fluorescence in situ hybridization (EL-FISH) and NanoSIMS (nano secondary ion mass spectrometry)." *Appl. Environ. Microb.* **74**, 3143. LLNL-JRNL-407918.

Pett-Ridge, J., et al., 2008. "Profiling microbial identity and activity: Novel applications of NanoSIMS and high-density microarrays." *Proc. Am. Soc. Microbiology 108th General Mtg.* LLNL-POST-403719.

Identification of Pathways Critical to Quorum Sensing and Virulence Induction

Ted Ognibene   07-ERI-001

Abstract

Therapeutic compounds that interfere with quorum sensing in pathogens should either increase the window of opportunity for more traditional antibiotic intervention or attenuate

the pathogen such that the host immune system can clear the infection. We propose to utilize carbon-14 accelerator mass spectrometry to quantitate autoinducer molecules (homoserine lactones) derived from the in vivo carbon-14 labeling of S-adenosylmethionine in *Yersinia pestis* and *Vibrio harveyi* to identify pathways critical to quorum sensing and to ascertain the role that quorum sensing may play in virulence induction. This will establish a platform in which the efficacy of novel therapeutics can be assessed.

We will demonstrate the effectiveness of using isotope labeling and quantitation by accelerator mass spectrometry to study biochemical pathways. We will also use mass spectrometry, along with gene-knockout studies of *Y. pestis*, to identify pathways critical to quorum sensing. The success of this project will lay the groundwork for metabolite analysis of pathogens based on accelerator mass spectrometry, which has several potential biodefense applications.

Mission Relevance

This project supports the Laboratory's national and homeland security missions by creating a capability to quantitate autoinducers in potential biowarfare agents. Autoinducer quantitation will help identify the pathways critical to quorum sensing and pathogen viability and could assist in identification of novel therapeutic targets for proteins associated with those pathways, as well as the assessment of therapeutic efficacy.

FY08 Accomplishments and Results

In FY08, we studied how to quantitate the small homoserine lactone molecules selected for this study, with a focus on completing the requisite step of characterizing the gas-accepting ion source connected to the mass spectrometry system. We constructed instrumentation to handle and transport nanomole-to-micromole quantities of carbon dioxide and injected known amounts of carbon dioxide gas, then measured the ion source response. We achieved excellent ion source efficiencies ranging from 0.2 to 10%—depending on the quantity of gas injected— and extremely rapid ion source response and fast rise times (<0.5 s). This project furthered the development of a directly coupled accelerator mass spectrometry and high-performance liquid chromatography interface to provide high-throughput analysis of small quantities of biochemicals. The National Institutes of Health is pursuing the next-stage development of this interface technology.

Quantification of Radiation-Induced Protein Expression

Matthew A. Coleman   07-LW-043

Abstract

This project will provide a new research tool, based on accelerator mass spectrometry (AMS), for the quantitative analysis of protein expression induced by ionizing radiation. Living

systems have evolved mechanisms to detect and repair damage using special repair enzymes. The biological response to low-dose ionizing radiation is difficult to quantify. Many ionizing radiation–induced genes have been identified, but messenger RNA (mRNA) expression correlates poorly with protein levels. Response to radiation is therefore better quantified by protein expression, rather than the direct damage to genomic DNA or the mRNA expression. The high sensitivity of AMS—combined with the specificity of antibodies against targeted, putative radiation–induced proteins—will enable quantitation of protein expression after radiation exposure.

First, we expect to demonstrate the quantitative ability of the affinity capture of proteins to selectively isolate expressed proteins that are metabolically isotope-labeled and quantified by AMS. We will subsequently quantify protein expression response to ionizing radiation using human-derived cell lines, pulse-labeling with carbon-14 amino acids, affinity capture of targeted proteins, and AMS as functions of radiation dose and time. Quantified protein expression will be compared with mRNA expression to validate protein biomarkers of radiation. These approaches will be crucial for expanding the sensitivity of measuring proteins within a single cell.

Mission Relevance

By providing a significant new research tool for quantitative protein expression that bridges the gap between large proteomic data sets and the interactions of DNA-damage proteins, this project contributes to the development of better tools and capabilities for the Laboratory's homeland security and national security missions. The sensitivity of this AMS tool will also be applicable to low-dose radiation research and general investigations of proteins and their interactions.

FY08 Accomplishments and Results

In FY08, we developed a protein-expression array for looking at selected proteins produced in response to ionizing radiation in human-derived cell lines. Although the arrays were robust, optimized methods are still needed for quantifying specific proteins using AMS. This is because of high background noise between capture antibodies and the selected substrate matrix. However, this challenge led us to develop a novel schema that does not require the direct labeling of protein samples. In conclusion, this project demonstrated that protein-expression arrays are a viable option for robust identification of protein responses to ionizing radiation in humans. The next step is to adapt this technique for label-free studies.

Publications

Bourguet, F., et al., 2007. "Identification of novel TP53-regulated genes induced by ionizing radiation." *Environ. Mol. Mutagen.* **48**, 7. UCRL-JRNL-236340.

Bourguet, F., et al., 2007. *Low-dose IR pathways associated with chromatin structure.* UCRL-POST-235657.

Stem-Cell Fate Decisions

Amy L. Hiddessen   07-LW-098

Abstract

We seek to understand the biological functions of stem cells to harness their power for tissue regeneration. Currently, internal and external factors that regulate stem-cell fate are poorly understood. We aim to determine the roles and significance of immobilized factors like extracellular matrix and signaling peptides, synergystic and opposing soluble factors and signals, and cell-to-cell communication in stem-cell fate decisions. Cell microarrays will be developed to capture single or clusters of cells onto substrate-bound signals and proteins. Commitment to proliferation and/or differentiation will be assessed using time-lapse microscopy, study of cell surface antibodies versus differentiation markers, and use of cell-division tracking dyes during exposure to immobilized and soluble signals.

We expect to provide a greater understanding of how the cell microenvironment controls fate and signaling, information that can shed light on disease states and the therapeutic potential of stem cells in regenerative medicine. Single-cell data from our research will contribute to development of computational models for predicting cell behavior. Developmental and cancer biology will benefit from insights into the function of stem cells, and we expect our research to be aligned with National Institutes of Health and National Aeronautics and Space Administration interests, as well as with California's three-billion-dollar stem-cell initiative, among others. In addition, this effort will help advance stem-cell research effort at LLNL, attracting top-quality scientists to the Laboratory.

Mission Relevance

This research will support DOE and LLNL missions in biosciences to improve public health by advancing technologies for investigating cell signaling and response as well as medical treatments based on tissue regeneration. This work will apply and build upon technologies and techniques previously developed at LLNL, thus leveraging prior efforts and investments.

FY08 Accomplishments and Results

In FY08, we (1) developed off-array cell phenotyping and sorting assays, a custom signal peptide, and a subcellular reporter; (2) modified the array chemistry because early experiments indicated stronger bio-resistance was required to maintain cells in the array, and used Protein A/G coupling to immobilize custom peptides on the arrays; (3) completed on-array viability tests by conventional methods and tests of baseline cell behavior by immunofluorescence assays that indicate correct cell polarity, localization of junctional proteins, and phenotype; and (4) initiated experiments with peptide arrays. This project has enabled development of custom tools for novel measurements of single mammary stem-cell behavior, which will enable better understanding of dysregulation of fate decisions during breast cancer development.

A New Selectable Marker System for Genetic Studies of Select Agent Pathogens

Patrick S. Chain   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 both basic and applied research on select agent 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.

If successful, this project will constitute the first important step towards developing technologies suitable for the application of standard bacterial genetic manipulations in studying select agent pathogens. Because no methodology for performing such manipulations currently exists, this achievement will advance all select agent pathogen research as well as numerous other fields of research. In addition, we plan to demonstrate the use of this novel technology in manipulating the genomes of two select agents that have been designated as highly important in counterterrorism—*Yersinia pestis* and *Francisella tularensis*, which cause plague and tularemia, respectively. This project will further our understanding of which genes are involved in virulence in the organisms and thereby help identify ideal 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.

FY08 Accomplishments and Results

In FY08, we worked to develop a system for the mutation of select agent pathogens without the use of antibiotic selection. Specifically, we (1) obtained and engineered the toxin–antitoxin system of *Streptococcus* pyogenes pSM19035 to be inducibly expressed with an arabinose and tested it in *Escherichia coli*; (2) devised a strategy to test this system in *Y. pestis*–attenuated mutants excluded from the select agent list; (3) engineered vectors for delivery of the toxin gene to antitoxin-containing bacteria; (4) successfully targeted *Y. pestis* genes for knockout with linear DNA flanked by target sequences with a recombinase enzyme and are assessing this without the use of a recombinase; and (5) successfully tested a plasmid-based red fluorescent protein for use in *Y. pestis* and will ascertain if it can be used in single copy for screening colonies or cells.

Proposed Work for FY09

Our primary goal for FY09 is to successfully introduce the bacterial toxin into a population of bacteria containing the antitoxin to validate that selection takes place. Because we will introduce the toxin via the conjugation method, we will develop strains with the toxin under the control of inducible promoters and engineer the toxin-encoding plasmid (or the *E. coli* donor strain) for downstream elimination. We will also test our validated plasmid containing the toxin to verify that it kills bacteria that do not contain the antitoxin. Once this step is verified, we will be able to selectively delete genes in *Y. pestis*.

The Elegant Molecular Syringe: Characterizing the Injectisome of the *Yersinia pestis* Type III Secretion System

Brett A. Chromy   **08-ERD-020**

Abstract

Currently, the pharmaceutical industry is not actively pursuing the development of antimicrobial compounds from natural products. Reasons include the 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. Therefore, 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.

We propose to examine the type III secretion system of *Yersinia pestis* (the agent that causes plague), which delivers virulence proteins into host cells using a macromolecular protein complex called the injectisome. Specifically, we will (1) develop antibacterial screens based on cell viability and induction of the type III secretion system of *Y. pestis*, which will test the effectiveness of natural products to kill it and other select-agent bacteria, (2) test a large number of natural products and attempt 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 pharmaceutical or biotechnology companies. 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, leading to new screening technologies, and by improving the understanding of the bacterium's key virulence mechanism, the type III secretion system.

FY08 Accomplishments and Results

In FY08, we (1) developed a screen for antimicrobial activity testing of approximately 5,000 crude extracts from marine sponges against bacterial pathogens of biodefense and military interest including *Y. pestis*, *Y. pseudotuberculosis*, *Bacillus anthracis*, *Acinetobacter baumannii*, *Pseudomonas aeruginosa*, and *Francisella tularensis*—we obtained 16 positive results from 9 unique extracts; (2) developed conditions to enhance this screen to test for blocking of the type III secretion system; and (3) developed methods to purify injectisome fractions from *Y. pestis* cells and began separating the protein components using proteomic technologies.

Proposed Work for FY09

In FY09, we propose to (1) utilize our natural product screen developed in FY08 to screen additional compounds obtained from the National Cancer Institute against a larger panel of bacteria, including select-agent microbes; (2) characterize the positive hits from our screen of natural products using high-performance liquid chromatography and mass spectrometry to better understand the secondary metabolite compounds found; (3) use our methods for purifying injectisomes from *Y. pestis* cells to characterize the injectisome proteins using gel-based and liquid chromatography–based proteomic methods; (4) create bacteria containing a fluorescently tagged *Y. pestis* protein; and (5) use stimulated emission depletion microscopy to detect fluorescence within the cells.

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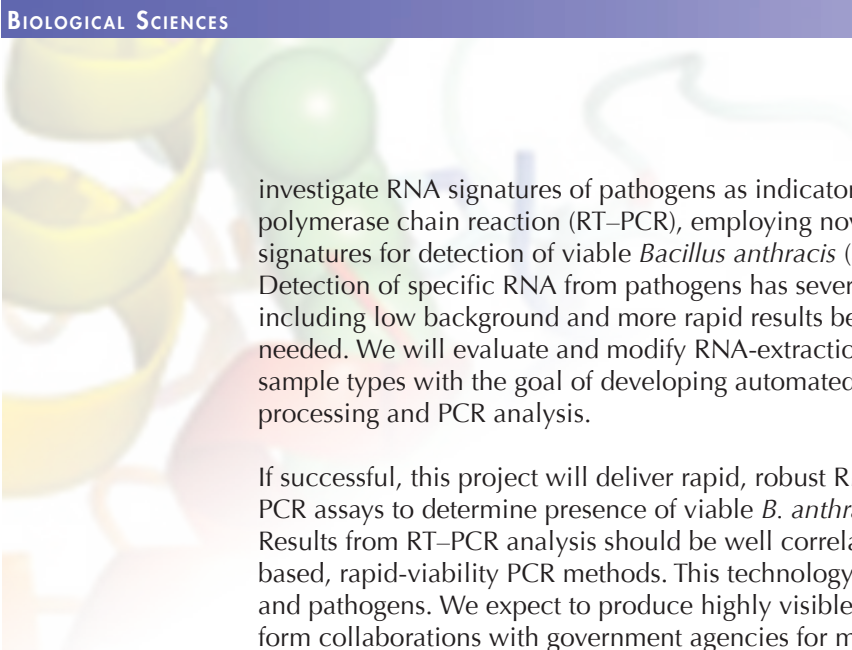
Evans, L., et al., 2008. *Undersea medicine: Screening marine natural products for anti-bacterial properties.* LLNL-POST-406137.

Viability-Based Detection Methods for Pathogens in Complex Environmental Samples

Staci R. Kane   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

investigate RNA signatures of pathogens as indicators of viability using reverse transcriptase–polymerase chain reaction (RT–PCR), employing novel RNA extraction technology, and using 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 highly visible 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 prominent role in next-generation development of 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.

FY08 Accomplishments and Results

We (1) finished generating unique RNA signatures for *B. anthracis* and *Y. pestis*; (2) obtained preliminary RT–PCR results and bioinformatics data on the basis of which we selected eight assays for *Y. pestis* and *B. anthracis* RT–PCR analysis with amplified and unamplified RNA; (3) conducted analysis that showed sensitivity differences with cells from different growth phases or germination times and demonstrated the ability to detect *Y. pestis* cells and *B. anthracis* spores at concentrations of 10^4 to 10^5 cells and 10^6 spores, respectively, per milliliter of unamplified RNA extracts (non-RT controls were negative); (4) continued analysis of amplified RNA, with two different methods being evaluated; (5) evaluated different combined RNA and DNA extraction kits for RNA yield and quality; and (6) developed preliminary protocols for *B. anthracis* spores and *Y. pestis* cells that are compatible with automated nucleic acid extraction and RT–PCR analysis.

Proposed Work for FY09

In FY09, we will (1) investigate RNA extraction from *Y. pestis* on surface samples and aerosol-wet collector samples; (2) optimize extraction protocols to maximize RNA yield and quality; (3) integrate RNA amplification protocols into extraction and analysis protocols and determine detection for both organisms; (4) complete development of RT–PCR protocols for *B. anthracis* using automated sample processing and a high-throughput RNA analysis platform, comparing results from RT–PCR analysis with traditional viability analysis and DNA-based rapid-viability

protocols; and (5) extend RT–PCR integrated protocols for detection of viable *Y. pestis* in surface samples and aerosol-wet collector samples for comparison with traditional viability methods.

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

Richard J. Law   08-ERD-037

Abstract

Biological action involves dynamic proteins that convert between multiple functional states. For example, different states of potassium channels have been implicated in a host of neuromuscular, cardiac, and other diseases. Molecular dynamics based on empirical force fields enables the study of the complex energy landscapes in molecular biology, yet there is a local minima limit for timescales and transition sizes. Normal mode analysis can suggest large conformational changes that are of vital importance to the protein's function, but only in a qualitative fashion. With this project, we propose to create a rigorous new method to use normal mode analysis to remove limits of molecular dynamics simulation. We will use this to quantitatively study, for the first time, the closed potassium channel.

We will design a novel Monte Carlo algorithm, which we call the projected importance-sampling Monte Carlo (PISMC) scheme. We will prove the efficacy of this method by driving a closed potassium channel to an open state. This study will provide illustrative predictions of how biological enzymes, receptors, and transmembrane ion channels alter their conformation to perform their function and will provide the atomic structures of transition and active and open states of these proteins. We expect our results to yield high-profile publications, and our method could be integrated into freely available molecular-dynamics codes, such as the Nanoscale Molecular Dynamics code (NAMD), and provide numerous applications for bioscientists.

Mission Relevance

The use of computer simulation to understand a complex biological process clearly fits the DOE goal of continuing the advancement of U.S. dominance in computations innovation by being able to simulate across multiple length scales. This project represents an important component in the future multiscale computing effort at Lawrence Livermore, and would increase the Laboratory's impact in computational biology and new materials in support of technology to improve human health. In addition, 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.

FY08 Accomplishments and Results

In FY08, we (1) reformulated the PISMC algorithm in terms of molecular dynamics with a bias potential, (2) created a stand-alone code for bias potential molecular dynamics along a single mode, (3) evaluated the NAMD code for augmentation, (4) began to develop the initial NAMD interface code for single-mode bias potential molecular dynamics, and (5) developed

a novel algorithm to extract normal modes of proteins from finite temperature molecular dynamics simulations.

Proposed Work for FY09

For FY09, we will (1) develop the input and output code for our new routines, (2) develop a new interface for the PISMC code, (3) develop code for a stand-alone PISMC routine for multiple modes, (4) apply the force-field interface code CHARMM to our PISMC code, and (5) develop an interface to NAMD to achieve multiple-mode PISMC.

New Molecular Probes and Catalysts for Bioenergy Research

Michael P. Thelen   08-ERD-071

Abstract

Harnessing biological systems for energy requires innovative tools to monitor and catalyze the hydrolysis of plant cellulose, lignin, and other major cell wall polymers. 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—aptamers—that are designed to either detect or hydrolyze key polymers for improving monomer production. This work will provide the basis for the future development and patenting of molecular tools that recognize target molecules sought in bioenergy, medicine, and chemical and biological defense applications.

Aptamers—short, single strands of DNA—that bind specifically to plant cell wall disaccharide and polymer targets will be developed 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 these aptamers will be patented and used in future biofuels efforts at LLNL and in collaborations with both the DOE Joint BioEnergy Institute and with industry. Aptazymes—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 becoming increasingly important 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 the 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.

FY08 Accomplishments and Results

We (1) synthesized end-tagged, randomized-nucleotide 40-monomer aptamers and tested both a single-microbead method and pooled magnetic microbeads for selection of initial binding to cellobiose and cellulose; (2) amplified and sequenced bound aptamers, then predicted secondary structures for functional significance; (3) examined fluorescently labeled candidates in both purified cellulose assays and plant cell walls; and (4) tested the aptamers by circular dichroism before and after the adding of target cellobiose, finding that conformational change occurs upon binding.

Proposed Work for FY09

In FY09 we plan to (1) synthesize further DNA libraries and select aptamers that bind specifically to monomeric glucose, cellotetraose, digalacturonic acid, and pectin (containing glucuronic acid, arabinogalactan, xylan, and other hemicellulosic polymers); (2) sequence selected candidates that bind with high affinity; (3) test aptamers that are specific for glucose, cellobiose, cellotetraose, and digalacturonic acid in biochemical (in vitro) assays for the release of these products after enzymatic hydrolysis of cellulose and pectin; and (4) perform confocal microscopic imaging of plant cell walls using the pectin-specific aptamers.

Publications

Lacayo, C., et al., 2009. *Imaging plant cell wall deconstruction in single cells from* Zinnia elegans. Keystone Symp., The Future of Biofuels, Snowbird, UT, Apr. 4–8, 2009. LLNL-ABS-409171.

Rowe, A., et al., 2008. *Aptamer selection and electrochemical biosensors for small analyte detection.* LLNL-PRES-408294-DRAFT.

Rowe, A., et al., 2008. *Selection of aptamers that bind to saccharides as probes for plant cell wall degradation.* LLNL-POST-407495.

Regulation of *Yersina pestis* Virulence by Autoindicer-2 Mediated Quorum Sensing

Brent W. 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, the most devastating disease in human history, and it is a recognized biothreat agent. Virulence-factor gene expression and AI-2 quorum sensing are correlated in *Y. pestis*. Other pathogens are also believed 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 the AI-2 signaling

pathway(s) 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–to-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. In addition, we expect to create genetic knockouts for the AI-2 signaling pathway and produce synthetic AI-2 to enable expression array experiments. This research will likely result in publications in high-profile peer-reviewed journals.

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 research capabilities and facilities at LLNL.

FY08 Accomplishments and Results

We (1) completed the synthesis of AI-2 and achieved the ability to routinely prepare carbon-14 AI-2, (2) made expression constructs for all of the *Y. pestis* genes known to be involved in AI-2 quorum sensing as well as several that we hypothesize to be involved, (3) carried out small-scale expression testing of all of the cloned genes that were successfully transformed into expression cell lines (6 of 11 genes), (4) conducted preparative scale expression and purification of four genes and purified them to near homogeneity, and (5) continued efforts to generate genetic knockouts, including working to develop new approaches to genetically manipulating *Y. pestis* that comply with new regulations.

Proposed Work for FY09

For FY09, we will (1) use real-time polymerase chain reaction techniques to determine the effects of gene knockouts on the expression of known virulence factors, (2) investigate the number and quantity of AI-2 metabolites in *Y. pestis* culture grown with carbon-labeled AI-2, (3) continue our efforts to identify metabolites from in vitro experiments using purified AI-2 signaling enzymes, (4) use site-directed mutagenesis and enzyme inhibition with synthetic-substrate analogs to test the hypotheses about enzyme function that we expect to result from in vivo and in vitro metabolite studies, and (5) publish our results on AI-2 signaling effects on virulence-factor expression.

Publications

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

Gryshuk, A., et al., 2008. Yersinia pestis *processing of quorum sensing signaling molecule AI-2.* LLNL-POST-403521.

Bacteria–Mineral Interactions on the Surfaces of Metal-Resistant Bacteria

Alexander J. Malkin   08-LW-027

Abstract

We propose to combine atomic force microscopy and synchrotron infrared spectromicroscopy techniques to investigate the surface chemistry, structure, and environmental dynamics of metal-resistant bacteria in response to various chemical stimuli. In addition, 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 metals, including radionuclides.

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 would profoundly enhance insights into molecular architecture, structural, and environmental variability of cellular and microbial systems. We also expect that our proposed work will improve the fundamental understanding of mechanisms of environmental remediation 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 to 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.

FY08 Accomplishments and Results

We (1) developed procedures for atomic force microscopy analysis of single cells in fluid, (2) conducted initial in vitro topographical high-resolution and chemical characterization of native bacterial surface structures of two bacterial species—*Arthrobacter oxydans* and *Thiobacillus denitrificans*—that are of great importance to subsurface bioremediation,

(3) initiated studies of stress-induced structural responses on cell surfaces, and (4) began studying the mechanisms and dynamics of the formation of biogenic metal phases on cell surfaces of *A. oxydans* in response to physicochemical stimuli.

Proposed Work for FY09

In FY09, we will (1) complete experiments on the mechanisms and dynamics of the environment-dependent formation of biogenic metal phases on cell surfaces; (2) characterize the mechanical properties of biogenic metal phases on cell surfaces through atomic force microscopy nano-indentation, x-ray diffraction, scanning electron and transmission electron microscopy, and energy-dispersive x-ray spectroscopy; (3) establish a direct correlation between the stress-induced ultrastructure of cell surfaces and environmental stimuli; and (4) establish direct correlations between the formation mechanisms and properties of the biogenic metal phases on cell surfaces and environmental stimuli.

Publications

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.

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

Paul T. Henderson   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. We will measure platinum-induced DNA damage sites (adducts) in cancer patients using the radiocarbon-labeled anticancer drug carboplatin and accelerator mass spectrometry, which is the most sensitive method for studying long-lived isotopes. 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 at Davis Cancer Center, which will help design the study and recruit patients for the clinical trial at Davis.

We expect to observe three types of patients: (1) responders—those with high DNA adduct levels, (2) persons 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. Questions we will address include: 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.

FY08 Accomplishments and Results

In FY08 we focused on obtaining radiocarbon-labeled compounds and complying with Food and Drug Administration requirements prior to Livermore's Institutional Review Board review. Specifically, we (1) obtained carbon-14-labeled carboplatin in large enough quantities for the clinical study; (2) performed preclinical experiments in cell culture and with mice bearing human tumors, which resulted in determination of the approximate dose required for human use; (3) developed a protocol by which a tumor sample can be isolated and cultured over several hours to measure cellular repair of the drug–DNA adducts after intravenous infusion of the drug—this protocol is required to obtain Institutional Review Board approval prior to use with humans; and (4) developed protocols to monitor the stability of the drugs to be used for human studies, which is required by the Food and Drug Administration.

Proposed Work for FY09
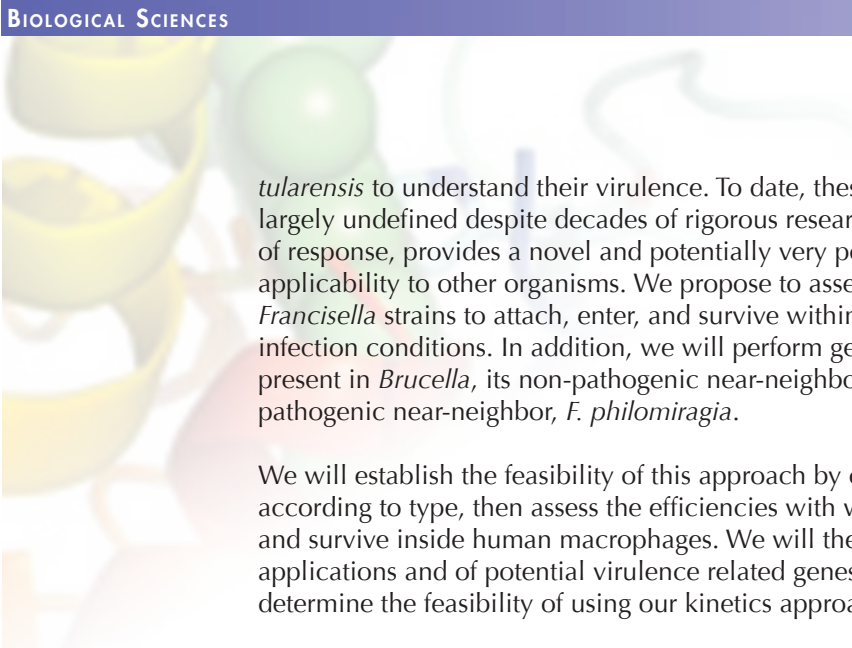
We propose to test our hypothesis that concentrations of DNA damage caused by a single dose of an anticancer drug will correlate with patient outcomes such as tumor shrinkage and mortality, which future clinicians will be able to use to minimize toxicity while optimizing doses and scheduling chemotherapy by analyzing pharmacokinetic profiles derived from individual patients. We will use accelerator mass spectrometry to quantitate cellular responses to carbon-14-labeled drugs in cells, animals, and humans at extremely low doses. This analysis will allow determination of the ability of a patient's cells to uptake the drug and to repair DNA damage.

Understanding Virulence in *Brucellae* and *Francisellae*: Towards Efficacious Treatments for Two Potential Biothreat Agents

Amy Rasley   08-FS-011

Abstract

We propose to assess the feasibility of utilizing the kinetics of the early host response during infection with the fully pathogenic gram-negative organisms *Brucella abortus* and *Francisella*

tularensis to understand their virulence. To date, these pathogens' mechanisms of virulence are largely undefined despite decades of rigorous research. Our approach, utilizing the kinetics of response, provides a novel and potentially very powerful technique that could have broad applicability to other organisms. We propose to assess the ability of specific *Brucella* and *Francisella* strains to attach, enter, and survive within human macrophages using in vitro infection conditions. In addition, we will perform genomic comparisons of key virulence genes present in *Brucella*, its non-pathogenic near-neighbor *Ochrobactrum*, *F. tularensis*, and its non-pathogenic near-neighbor, *F. philomiragia*.

We will establish the feasibility of this approach by characterizing and grouping the strains according to type, then assess the efficiencies with which disparate strains can attach, enter, and survive inside human macrophages. We will then derive unique regions for diagnostics applications and of potential virulence related genes in *Brucellae* and *Francisellae* and thereby determine the feasibility of using our kinetics approach for diagnosing virulence.

Mission Relevance

Understanding virulence is central to many biosecurity efforts. Establishing the feasibility of this approach will allow us to interact in a meaningful and collaborative manner with leaders in the fields of bacterial pathogenesis, lending strength to existing capabilities in the areas of bacterial pathogenesis and host–pathogen interactions—both key to our national security efforts. In addition, this project establishes stronger collaborations with researchers at universities having biosecurity level 3 facilities, which are critical for achieving these mission goals.

FY08 Accomplishments and Results

In FY08 we (1) characterized nine clinical *F. tularensis* isolates as Type A and one isolate determined to be non-*F. tularensis* using the IS100 insertion sequence element analyses; (2) characterized the ability of both virulent and avirulent strains of *F. tularensis* and *Brucella* to infect and survive inside human monocytes; (3) identified, by comparative genomics, unique genes and regions in each species; and (4) analyzed infections of human monocytes with *Y. pestis*, another immune evader and intracellular pathogen that preferentially infects human monocytes. Our comparative analyses laid the foundation for further work to develop rapid therapeutics against biothreat agents.

Computational Biology for Drug Discovery

Felice C. Lightstone   08-FS-013

Abstract

We propose to determine the underpinnings of a high-throughput computational infrastructure that would support future efforts in therapeutics against biothreat pathogens. Existing modeling capabilities focus on pathogen detection, but extending such capabilities to high-throughput molecular docking would lead to a proactive method to guide the development of therapeutics. This project will focus on determining the feasibility of extending current databases to accommodate molecular docking and will also examine the feasibility of massive parallelization of docking algorithms and the utility of docking libraries. Transferring this new technique to a high-performance computing platform at LLNL would result in a unique capability not available elsewhere in the country—high-throughput virtual screening for the design and development of new pathogen therapeutics.

Mission Relevance

If successful, we will lay the groundwork for a high-throughput system to design and develop broad-spectrum therapeutics as countermeasures to known and emerging and engineered biothreat organisms, in support of the Laboratory's homeland security mission.

FY08 Accomplishments and Results

We (1) successfully defined the feasibility of using three different small-molecule databases for high-throughput docking; (2) analyzed the accuracy and parallelization capabilities of six separate docking programs, finding each to be completely amenable to parallel execution (the fastest code was eHiTS, and Glide was the most accurate); and (3) created scripts for quality- and job-control functions. This project enabled a high-throughput computational docking capability—utilizing LLNL's high-performance computing resources for significant gains in performance—and led to a cooperative research and development agreement with an industrial partner (funded by the National Institutes of Health) that will fully utilize this technology for therapeutic design and development for biodefense applications.

Laboratory Directed Research and Development

Chemistry
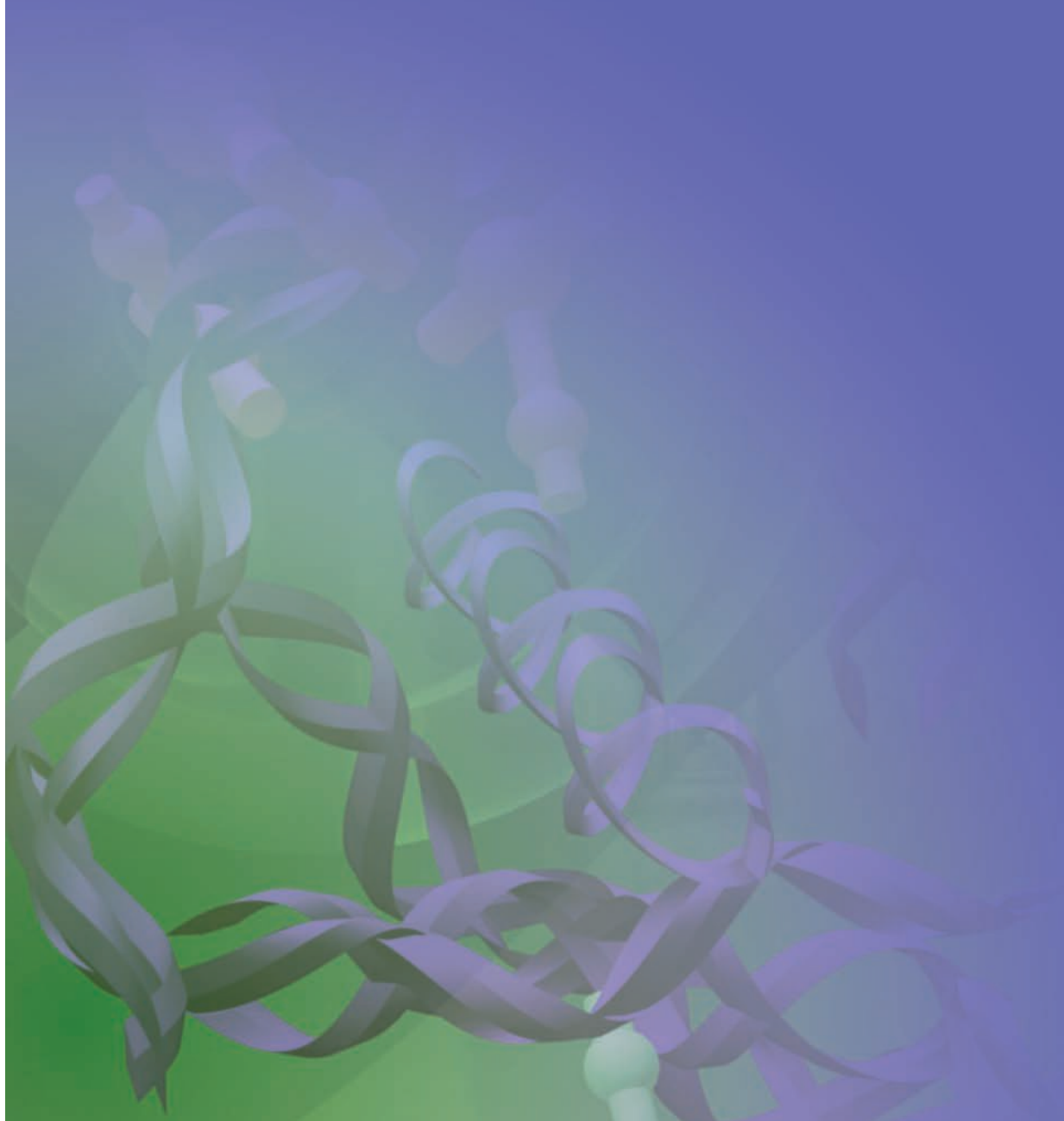
Discovering the Folding Rules that Proteins Obey

Olgica Bakajin   05-ERD-078

Abstract

Protein folding is a fundamental cellular process. Proper folding is required for a protein to carry out its functions, while improper folding can be a source of disease. We propose to use a combination of simulations and experiments to significantly advance our understanding of the molecular mechanisms of protein folding. We will develop a robust microfluidic mixing device, conduct long-time simulations on supercomputers, and perform measurements on the systems that exhibit a fast folding and fast hydrophobic collapse. Our results will be used to answer the following questions: Can traps and intermediate states be observed? Why are some molecules such fast folders? Are there multiple folding pathways, a few, or just one? And is folding hierarchical?

We expect to elucidate the mechanisms of protein folding through a combination of complementary experimental and simulation studies. In addition, the equipment and technology developed for this project will provide new capabilities that will be applicable to numerous projects at LLNL. This research will establish and strengthen collaborations between LLNL scientists and leading researchers in academia and industry. Because of the fundamental nature of this project, it should result in publications in high-impact, peer-reviewed journals.

Mission Relevance

By preparing the scientific basis for understanding and controlling protein function, this project is highly relevant to the Laboratory's mission in biodefense. The knowledge base created in this project also will support the Livermore's mission in bioscience to improve human health.

FY08 Accomplishments and Results

For FY08, we (1) developed and demonstrated microfluidic mixers that can initiate folding reactions in less than 1 μs; (2) measured, in collaboration with scientists at Michigan State, early folding in an ultrafast-folding, relatively small protein known as the lambda repressor using ultraviolet fluorescence—results suggest a multidimensional folding landscape; (3) used microfluidic mixers to measure fast folding events of other proteins labeled by fluorescence resonance energy transfer; (4) developed a mixer that can be used in combination with synchrotron radiation circular dichroism measurements; and (5) performed simulations, in collaboration with IBM, on the lambda repressor. The successful conclusion of this project is evidenced by the fact that a federal agency has expressed interest in our results and in providing support for further research on early events in protein folding.

Conversion of Plutonium and Enriched Uranium

Thomas W. Trelenberg   06-ERD-012

Abstract

This project seeks to determine the mechanisms governing hydride and oxide conversions of uranium and plutonium. The unpredictable nature of conversion processes raises long-term storage and retrieval concerns for these materials and highlights a lack of understanding about how impurities serve to catalyze the reactions and what effect they might have on archived scientific samples. Both macroscopic (coupon tests) and microscopic surface-science experiments (photoemission) will be used to characterize reaction rates (with and without catalysts) and mechanisms that convert plutonium and uranium into their respective hydrides and oxides. Computer simulations using relativistic quantum models will guide the experimental program. In turn, data collected for this project will help verify the modeling results.

The integration of our experimental and theoretical findings will lead to a predictive capability for these reactions and will begin the process of defining the mechanisms governing these conversions, providing insight into their proper application to the storage and retrieval of plutonium and uranium.

Mission Relevance

Actinide compounds (such as hydrides or oxides) are of interest for the storage and recovery and retrieval of nuclear materials in support of the Laboratory's national security missions in stockpile stewardship and nonproliferation.

FY08 Accomplishments and Results

In FY08, we (1) completed quantum chemical modeling of a pure plutonium matrix as well as impure plutonium metal with one substituted atom—for the pure metal we calculated an activation barrier of 7.5 kcal/mole hydrogen and for two of the selected impurities, we eliminated this barrier; (2) completed modification of our coupon testing apparatus and conducted tests that confirmed our modeling predictions; and (3) expanded experiments to

investigate a full range of temperatures. Overall, we identified and quantified a number of kinetic processes important to the recovery of plutonium though forced hydriding. With these successes, we have been able to scale these processes up to high-volume production levels because of interest from several Livermore programmatic areas.

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 method, 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 the multiscale shock method 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 study will represent the first use of a state-of-the art quantum mechanical simulations code to study shocked, highly reactive materials. If successful, 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. We have already published in a peer-reviewed journal and have several more publications in preparation.

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.

FY08 Accomplishments and Results

In FY08 we (1) conducted the first simulations of shock-compressed interstellar ices over a wide variety of shock velocities, showing that peptide bond formation can occur at pressures of up to 60 GPa and temperatures as high as 4000 K—significantly higher than previous estimates—and

observing the extremely fast breaking and forming of covalent bonds; (2) calculated kinetic rates for covalent bond formation, determining that long carbon chain amino acids can form at high temperatures and pressures and that a reducing environment in the interstellar ices promotes peptide bond formation; and (3) concluded our studies of shock-compressed astrophysical ices by investigating compositional effects—such as varying ice composition—and by exploring the results of placing interstellar ice in reducing rather than oxidizing conditions.

Proposed Work for FY09

In FY09, we plan to conclude our studies of shock-compressed astrophysical ices by investigating compositional effects, such as varying ice composition, and by exploring the results of placing interstellar ice in reducing versus oxidizing conditions. Based on previous publications in this area of astrobiology, this work could result in articles in high-profile journals such as *Science* or *Nature*.

Publications

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., in press. "A microscopic picture of electrical conductivity of H_2O 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.

Mundy, C. J., et al., 2008. "Ultrafast transformation of graphite to diamond: An ab initio study of graphite under shock compression." *J. Chem. Phys.* **128**, 184701. UCRL-JRNL-235688.

A Novel Approach to Investigate the Mechanism of *Yersinia Pestis* Pathogenicity in Real Time and at the Single-Cell Level

Julio A. Camarero   07-ERD-050

Abstract

The main objective of this proposal is to study the pathogenicity of *Yersinia pestis* in real time and at the single-cell level. A key to our approach is development of new molecular tools based on protein splicing, which will allow reconstitution and site-specific labeling of *Y. pestis* cytotoxic proteins inside the host cell with temporal and spatial control. This approach will also be used for the simultaneous, multicolor site-specific labeling of *Y. pestis* cytotoxic effectors and their target proteins in vivo. This will allow, for the first time, study of multiple interactions in vivo between the *Y. pestis* cytotoxic proteins and their host target proteins to better understand the virulence mechanisms of *Yersinia* during infection of its natural hosts.

This multidisciplinary project will allow the development of a new set of biomolecular tools for the study of proteins and their interactions in vivo with minimal perturbation on the protein function, and determine the primary factors of temporal and spatial control. This set of tools will be used for the first time to elucidate the action mechanism of YopM, a key effector protein for *Yersinia* pathogenicity, within the host cell. We will address key questions regarding the pathogenicity of YopM. Specifically, is the tetrameric structure of YopM required for nuclear delivery and for biological activity? What is the temporal mechanism for RSK1 and PRK2 *Yersinia* outer-protein-mediated activation? What other proteins interact with YopM in the cytoplasm?

Mission Relevance

Successful completion of this project would provide a new way to study pathogenicity in living cells with temporal and spatial control. It would enable real-time, single-molecule-level studies on host–pathogen interaction biology. This research is aligned with the Laboratory's missions in homeland security and in biosciences to improve human health, and with the National Institute of Allergy and Infectious Diseases strategic plan for biodefense research.

FY08 Accomplishments and Results

In FY08 we (1) successfully cloned the gene encoding YopM, a protein known to be essential for *Y. pestis* to cause disease, into a pTXB1 expression vector as a first step towards the goal of achieving protein trans-splicing—the pTXB1 expression vector is a commercially available, circular DNA molecule designed for producing proteins linked to an intein, which is the key element of the trans-splicing event; (2) demonstrated proof-of-concept in vitro photomodulation with maltose binding protein and detected a signal indicating that a successful splicing event occurred; (3) made initial attempts to clone RSK1 and RSK2 kinases, two proteins that form a complex with YopM during *Y. pestis* infection; and (4) began the process of cloning these two kinases as fusion proteins to both DnaE and DnaB C-intein polypeptides—the fusion proteins are meant to facilitate the trans-splicing in vivo. This work was not completed in FY08, but fusion constructs as proposed will likely be successful based on the proof-of-concept studies with maltose binding protein.

Publications

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The Structure and Transport of Water and Hydrated Ions within Hydrophobic, Nanoscale Channels

Jason K. Holt   07-LW-056

Abstract

Although recent studies have examined fluid and ion confinement in nanoscale materials, no consensus exists about the length scale below which nanoscale effects become important, nor is the interplay between ordering and transport clear. Because of their size and hydrophobic nature, carbon nanotubes are nanoscale materials that can serve as analogues for biological channels that regulate water and ion conduction in cells. We plan to study the structure and transport of water and hydrated ions in carbon nanotubes using proton (^{1}H) nuclear magnetic resonance, x-ray absorption spectroscopy, and molecular simulations. Our goal is to define length scales and probe the consequences for molecular transport. Answers to fundamental scientific questions about how solutions flow through these structures will impact future generations of filters and other devices that operate on this scale.

This project aims to define the length scale for ordering of water molecules in artificial hydrophobic channels. Another objective is to determine how ion hydration is altered by confinement in these channels. The interest in these phenomena stems from our recent observations of enhanced flow in carbon nanotubes. We will determine if the flow enhancement can be attributed to molecular ordering within the channel. This research will enhance our understanding of transport in carbon nanotube systems and aid in the development of high-throughput membranes for applications such as desalination.

Mission Relevance

This project brings cutting-edge science to the Laboratory at the intersection of chemistry, materials science, and biology. The project will foster collaboration with researchers at the DOE's Stanford Synchrotron Radiation Lightsource. The research will generate publications in high-profile journals, and develop technologies that will enable new research opportunities of value to biosecurity, in support of the Laboratory's homeland security mission, and water purification, in support of environmental management and remediation.

FY08 Accomplishments and Results

During FY08, we (1) succeeded in identifying a ^{1}H nuclear magnetic resonance signature associated with interior water in single-wall carbon nanotubes channels of 1 nm diameter; (2) performed, in collaboration with researchers at the Synchrotron Radiation Lightsource, extended x-ray absorption fine structure and x-ray fluorescence measurements on bromide-treated carbon nanotubes and discovered the presence of a basic site on the nanotubes (both

single-wall and multiwall) that selectively binds bromide over cations present in solution; (3) performed computational modeling that revealed an upfield shift in the ^{1}H nuclear magnetic resonance spectrum for water confined within the nanotubes; (4) obtained water adsorption isotherms for carbon nanotubes of 1 nm diameter and smaller to better understand the nature of water and nanotube interactions and confirm that below a certain size, molecular ordering effects will come into play; and (5) performed x-ray absorption spectroscopy experiments examining how other halide species interact with carbon nanotube surfaces.

Publications

Chen, Q., et al., 2008. "Identification of endohedral water in single-walled carbon nanotubes by ^{1}H NMR." *Nano Lett.* **8**(7), 1902. LLNL-JRNL-401662.

Holt, J. K., 2008. "Methods for probing water at the nanoscale." *Microfluid. Nanofluid.* **5**(4), 425. LLNL-JRNL-402473.

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The Viral Discovery Platform

Christopher G. Bailey   08-SI-002

Abstract

A top national priority for homeland security is to develop systems and supporting assays for detecting engineered biothreats. These threats range from modifications of existing organisms to totally new organisms created, for example, by de novo synthesis or by synthesis of hybrids or chimeras that may require new paradigms for detection. 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. If successful, 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) develop the first-ever bioinformatic system to design multiplexed primer sets that are optimized to work in combination, (2) provide design parameters and analysis for next-generation microarrays, (3) validate the assays and arrays for viral families predicted by bioinformatics for rapid virus identification in clinical samples, (4) optimize short primer sets to generate expected banding patterns that can be used for identification of known and unknown

threats, (5) demonstrate microfluidic isolation of virus particles in complex biological samples, and (6) develop systems for precise fluid manipulation, droplet sorting, and polymerase chain reaction.

Mission Relevance

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

FY08 Accomplishments and Results

In FY08, we achieved all of our proposed tasks. Specifically, we (1) designed, fabricated, and tested two generations of viral-discovery microarrays; (2) collaborated with three universities on microarray applications; (3) employed microfluidic technologies to separate viruses from complex samples; (4) demonstrated the use of digital microfluidics to detect viruses; (5) used custom bioinformatics to design short primers for viral identification; and (6) demonstrated multiplex polymerase-chain-reaction amplification and identity of predicted bands for identifying viruses.

Proposed Work for FY09

In FY09 we will continue developing our approach to high-throughput, rapid analysis for known and unknown viruses in clinical samples. Specifically, we will (1) use lessons from our first generation of microarrays to develop optimized and expanded arrays to include bacterial and fungal species as well as probes for detecting signatures of genetic engineering, (2) increase our microdroplet generation and detection capability from the current hundreds-of-droplets per hour to millions per hour for complete sample analysis, (3) incorporate additional microfluidic sample preparation steps to separate bacteria and free nucleic acid from viruses, and (4) expand the bioinformatic and experimental assay development to include discovery using next-generation, high-throughput sequencing techniques.

Publications

Beer, N. R., et al., 2007. "On-chip, real-time, single-copy polymerase chain reaction in picoliter droplets." *Anal. Chem*. **79**(22), 8471. UCRL-JRNL-230233.

Beer, N. R., et al., 2008. "On-chip single-copy real-time reverse-transcription PCR in isolated picoliter droplets." *Anal. Chem.* **80**(6), 1854. LLNL-JRNL-403189.

Jung, B., et al., 2008. "Acoustic particle filter with adjustable effective pore-size for automated sample preparation." *Anal. Chem.* **80**(22), 8447. UCRL-JRNL-237328.

Kiss, M. M., et al., 2008. "High-throughput quantitative polymerase chain reaction in picoliter droplets." *Anal. Chem.* **80**(23), 8975. LLNL-JRNL-401219.

Rapid Radiochemical Separations for Investigating the Chemistry of the Heaviest Elements

Dawn A. 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 than their neighbors. This project will study the chemical and physical properties of heavy elements. For elements 104 and 105, chemical separations and automated techniques will be developed, and the results will indicate if the transactinides follow the lighter homologues in the periodic table, or if relativistic effects induced by nuclear charge alter predicted chemistries. The combination of physics and chemistry will provide insight into the chemical behavior of heavy elements and potentially result in discoveries of new elements and isotopes.

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, will be used in accelerator-based online experiments with elements 104 and 105, and will also 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 security 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.

FY08 Accomplishments and Results

In FY08 we (1) produced hafnium tracer material at Livermore's Center for Accelerator Mass Spectrometry and began development of a chemical separation for elements 104 and 105 using their homologues zirconium, hafnium, niobium, and tantalum with Eichrom diglycolamide (DGA) resins in various acid systems; (2) continued to evaluate organophosphorous and crown ether extractants for separation of elements 104 and 105; (3) adapted element 105 separations to an automated chemistry platform; and (4) began construction of a computer-controlled prototype automated chemistry system designed to perform column chromatography while simultaneously regenerating and preparing the resin beds.

Proposed Work for FY09

In FY09 we plan to (1) continue DGA extraction studies on intra- and inter-group separations of groups IV and V under varying acid concentrations to establish a chemical method for separation of elements 104 and 105; (2) construct a prototype of the automated chemical apparatus and begin tests with tracers; (3) perform online chemistry tests at Berkeley's 88-inch cyclotron or another suitable facility; and (4) collaborate with researchers at the University of Nevada, Las Vegas to conduct joint chemistry experiments based on results of our DGA work and their work on crown ether extraction.

Publications

Henderson, R. A., and K. J. Moody, 2008. $^{243}Am + ^{48}Ca$: *A second look at the Rf/Db data set.* LLNL-TR-400981.

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Henderson, R. A., K. J. Moody, and D. A. Shaughnessy, 2008. *Automated radiochemistry efforts at LLNL.* Interagency Laboratory Working Group 42, Atomic Weapons Establishment, Aldermaston, England, Sept. 16, 2008. LLNL-PRES-406833.

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Probing the Organization of the Cell Membrane

Peter K. 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. We will provide fundamental data that have broad implications, from host–pathogen interaction to next-generation sensors. Lipid interactions through the formation

of lipid rafts in the cell membrane are believed to play a key role in organizing the cell 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. The proof-of-concept results we demonstrated in 2006 were selected by *Chemical and Engineering News* as one of the top research advances of the year, so 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 characterization of nano-lipoproteins for such sensors. In addition, the project will advance our capability for NanoSIMS analysis of bioweapon particles.

FY08 Accomplishments and Results

Molecule-specific labeling (using ^{18}O) and lipid raft experiments showed that cholesterol partitions preferentially to the fluid phase of unsaturated lipid. This result was significant because conventionally, nonfluid membrane domains had been predicted to be enriched in cholesterol. We also tested molecules labeled with fluorine, sulfur, and deuterium and used NanoSIMS to imaged gradients made by electric fields; expressed and purified green fluorescent protein and subunit B of the cholera toxin labeled with ^{13}C and ^{15}N and successfully detected these labeled proteins using NanoSIMS; and cultured cells, developed protein tags, and tested cholesterol incorporation methods.

Proposed Work for FY09

In FY09, we will (1) continue our work on multicomponent model membranes to validate our hypothesis that lipids play a key role in membrane organization, (2) initiate a new effort with DNA-tethered membranes to enable work with membrane-bound proteins, and (3) perform our first experiments with natural cell membranes to validate our work with model membranes.

Collection of Solid Debris from Fusion-Class Lasers for Radiochemical Diagnostics and Measurements

Dawn A. Shaughnessy   08-FS-001

Abstract

Designs for an effective system for collecting solid post-explosion debris samples from fusion-class laser experiments are the first step toward radiochemical measurements relevant to fusion ignition diagnostics, stockpile stewardship, and nuclear science. In this project, we will demonstrate the feasibility of a system for collecting solid debris from the National Ignition Facility target chamber. We will also determine which radiochemical measurements would be possible given such factors as collector–debris material interaction. If the debris that condenses out of the fusion plasma can be collected and radiochemically analyzed, the number and type of nuclear reactions that occurred in the capsule material could be determined. This is important both for ignition capsule diagnostics and radiochemical measurements relevant to basic science and stockpile stewardship applications.

If successful, this project will produce design prototypes for a solid collector for use at fusion-class lasers facilities. We will identify issues regarding collector size, collector–debris material interactions, and how the collector will be introduced and extracted from laser target chambers. Input from relevant engineers, capsule designers, target design and fabrication scientists, and materials scientists will be included. In addition, the need for new techniques in radiochemical processing, detection methods, and chemical automation will be considered.

Mission Relevance

Collection of solid debris from laser–matter interactions and sample processing are critical skills for radiochemical diagnostics, actinide chemistry, and radiochemical process development, which are important for stockpile stewardship and nuclear forensics, in support of LLNL's missions in national security and homeland security.

FY08 Accomplishments and Results

For FY08 we (1) identified major issues related to the introduction and extraction of the collector, the chemical form of post-explosion capsule debris, and collector–debris material interactions; (2) produced designs for prototype collection and testing systems; (3) prioritized the list of collector designs according to issues identified by debris modelers and engineers; (4) performed sensitivity studies for some proposed measurements to determine whether their detection in capsule debris would be feasible; and (5) developed a prioritized list of radiochemical measurements. This project has laid the groundwork for developing solid debris collection systems at the National Ignition Facility over the coming few years. The next step is to produce and test the prototype solid debris collectors.

Laboratory Directed Research and Development

Earth and
Space Sciences
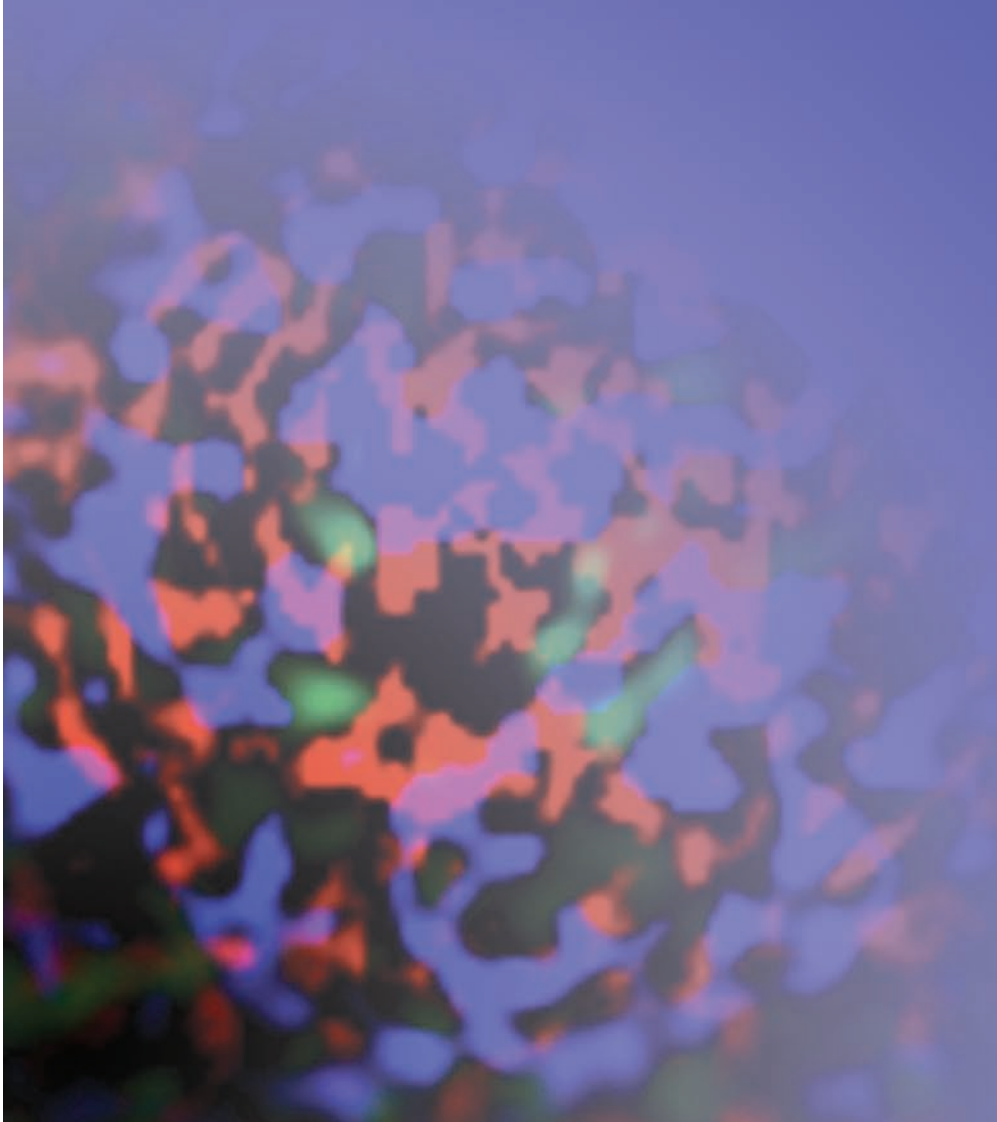
The Physics of Recombining Plasmas in Celestial Sources

Gregory V. Brown   06-ERD-010

Abstract

Recombining highly charged ions with bound electrons to produce x rays plays an important role in laboratory plasmas and is the dominant x-ray production process in many celestial objects. Interpretation of recombination spectroscopy has been challenging because few targeted laboratory data are available. Lawrence Livermore is the only facility able to provide high-resolution spectra, measured under well-controlled conditions, from recombination reactions. This project uses LLNL's Super Electron Beam Ion Trap and a National Aeronautics and Space Administration (NASA) microcalorimeter to measure spectra following bare ion recombination with electrons bound to atomic and diatomic hydrogen and helium. This work provides a complete set of experimental x-ray spectra from recombining plasmas for interpreting spectra from laboratory and celestial sources, as well as benchmarking atomic theory.

We will provide an improved understanding of the spectral dependence of the neutral donor (hydrogen and helium) by observing the x-ray spectra following the interaction of each neutral projectile with bare ions. We have already observed the dependence of bare ions on atomic number in the measured x-ray spectra. By measuring the spectral signature of each of these interactions and understanding the spectral signatures of different donor material and the dependence of the bare target ion on atomic number, we will be able to diagnose physical processes taking place in a variety of celestial sources including the Galactic Center, low-mass x-ray binaries, and supernova remnants, as well as complex laboratory sources such as tokamaks.

Mission Relevance

Because the thermonuclear phenomena found in stars are the same as those that occur in nuclear explosions and in fusion reactors, this project will benefit numerical simulation and contribute to fundamental experimental research that supports the Laboratory's national security and energy security missions.

FY08 Accomplishments and Results

Because of uncertainties in the x-ray spectra produced by the aurora of Jupiter, the cosmic x-ray background, cometary atmospheres, and the Earth's magnetosheath, we focused our FY08 efforts on measuring the charge-exchange-produced x-ray emission from L-shell transitions in highly charged sulfur ions. Compared to the direct excitation spectrum, we found an enhancement in x-ray transitions originating in levels with a high-n principle quantum number ($n > 5$) and the 3s levels. We also measured the signature of double electron capture following charge exchange onto bare and hydrogenic argon. These spectral signatures, especially those from L-shell sulfur ions, are already being used to interpret spectra measured by orbiting observatories such as Suzaku and Swift. The successful conclusion of this research projected LLNL to the forefront of experimental work on x-ray emission produced by charge-exchange recombination and attracted support from NASA to continue studies of charge-exchange recombination. As part

of this work, we found that our calorimeter can be used in conjunction with the LLNL electron beam ion trap to calibrate x-ray blocking filters employed by high-resolution spectrometers used to diagnose high-energy-density plasmas produced at the Omega laser facility and the National Ignition Facility, in addition to applications for spectrometers for future NASA x-ray missions.

Publications

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Frankel, M., et al., 2008. *Simulating Jupiter's x-ray emission in the laboratory.* 212th Mtg. American Astronomical Society, St. Louis, MO, June 1–5, 2008. LLNL-ABS-402453.

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Urban Atmospheric Turbulence: Improved Turbulence Closure Models through Observations and Simulations

Julie K. Lundquist   06-ERD-026

Abstract

We propose to test advanced turbulence models and numerical methods for urban simulations and then integrate them into a numerical model that is widely used for weather forecasting, transport modeling, and dispersion prediction. This project is motivated by the inadequacy of current turbulence models (compared to observations) and the demand for complex time- and space-varying boundary conditions for urban-scale models. Improved models are essential for national security purposes in the case of accidental or intentional urban atmospheric release of hazardous materials. Project success will be determined by comparing dispersion simulations to a refined field dataset from the Joint Urban 2003 field study.

New, more accurate turbulence models for urban areas developed in this project will provide improved plume predictions for national security applications. These improved numerical methods will allow the seamless integration of urban-scale simulations with appropriate coarser-scale simulations to provide the best available forcing of urban models. This project will enable better population protection by providing higher fidelity simulations for emergency response, sensor siting, and forensic studies in urban areas. Our improved simulation capability will also be applicable for estimating winds in complex terrain and will therefore be suitable for wind power applications such as turbine siting.

Mission Relevance

Our project supports LLNL's national and homeland security missions by improving capabilities to provide emergency response for atmospheric releases of hazardous materials, in addition to supporting Laboratory efforts in energy and the environment.

FY08 Accomplishments and Results

In FY08, we (1) implemented the immersed boundary method for two-dimensional flow; (2) implemented a third subfilter turbulence model, the Nonlinear Backscatter and Anisotropy model, that appears to be more accurate and is much more computationally efficient than the dynamic reconstruction model; (3) conducted extended immersed boundary method simulations for the complex terrain of the Owens Valley of California; (4) simulated flow

and dispersion using our models in canonical cases; and (5) prepared journal publications quantifying the improvements afforded by our models. Our set of subfilter turbulence parameterizations are scheduled for release to the atmospheric science community via the March 2009 Weather and Research Forecasting model distribution. The successful conclusion of this project enabled accurate and computationally efficient large-eddy simulations of atmospheric flow in a range of atmospheric stability conditions, enabling accurate predictions in urban and complex terrain for wind energy resource assessment, operational forecasting, and atmospheric dispersion consequence assessment. We obtained funding for multiple follow-on projects, including a Cooperative Research and Development Agreement with an industrial partner to develop an operational forecasting capability for wind energy projects as well as DOE support for analysis of wind farm power data.

Publications

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Atmospheric Carbon Dioxide-14 Constraints on and Modeling of Net Carbon Fluxes

Thomas P. Guilderson   06-ERD-031

Abstract

Carbon dioxide (CO_2) is the most important anthropogenic greenhouse gas influencing global climate. Sources and sinks impart their signature on the distribution, concentration, and isotopic composition of CO_2, while spatial and temporal variability provide information on net surface fluxes. Observations of carbon and oxygen isotope tracers and their rate of change in the atmosphere can be used to constrain global and regional contributions of different carbon sources and sinks, because each bears a different isotope or elemental ratio signature. We propose to measure $^{14}CO_2$ samples from a suite of clean air locations and use these results in inversion estimates to constrain unidirectional carbon fluxes.

This project is expected to produce the best possible estimates of surface carbon sources and sinks on a regional scale using atmospheric observations of CO_2 partial pressure, ^{13}C, ^{14}C, and oxygen-to-nitrogen ratios; atmospheric transport based on the range of Atmospheric Tracer Transport Model Intercomparison results; and the best possible representation of isotopic composition of exchangeable carbon pools and associated isotopic fractionation factors.

Mission Relevance

By investigating size and variability of the dynamic reservoirs and fluxes of carbon within the Earth system, this research supports Laboratory missions in energy security and long-term energy needs. The synergy between field data and computational models offered by this project will contribute to DOE's missions in energy security and carbon management.

FY08 Accomplishments and Results

Our data analysis showed a clear change in the latitudinal gradient, particularly in the Southern Ocean, which we interpreted as reflecting a change in the air–sea CO_2 flux. Low-latitude atmospheric values were higher than at either poles, consistent with release of terrestrial carbon fixed in the late 1960s and 1970s. The model inversion successfully interpreted the $^{14}CO_2$ observations and directed us towards a bias in the underlying Southern Hemisphere background CO_2 flux fields. In summary, this successful project enabled and demonstrated the ability of accelerator mass spectrometry to make measurements accurate to less than two parts per thousand on atmospheric CO_2 samples, opening up a new area of carbon cycle research and CO_2 attribution in the atmosphere. The next step is to include this atmospheric $^{14}CO_2$ measurement into efforts on climate forcing for DOE's Office of Biological and Environmental Research.

Publications

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Regional Climate

David C. Bader   06-ERD-066

Abstract

Understanding regional climate depends on gaining knowledge about climate variability at similar scales. The proposed research will contribute to this understanding by developing an integrated, multimodel capability for regional climate change impact and adaptation studies, and by using the model to examine climate change impacts on regions as small as watersheds and cities. The emphasis of this project is to develop and establish a scientifically strong and peer-accepted regional climate modeling capability through studies focusing on the effects of climate change on California. Our first focus area is the effect of climate change on water resources, and our second is the relationship between climate change and air quality.

Our project will use observations of atmospheric variables to examine the ability of climate models to simulate this variability. We will leverage Livermore's climate-modeling expertise for further analysis of California climate change. The modeling capability we develop will enable the Laboratory to design and execute simulations of important climate change impacts such as the frequency and intensity of flooding in regions as small as individual cities or watersheds. In addition, our efforts complement global modeling used for forming national and international energy, air quality, and water management policies.

Mission Relevance

In support of LLNL's missions in energy and water security and environmental management, we will develop an integrated, multimodel capability for regional climate change analysis and for impact and adaptation studies. This suite of simulation tools will provide a new capability for managing regional water resources in California that can be applied to other regions in the U.S.

FY08 Accomplishments and Results

Based on results from our simulations, we modified some tasks originally planned for FY08. Specifically, we (1) ran a 40-year regional climate simulation forced by the control run from the Community Climate System Model for present-day conditions; (2) performed a detailed comparison of the results from downscaled regional simulation to observations in California—the model tends to over-predict wintertime precipitation, particularly in the mountains; (3) performed a global climate model experiment to evaluate the effect of irrigation on temperatures in several regions of the world—results indicate substantial regional differences in the magnitude of irrigation-induced cooling, which are attributed to three primary factors: differences in extent of irrigated area, differences in the simulated soil moisture, and the nature of cloud response to irrigation; and (4) prepared two journal articles that detail our results. The successful completion of this project produced the longest, highest resolution, and most

rigorously analyzed global-downscaled simulation of California climate performed to date. These results provide the basis for a decadal prediction concept that is currently being further developed at LLNL.

Publications

Caldwell, P., et al., 2008. *Evaluation of a WRF dynamical downscaling simulation over California.* LLNL-JRNL-403431.

Lobell, D., et al., in press. "Regional differences in the influence of irrigation on climate." *J. Climate.* LLNL-JRNL-401185.

Development of Integrated Microanalysis of Nanomaterials

John P. Bradley   06-ERI-001

Abstract

In recent years there have been significant advances in detection and imaging capabilities using electron microscopy and ion microprobe techniques. We propose to develop an integrated microanalysis capability utilizing these advances with the state-of-the-art instrumentation at Lawrence Livermore to enable a new level of investigation into the mineralogical, chemical, and isotopic properties of nanomaterials. The initial development will be carried out on natural nanomaterials captured at hypervelocity speeds by low-density silica aerogels. The analytical studies of these captured particles will provide new insights into cosmically primitive extraterrestrial material and develop synergistic capabilities that are complimentary to multiple mission-relevant analytical needs.

The National Aeronautics and Space Administration Stardust samples are the first solid-matter materials to be returned to Earth since the Apollo missions of the 1970s. New insights into early solar system processes will be gained by analyzing these "fresh" materials in contrast to materials (e.g., interplanetary dust particles) that have encountered space weathering and atmospheric entry alteration before analysis in a laboratory setting. Stardust samples will enable comparisons between astronomical spectral observations of comets and laboratory observations of astromaterials. Stardust samples will give insights into the role comets played in bringing life to early Earth and if cometary dust is composed of interstellar dust, inner solar system dust, or both.

Mission Relevance

The proposed work will develop and investigate new analytical techniques for nanoscale materials characterization that are directly applicable to the Laboratory's missions in stockpile stewardship and homeland security. The project also supports the Laboratory's mission in breakthroughs in fundamental science and applied technology, specifically in the area of astrophysics and space science, which includes the exploration of Kuiper Belt objects such as Comet Wild 2.

FY08 Accomplishments and Results

We conducted light gas-gun shots of mineral grains into aerogel and atomic-scale scanning transmission electron microscope (STEM) studies of Stardust comet grains, finding that capture damage to the Stardust samples was significant but that important scientific information can still be found at the nanometer scale. The Comet Wild 2 sample did not contain what was expected in a comet. As we reported in *Science*, the sample appeared to contain inner solar system materials similar to those found in meteorites (most meteorites are from the asteroid belt in the inner solar system). This totally unexpected finding, after roughly two years of careful examination of the returned sample, essentially redefined the direction of comet science. The next step in this work is to fully integrate the state-of-the-art analytical instruments: the focused ion beam, field emission scanning electron microscopy, nanometer-scale secondary-ion mass spectroscopy, and SuperSTEM, the Laboratory's advanced scanning transmission electron microscope. This will enable precious samples, whether Stardust or one-of-a-kind nuclear forensics samples, to be analyzed with multiple analytical techniques, thereby maximizing the science yield.

Publications

Bradley, J. P., and H. A. Ishii, 2008. "Comment on the shape and composition of interstellar silicate grains." *Astron. Astrophys.* **486**, 781. LLNL-JRNL-402474.

Grahan, G., 2008. "Applied focused ion beam techniques for sample preparation of astromaterials for integrated nano-analysis." *Met. Planet. Sci.* **43**, 561. LLNL-JRNL-228355.

Ishii, H. A., et al., 2008. "Comparison of Comet 81P/Wild 2 dust with interplanetary dust from comets." *Science* **319**, 447. LLNL-JRNL-234616.

Ishii, H. A., et al., 2008. "Recovering the elemental composition of Comet Wild 2 dust in five Stardust impact tracks and terminal particles in aerogel." *Met. Planet. Sci.* **43**, 215. LLNL-JRNL-227089.

The Chemistry of Core Formation

Frederick J. Ryerson   **06-ERI-002**

Abstract

Core formation represents the major chemical differentiation event for terrestrial planets. Generation of the Earth's magnetic field is related to core formation and is important in establishing planetary habitability. The depth and temperature of core segregation controls its chemistry, and high-pressure experiments can be used to simulate metal–silicate segregation. In this project, we will develop methods that link the diamond anvil cell with analytical systems such as a secondary-ion mass spectrometer with nanometer-scale spatial resolution, a focused ion-beam system, and a transmission electron microscope to determine the partitioning of elements such as sulfur, silicon, oxygen, carbon, hydrogen, vanadium, tungsten, molybdenum, ruthenium, and lead at extreme conditions relevant to the Earth's lower mantle.

Results of this research will help to explain the low density of the Earth's core relative to pure iron and the overabundance of siderophile elements (i.e., chemical elements that partition strongly into a metal-rich phase) in the silicate mantle. This explanation will constrain the potential range of core-forming processes on the Earth. Because the core is responsible for generating the Earth's magnetic field, constraining composition of the core may provide clues to the absence of magnetic fields on other terrestrial planets and the influence of magnetic fields on planetary habitability.

Mission Relevance

The extreme conditions of temperature and pressure present in the Earth's core overlap those found in the stars and in exploding nuclear weapons. The microanalytical methods, materials characterization techniques, microanalysis, and high-pressure experimentation that will be developed in this project to understand the Earth's core are applicable to LLNL's stockpile stewardship mission and to forensics efforts for the nonproliferation mission. This project also contributes to the Laboratory's mission in basic science.

FY08 Accomplishments and Results

In FY08, we (1) performed metal–silicate partitioning for moderately siderophile (molybdenum, arsenic, germanium, tungsten, phosphorous, nickel, and cobalt), slightly siderophile (zinc, gallium, manganese, vanadium, and chromium), and refractory lithophile (niobium and tantalum) elements using a new piston-cylinder assembly at 3 GPa from 1600 to 2600°C; (2) investigated the effect of pressure on partitioning through a combination of piston cylinder and multi-anvil experiments from 0.5 to 18 GPa at 1900°C; (3) determined that models of core segregation constrained by our data preclude a single-stage model for terrestrial core formation; (4) developed analytical data on oxygen, carbon, silicon, and sulfur using the electron microprobe; and (5) determined the partitioning of transition metals between ferropericlase, perovskite, and post-perovskite, and observed metallic phases in some runs during transmission electron microscopy analysis. The experimental and analytical methods developed in this project now allow trace element analysis of planetary materials at extreme pressures and temperatures, extending the reach of experimental geochemistry into the earth's deep mantle. We have established an ongoing collaboration with colleagues at the Institute de Physique du Globe de Paris to utilize these methods in probing planetary interiors and have obtained support from the DOE Office of Basic Energy Sciences' Geoscience Research Program for further geochemical applications of high-spatial-resolution secondary-ion mass spectrometry.

Publications

Auzende, A-L., et al., 2008. "The role of iron chemistry on the interpretation of lower mantle heterogeneities." *Eos Trans. AGU Fall Meet. Suppl.*, **89**(53), V13D-2145. LLNL-PROC-408208.

Putrika, K. D., and F. J. Ryerson, 2008. "Olivine compositions from the Hawaii scientific drilling project, phase 2: Evidence for a peridotite mantle source region." *Eos Trans. AGU Fall Meet. Suppl.*, **89**(53), DI34A-07. LLNL-PROC-408209.

Putrika, K. D., et al., 2007. "Ambient and excess mantle temperatures, olivine thermometry, and active vs. passive upwelling." *Chem. Geol.* **241**, 177. LLNL-JRNL-408210.

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Watkins, J., D. J. DePaolo, and F. J. Ryerson, 2008. "Diffusive isotope fractionation experiments and the structural components of silicate liquids." *Geochim. Cosmochim. Acta* **72**, A1009. LLNL-ABS-401871.

Evidence for Stratospheric Downwelling Associated with High-Elevation Topography

Robert C. Finkel   06-ERI-005

Abstract

The continued presence of nuclides such as ^{36}Cl in streams in the Sierra Nevada has been interpreted to be residual nuclear fallout, but the fallout reserve required implies groundwater storage that contradicts current hydrologic models. Here we test the hypothesis that the source of the unexpectedly high concentration of these nuclides in the Sierra Nevada is downwelling from the stratosphere during stratocumulus storms. We will measure ^{7}Be, ^{10}Be, and ^{36}Cl in precipitation and soil samples from the Sierra Nevada. Because these nuclides are produced in the upper atmosphere, their measured abundance should serve as an indicator of stratospheric input to the hydrologic system. We will collaborate with researchers at the U.S. Geological Survey and the University of California at Merced to collect these samples. This project will either substantially change hydrologic models or reveal an unrecognized pathway for stratosphere–troposphere exchange that will have significant impact on our understanding of atmospheric circulation, chemistry, and regional climate.

The test of the hypothesis is straightforward. If stratospheric downwelling occurs to the extent necessitated by the observed ^{36}Cl levels in Sierran streams, it should be straightforward to prove it by direct measurement of ^{7}Be, ^{10}Be, and ^{36}Cl in precipitation samples collected from an established array of sampling locations. If elevated levels of these nuclides are not found, it would cast severe doubt on our hypothesis. In this case, Sierran hydrologic models will have to take high levels of groundwater storage into account or appeal to another, unknown mechanism. If elevated levels of these nuclides are found in Sierran precipitation, it could only be from stratospheric input, both because nuclear fallout is no longer occurring and because ^{7}Be and ^{10}Be are not produced by atmospheric nuclear tests.

Mission Relevance

This project supports the Laboratory's national security mission because of its relevance to atmospheric dispersal monitoring for nuclear and other releases. The work also supports the environmental-management mission areas of atmospheric and climate modeling and atmospheric protection from ozone-depleting and greenhouse gases. An ability to characterize certain types of stratosphere–troposphere exchange pathways using relatively inexpensive ground level measurements, as opposed to airborne tropopause measurements, would enhance LLNL's capabilities for testing regional atmospheric and climate models.

FY08 Accomplishments and Results

In FY08, we (1) monitored the network of precipitation samplers installed in FY07 in collaboration with colleagues from the University of California at Merced and the U.S. Geological Survey; (2) collected stream and lake samples to monitor the relationship between precipitation and elevated ^{36}Cl levels; (3) conducted monitoring of high-elevation lakes and streams and determined isotopic tracers, including ^{36}Cl in rainwater, snow, lake, stream, and soil samples; and (4) began compiling and interpreting the results to draw conclusions about the validity of the downwelling hypothesis, which could substantially change hydrologic models or even reveal an unrecognized pathway for stratosphere–troposphere exchange that would significantly impact our understanding of atmospheric circulation, chemistry, and regional climate.

Broad-Area Search for Proliferant Infrastructure

David B. Harris   07-ERD-011

Abstract

This project will determine the feasibility of using long-term observations of ambient noise to detect, locate, and characterize industrial infrastructure. We will use very long-term (1- to 100-day) estimates of coherent noise structures across networks of sensors to detect and locate infrastructure and vehicular and rail traffic that radiate continuous noise-like signals. The ultimate application of this technology is to detect and locate proliferant infrastructure and traffic supporting possible sites of weapons of mass destruction (WMD) development.

We propose to develop (1) methods to detect and enumerate narrowband sources, (2) robust methods to locate narrowband sources, (3) methods to extract source time histories for characterization, and (4) calibration methods for matched field processing to track traffic. We expect to demonstrate the ability to detect and locate the larger components of infrastructure that operate continuously over long intervals and to provide a calibrated capability to track vehicle movement with sensor networks. Examination of long-term ambient noise covariance over sensor networks may select for such sources.

Mission Relevance

This project supports LLNL's nonproliferation mission by providing techniques to implement an indirect strategy of broad-area search for WMD development facilities through detection and location of supporting infrastructure (e.g., power generation). While not likely to directly identify WMD production processes, the techniques could assist in the development of target lists for more specific, shorter-range process-identification methods. These techniques also could help to characterize whether a specific process, once identified, is in operation at a given time and provide some information on power level from relatively far-field observations.

FY08 Accomplishments and Results

We (1) developed a successful detection method that eliminates the need for propagation models and for detailed knowledge of sensor positions, using independence among sources and background noise to achieve processing gain across a network of individual sensors or sensor arrays; (2) deployed a sensor array in a remote rural location and demonstrated that the method works moderately well in such locations; (3) used the method in an urban region to locate and characterize a source from a distance of 70 km; (4) demonstrated the ability of matched field processing to resolve the signal generated by an individual vehicle in a convoy of other vehicles; and (5) experimented with traditional beam-forming methods in realistic field test environments, establishing that such methods exhibit poor performance in detecting and locating industrial machinery because of significant scattering. In summary, this project established the potential for detecting industrial machinery with coherent processing methods operating on networks of sensors and sensor arrays distributed across broad (10,000-km^2) regions. A government agency has expressed interest in the methods developed.

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. There is currently 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 buildings and gas density can produce misleading predictions of plume magnitude, location, or even direction. We are developing an urban dispersion modeling capability that will include both the appropriate dense gas physics and the effects of buildings and complex terrain on atmospheric transport and dispersion, including appropriate source terms. We will validate the model using field data.

Dense gases suppress local atmospheric turbulence, whereas buildings and other obstacles generate atmospheric turbulence. Furthermore, heat transfer, affected by phase change, may either amplify or reduce turbulence. The new, validated denser-than-air simulation tool will represent 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 toxic chemical transport, LNG storage, and carbon dioxide sequestration.

Mission Relevance

This project supports the Laboratory's missions in homeland security, environmental management, and energy security, by enhancing our ability to respond 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.

FY08 Accomplishments and Results

In FY08 we developed and tested some of the physics-based models needed to resolve the effects of buildings and dense gas releases concurrently. Specifically, we (1) refined turbulence modeling with large-eddy simulation by introducing a state-of-the-science, nonlinear sub-grid-scale parameterization into our dense-gas dispersion model; (2) refined the phase-change model; (3) incorporated the capability to model heat transfer from the underlying surface; (4) continued code validation using data from field studies of atmospheric releases of LNG; and (5) completed an assessment of source-term modeling requirements.

Proposed Work for FY09

In FY09 we will (1) complete development of the new dense-gas simulation capability, (2) carry out extensive validation of the new capability using available data from field experiments on complex terrain, (3) continue development of the code's source-term capability, and (4) use the results of high-resolution dense-gas dispersion simulations to improve parameterizations of dense-gas effects for larger-scale models.

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. 10–13, 2007. UCRL-ABS-231188.

Cosmochemical Forensics

Ian D. Hutcheon   07-ERI-005

Abstract

This project uses nuclear forensics to investigate correlated isotopic anomalies associated with short-lived radionuclides (SLNs) and with ^{16}O in calcium–aluminum-rich inclusions (CAIs) from cometary material and meteorites to carry out four cutting-edge scientific tasks: (1) refine the

initial abundance of ^{26}Al in the solar system, (2) determine whether ^{26}Al and ^{16}O originated from a single supernova source, (3) use correlations between ^{10}Be and ^{36}Cl to evaluate the extent of spallation reactions in the nascent solar nebula, and (4) compare the signatures of SLNs and ^{16}O in cometary materials containing normal CAIs. 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) define the initial abundances of four SLNs: ^{10}Be, ^{26}Al, ^{36}Cl, and ^{53}Mn; (2) determine whether SLNs are correlated with ^{16}O; (3) use these data to constrain the relative contributions of massive asymptotic giant branch stars, supernovae, and spallation reactions to the solar nebula; (4) constrain the evolution of oxygen isotope reservoirs in the solar nebula; and (5) determine how CAIs found in samples returned from Comet Wild 2 are related to CAIs found in chondritic meteorites. 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 enhance and refine 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.

FY08 Accomplishments and Results

We analyzed ^{26}Al–^{26}Mn isotope systematics in three coarse-grained Type B Allende CAIs. The internal mineral isochrons yielded initial ^{26}Al–^{27}Al ratios indistinguishable within analytical uncertainty from the value inferred from our bulk Allende CAI measurements. Based on these observations, we inferred that the formation of Allende CAIs—including processes of evaporation, condensation, melting, and crystallization—occurred over a very short time interval, perhaps no more than 20,000 years and possibly as short as 8,000 years. Our new data underscored the need to understand quantitatively the extent to which deviations from an isochron often found with in situ measurement techniques (laser ablation multicollector inductively coupled plasma mass spectrometry and secondary-ion mass spectroscopy) reflect spatially localized diffusion and transport of magnesium isotopes.

Proposed Work for FY09

In FY09, we will develop absolute chronometry techniques to constrain the timing of events in the early solar system. This will provide a link between relative-age dating associated with the short-lived chronometers and the absolute-age dating derived from the application of long-lived isotopic systems. To accomplish this, we will apply a combination of aluminum–magnesium, manganese–chromium, and ^{146}Sm–^{142}Nd short-lived chronometers in conjunction with the long-lived chronometric systems of lead–lead and ^{147}Sm–^{143}Nd to the primitive achondrite meteorite

GRA 06129 and lunar sample 15415. This work will allow the short-lived and long-lived chronometric systems to be linked, thus permitting absolute chronometry to be derived from short-lived isotopic systems.

Publications

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: Eidence for isotopic exchange during nebular melting and asteroidal thermal metamorphism." *Geochim. Cosmochim. Acta* **72**, 2534. LLNL-JRNL-401571.

Makide, K., et al., 2008. "Correlated measurements of O and Mg isotopes in CR CAIs: Constraints on the duration of CAI formation and evolution of oxygen isotopes in the inner solar nebula." *Meteorit. Planet. Sci.* **43**, A88. LLNL-ABS-403768.

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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.

Coordinated Analysis of Geographic Indicators for Nuclear Forensic Route Attribution

Hope A. Ishii   08-ERD-065

Abstract

This project explores the feasibility of determining the route of smuggled nuclear materials via nuclear forensics by determining which types (and combinations of types) of signatures are optimal, as well as over what timescales they are optimal and why. The pathway and means of transport are critical to uncovering smuggling routes and potential distribution points of

illegal nuclear materials. Environmental and geological particulates and surficial deposits will be analyzed in coordinated studies using scanning electronic microscopy, nanometer-scale secondary-ion mass spectroscopy, scanning transmission electron microscopy, nuclear microprobes, gas-chromatography mass spectrometry, and synchrotron-x-ray fluorescence to extract geographically specific signatures (i.e., molecular and trace element chemistry and stable isotope abundances). Each method's accuracy and limitations will be analyzed using real-world materials. Sample recovery from radioactive materials and packaging will be developed using focused ion beams and scanning electronic microscopy micromanipulation and 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 of more efficient and effective route attribution. This project will leverage LLNL's capabilities and expertise in nuclear forensics.

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 analytic techniques.

FY08 Accomplishments and Results

In FY08, we (1) carried out chemical analyses on samples from two different locations and on reference samples of monazite, a rare earth phosphate mineral; (2) used the resulting data to begin building a reference database that will continue to be expanded as new samples are processed; (3) studied the use of differences in rare earth chemistry as a function of geography and the distribution of accompanying minerals as an aid in geolocation to make monazite a useful signature; (4) conducted exposure experiments that successfully demonstrated uptake by pollen, paper, and polymer packaging materials of readily detectable levels of organics used in nuclear materials processing; and (5) began experiments to explore the effects of humidity and desorption.

Proposed Work for FY09

In FY09, we propose to (1) continue organic exposure experiments using isotopically labeled hexadecane to determine adsorption sites by nanoscale secondary-ion mass spectrometry and to explore pollen carrier mechanisms, (2) begin collecting common route clues for comparison with crates used for the transport of nuclear material and collect samples for isotope studies on soil and plant fragments, (3) explore the possibility of using soil isotope signatures for geolocation and determine if plant signatures are correlated, (4) perform controlled oxidation studies with different oxygen isotopes and single and multiple events to determine if rust layers can be used to determine the location of oxidation events, and (5) perform oxygen isotope mapping of actual evidence from the capture of transported nuclear material to determine if existing oxidation layers are differentiable.

An Experimental and Theoretical Approach to Visualize Dechlorinating Bacteria in Porous Media

Walt W. 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, dechlorinating, bioaugmentation culture in a two-dimensional sandbox and in soil cores from an actual contaminated site using various microbiological and molecular biological techniques, and by developing a new mathematical model of bioremediation in chlorinated source zones.

If successful, this project will provide the experimental and theoretical means to approach the much larger problem of understanding how bioremediation works in the immediate vicinity of contaminant source zones. This will enhance LLNL's capabilities in this area and permit collaborations with organizations that specialize in the cleanup of solvent-contaminated sites. Furthermore, this project will result in the publication of the predictive and experimental results in a high profile peer-reviewed journal.

Mission Relevance

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

FY08 Accomplishments and Results

In FY08, we (1) identified candidate stains for visualizing *Dehalococcoides* and developed a protocol to maintain culture viability during tests; (2) successfully tested a visualization method in a two-dimensional sand column using fluorescing polymer beads as surrogates; (3) developed a two-dimensional flow and transport model (based on the finite-difference method and particle tracking), coupled with an ordinary differential-equation system solver, to quantify dehalogenation, bacterial growth, and attachment and detachment rates based on published data; and (4) calibrated our model to fluorescing polymer bead data.

Proposed Work for FY09

In FY09 we will (1) conduct genetic manipulation of the solvent-degrading bioaugmentation culture to produce a fluorescent protein, (2) begin experiments visualizing organisms using sand as a model porous media, (3) fit the numerical model of bioremediation to experimental data, and (4) visualize solvent-degrading organisms in soil cores obtained from a well-characterized site.

Energy Supply and Use
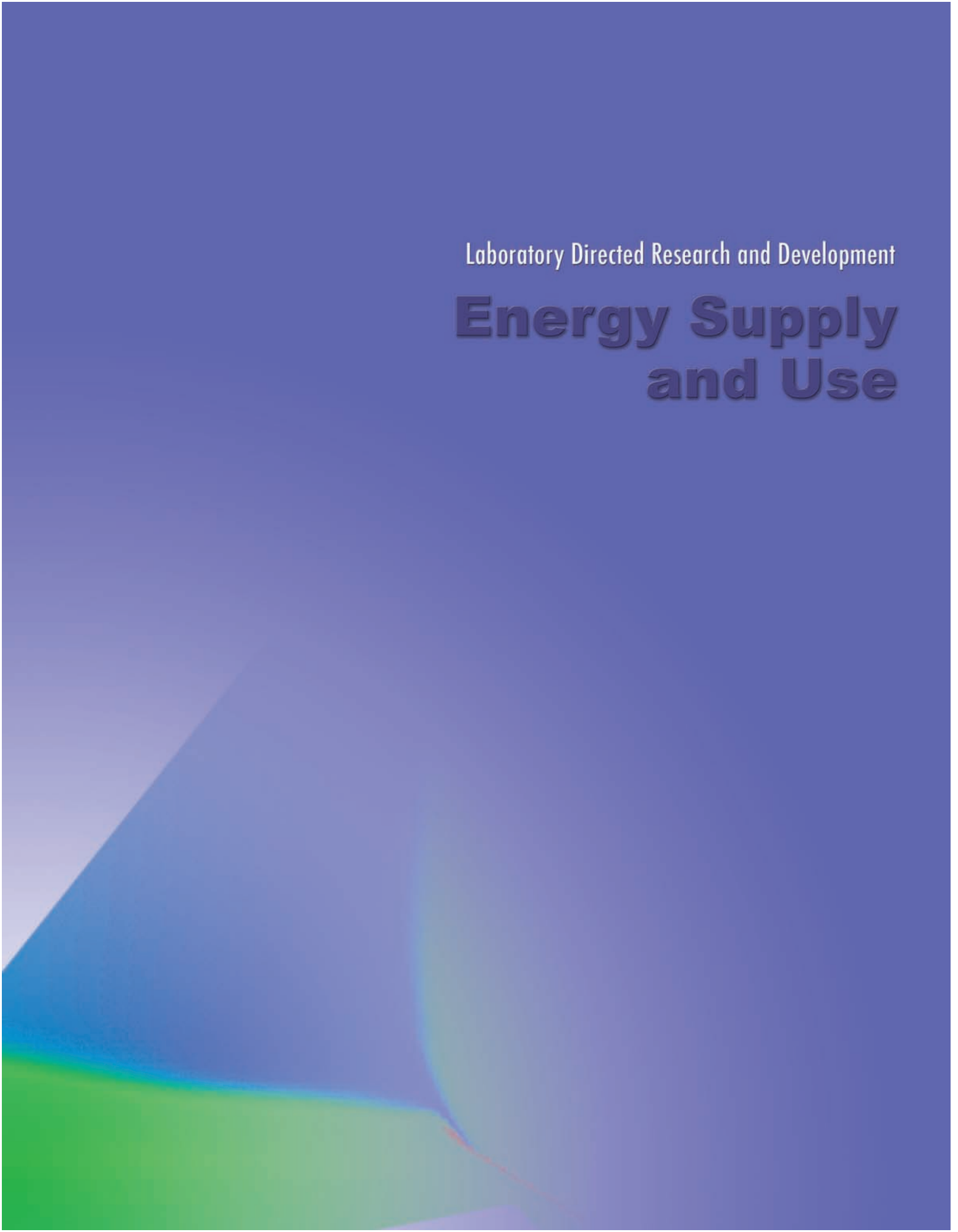
Separation of Carbon Dioxide from Flue Gas Using Ion Pumping

Roger D. Aines   06-ERD-014

Abstract

Cost-effective separation of carbon dioxide (CO_2) from combustion sources is the main limitation to lowering carbon emissions. In this project, we propose to separate CO_2 from flue gas by ionic pumping of carbonate ions dissolved in water. The ion pump dramatically increases dissolved carbonate ion in solution and hence the overlying vapor pressure of CO_2 gas, allowing its removal as a pure gas. This novel approach to increasing the concentration of the extracted gas permits new approaches to treating flue gas, because the slightly basic water used as the extraction medium is impervious to trace acid gases that destroy existing solvents, and no pre-separation is necessary. We will demonstrate the chemistry of the method through modeling and laboratory experiments.

We anticipate that our method will compete favorably with current chemical stripping systems used for CO_2 separation at power plants, which incur a 35% energy penalty. Thus we expect to offer a dramatically improved solution for removing carbon from hydrocarbon combustion. Our method can be demonstrated on small sources, which will enable us to conduct the demonstrations required to build confidence in the method. If successful, we will be in a position to advance a follow-on proposal for a demonstration at the 10-MW scale.

Mission Relevance

This project supports energy security and environmental missions by enhancing currently proposed carbon management options such as technology development for fuel efficiency via fuel cells, hydrogen fuel, and other methods; fossil-fuel recovery; and CO_2 sequestration.

FY08 Accomplishments and Results

In FY08, work on use of the ion pump to drive this process was limited by the ability to recycle the necessary buffer compound. Calculations showed that the cost of separating dissolved buffers would be prohibitive. We therefore developed a system using solid, slurried buffers derived from ion exchange media. These work better with thermal distillation methods than with the ion pump. Tests with the new buffers showed that seawater could be co-processed with flue gas, yielding 3 g of recovered CO_2 per 100 g of purified water. The successful completion of this project demonstrated that a single process can simultaneously separate CO_2 from flue gas (for disposal) and create fresh water (for sale or use as cooling water). This work has attracted interest from the Electric Power Research Institute to evaluate its use in managing CO_2 from power plants while providing water for cooling.

Fossil-Fuel Emission Verification Capability

Thomas P. 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 carbon dioxide emissions from fossil fuels. Accurate assessment of fossil-fuel carbon emissions require highly precise measurements of car emissions and a sampling program with geographic and temporal resolution adequate to determine regional emission profiles. 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 carbon dioxide emissions in California. Issues we will address include solving the inversion problem—numerically estimating the emission magnitude and distribution of chemical species given measurements of chemical concentrations at various locations in the domain.

This project will establish the fossil-fuel emission (carbon-14 dioxide) variability for a metropolitan region in California and create a simulation-based framework for locating and tracking fossil-fuel emissions for California. Completing these two tasks will provide the basis for a fossil-fuel emission verification program for California and establish LLNL as a key resource for implementing national carbon emission verification programs.

Mission Relevance

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

FY08 Accomplishments and Results

In FY08 we utilized the Weather Research and Forecast coupled with chemistry code (WRF-Chem), available meteorological data, and an estimate of fossil-fuel carbon dioxide emissions derived from California Air Resources Board carbon monoxide emissions measurements to explore a hypothetical sampling network design. The bounding meteorological data from one week in January 2006 provided the advective component for the simulation. The inversion solution is close to the input emission field with 10 to 12 idealized sensor locations and an approximately 3-h sampling frequency. We used Federal Aviation Administration hazard designations (transmitters and towers) as a potential network of opportunity for measurement stations and performed a similar inversion, however the hazard locations did not perform as

well as idealized locations. Finally, we initiated a pilot observation program at Walnut Grove, California in collaboration with Lawrence Berkeley National Laboratory and the National Oceanic and Atmospheric Administration, Earth System Research Laboratory. Discrete flask samples and subsequent analyses indicated about 8 to 30 ppm of carbon dioxide above background levels in these air samples was derived from fossil-fuel use.

Proposed Work for FY09

In FY09 we will focus nearly entirely on furthering our inversion methodology under different emission scenarios and atmospheric dispersal regimes (weather patterns). In particular, although state-of-the-art atmospheric models can now be run with a resolution of several kilometers with reasonable fidelity, the nonlinear interactions of some atmospheric chemicals, the chaotic nature of atmospheric equations, and sub-gridscale errors will require scientific advances in the inversion scheme to make it robust in the face of these realities. We will also compare ensemble-averaged emissions estimates with a more limited "real-time" capability.

Publications

Guilderson, T., et al., 2008. *Attribution of carbon in the atmosphere: A fossil fuel emission verification capability and a tool to reduce the uncertainties in the carbon budget.* California Climate Change Conference, Sacramento, CA., Sept. 8–10, 2008. LLNL-ABS-406850.

Direct Simulation of Dynamic Fracturing during Carbon Storage and Prediction of Potential Storage Failures

Joseph P. 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 CO_2 storage. The 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 the caprock, leveraging existing LLNL codes. Specifically, we will modify LDEC (a finite-distinct element code with dynamic fracture and fully coupled fluid-flow capabilities) to directly simulate potential damage within the 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 the 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 creation 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.

FY08 Accomplishments and Results

In FY08 we implemented and tested a fully coupled fluid-flow capability. Specifically, we (1) obtained suitable experimental results for validation and obtained field data from the In Salah Gas Development project; (2) implemented a fully coupled fluid network solver, which was shown to be unmatched in versatility by prior codes, (3) used field data to develop models for caprock and reservoir materials; (4) modified LDEC to simulate tensile and shear failure as being triggered by stress changes induced by a pressurized fluid; (5) compared our results against analytic solutions and began validating our model against recently obtained experimental work; and (6) modified FRAC–HMC for generalized fracture networks.

Proposed Work for FY09

For FY09, we propose to apply the new LDEC capability, coupled with FRAC–HMC, to field-scale problems. Specifically, we will (1) simulate pressurization of water within an existing fracture network—activating existing fractures and creating new fractures—using the LDEC component, (2) evaluate the field-scale impact of dynamic events on permeability using the FRAC–HMC codes, and (3) validate our simulations against field data.

Publications

Morris, J. P., and S. M. Johnson, 2008. *Direct numerical simulation of fluid driven fracturing events with application to carbon sequestration.* 42nd U.S. Rock Mechanics Symp., San Francisco, CA, June 28–July 2, 2008. LLNL-PROC-401947.

Morris, J. P., S. M. Johnson, and S. J. Friedmann, 2008. *Geomechanical simulations of caprock integrity using the Livermore distinct element method.* 7th Ann. Conf. Carbon Capture and Sequestration, Pittsburg, PA, May 5–8, 2008. LLNL-PROC-403056.

Morris, J. P., S. M. Johnson, and S. J. Friedmann, 2008. *Permeability evolution in a fractured rock mass in response to fluid injection.* 2008 Pittsburgh Coal Conf., Pittsburgh, PA, Sept. 29–Oct. 2, 2008. LLNL-CONF-406303.

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 energy efficiency of any internal combustion engine ever built. The engine will enable practical vehicles necessary for transitioning 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 about 80%, and in practice to about 50% after heat transfer and friction losses. Our goal of maximum engine efficiency will be accomplished by conducting fundamental research on basic issues such as ignition, flame propagation, and detonation that control efficiency at the operating conditions of this engine.

Demonstrating this proposed engine requires a fundamental 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 never before explored by theory, simulation, or experiment. We will therefore conduct basic research to characterize the relevant processes and to determine how to achieve optimum efficiency. This project will also pioneer the uncharted territory of the combustion science of hydrogen, oxygen, and argon at high pressures.

Mission Relevance

This research 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 also help in the development of efficient and inexpensive hydrogen-fueled vehicles, accelerating the transition to hydrogen, in support of LLNL's missions in energy security and environmental management.

FY08 Accomplishments and Results

For FY08, we (1) validated our detailed chemical-kinetics model for hydrogen combustion against experimental laminar flame speeds and ignition delay times; (2) constructed a mesh of the experimental engine at the University of California at Berkeley that resolves in-cylinder geometry, including intake and exhaust ports; (3) implemented spark ignition and single-step hydrogen chemical-kinetics models in the KIVA computational fluid dynamics code; (4) developed and used a system-level engine model to determine promising regions of operation for the experimental engine; (5) installed hardware and thoroughly tested the data acquisition code for the experimental engine at Berkeley; and (6) conducted preliminary experimental engine tests to determine ranges of satisfactory operation and produce data for our simulations.

Proposed Work for FY09

In FY09, we will (1) implement our chemical-kinetics model in the KIVA code, (2) implement a flame-propagation model in KIVA and validate it against experimental engine data from Berkeley on both homogeneous charge compression ignition and spark ignition, (3) refine the system-level engine model as we receive data from the experimental engine to further hone in on promising regions of operation for the experimental hydrogen–oxygen–argon engine, and (4) conduct experiments that will test model predictions and demonstrate engine performance, with the aim of reaching or surpassing the 50% efficiency goal and producing an engine performance map that demonstrates efficiency as a function of engine speed and percentage of hydrogen.

Toward More Intrinsically Secure Nuclear Fuel Cycles

Keith S. Bradley   08-ERD-056

Abstract

The rapid worldwide growth in nuclear fission energy poses dramatic risks for the proliferation of nuclear weapons materials. The objective of this project is to assess and enhance the proliferation resistance of advanced nuclear fuel cycles. We will build a process-based understanding and model that will include determining the dynamic and nuclear properties of fuel-cycle mixtures, assessing the attractiveness of various mixtures for use in nuclear explosive devices, and developing the means to reduce that attractiveness. We will focus on one characteristic fuel cycle and several mixtures at critical steps in the cycle.

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 that enhance the nation's ability to counter the 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.

FY08 Accomplishments and Results

In FY08, we (1) established methodologies for assessing nuclear fuel attractiveness and designing nuclear poisons to reduce the utility of nuclear fuels as a source of weapons material; (2) selected a representative set of nuclear weapon classes, developed appropriate equations of state for relevant complex mixtures, and calculated nuclear yield to assess attractiveness of

selected materials; (3) analyzed the effects of fuel burn-up and of varying the abundance of lanthanides resulting from reprocessing; and (4) used the Monteburn code to investigate the feasibility of doping fresh reactor fuel to reduce its utility for nuclear weapons. This led us, for example, to a parabolic mass chain, which ends in an isotope with a large capture cross section and long (90-year) half-life that could serve as a nuclear poison in the spent fuel for a significant period of time.

Proposed Work for FY09

We will (1) refine our understanding of the hydrodynamic properties of material mixtures according to sensitivity studies performed using our baseline numerical descriptions, (2) perform reactor burn calculations (accumulation and depletion) to determine if we can produce the poisoning properties we seek by loading appropriate concentrations of the candidate isotopes, and (3) explore means of making it considerably more difficult for a potential adversary to partition and separate any isotopes deliberately bred inside the nuclear fuel.

Laboratory Directed Research and Development

Engineering and Manufacturing Processes

Study of Transport Behavior and Conversion Efficiency in Pillar-Structured Neutron Detectors

Rebecca J. Nikolić   06-ERD-067

Abstract

A radiation detection device that can be easily fielded and offers high detection efficiency is vital to national security efforts. In this project, we will demonstrate 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 gas-based 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 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.

FY08 Accomplishments and Results

In FY08 we (1) developed methods to etch pillars with a high aspect ratio (i.e., 2-µm diameter versus 50-µm height) and spaced as closely as 2 µm apart and to deposit boron materials between these pillars with a high fill factor; (2) fabricated and characterized a 12-µm-tall pillar detector with a 7.3% thermal neutron detection efficiency; and (3) simulated the pillar detector, including both nuclear physics and semiconductor device physics for efficiency predictions based on geometry and discriminator setting.

Proposed Work for FY09

For FY09, we propose to (1) determine the fundamental scalability limitations of a conformal coating made by boron chemical vapor deposition, (2) study the scalability limitations of the pillar detector, (3) perform alpha and neutron measurements for the detector, (4) benchmark simulated efficiencies with experimental data of varying pillar height, and (5) update the physics-based pillar detector model to account for losses.

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.

Deo, N., et al., 2008. "Conformal filling of silicon micro-pillar platform with boron-10." *J. Vacuum Sci. Tech. B* **26**, 1309. LLNL-JRNL-401189.

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Nikolić, R. J., et al., 2007. "Pillar-structured thermal neutron detector with 6:1 aspect ratio." *Appl. Phys. Lett.* **93**, 133502. LLNL-JRNL-405940.

Standing-Wave Probes for Micrometer-Scale Metrology

Richard M. 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 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 the probe–surface interactions and the resulting uncertainty related to the measurement based on analytical models and experimental results, (3) an assessment of 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 characterizing the dimensional and material properties of low-density materials such as aerogels and metallic foams.

FY08 Accomplishments and Results

In FY08 we (1) implemented an upgrade to our probe and verified increased performance at the nanometer level, which represents a new capability at LLNL; (2) designed both a scaled probe and two-directional probe system based on our modeling efforts, an understanding of the contact physics, and the subsequent dynamics related to probe output and performance; (3) developed a design for two new (two-dimensional and scaled) probe types and initiated prototype development of our other probe systems; and (4) continued collaborations with the University of North Carolina at Charlotte and provided a method for testing the current probe design on geometries relevant to fusion-class laser targets.

Proposed Work for FY09

In FY09 we will (1) test and evaluate the scaled probe system, including addressing measurement issues of micrometer-scaled features, such as small holes; (2) evaluate multidirectional sensitivity by designing and prototyping an experimental system; (3) file a record of invention for the two-dimensional probe; and (4) investigate the proof-of-principle ability to determine properties in relevant materials (an "inverse model") and the ability to use the probe system to modify and measure the surface of foam materials.

Publications

Bauza, M., et al., 2008, "Microscale metrology using standing wave probes." *Proc. 3rd Intl. Conf. Micromanufacturing*, p. 120. LLNL-PROC-406066.

Seugling, R. M., et al., 2008, *Investigating scaling limits of a fiber based resonant probe for metrology applications*. 23rd Ann. Mtg. American Society for Precision Engineering, Portland, OR, Oct. 19–24, 2008. LLNL-PROC-407143.

Ultrahigh-Velocity Railgun

Jerome M. 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 design for achieving velocities of 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.

FY08 Accomplishments and Results

In FY09 we (1) continued simulations of the fixed hybrid armature experiment, (2) simulated actual three-dimensional railguns of a simplified geometry but with high speeds (6 km/s), (3) conducted additional experiments with the fixed hybrid armature apparatus, (4) developed a fiber-optic diagnostic for future experiments, and (5) began refining the magnetohydrodynamic and equation-of-state capabilities of our ALE3D code to reach the levels of detail needed to simulate full HELEOS (Hypervelocity Electromagnetic Launcher for Equation of State) railguns.

Proposed Work for FY09

In FY09 we plan to (1) continue our simulations, refining their agreement with existing data and using them to evaluate various alternative concepts under consideration; (2) obtain an appropriate capacitor bank and assemble a laboratory railgun with diagnostics derived from our fixed hybrid-armature experiment; (3) test our simulation capability on the most promising of the evaluated concepts; (4) refine our simulations and the associated code; and (5) continue, if our schedule permits, the fixed hybrid-armature experiments, further developing diagnostics and

obtaining additional temperature, pressure, and viscosity measurements. We intend to pursue collaborations with Department of Defense experimentalists.

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 Micro-Stereolithography for Advanced Target Fabrication

Christopher M. Spadaccini   08-ERD-053

Abstract

Target fabrication for future fusion-class lasers has been a factor in limiting the scope of potential experiments. Livermore efforts have focused on developing new fabrication techniques that can generate mesoscale to microscale targets with microscale or nanoscale precision. Although much progress has been made, several key target features have been elusive—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 in target fabrication using projection micro-stereolithography and then extend this technique to nanometer-scale resolution, multilayer 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 technique 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.

FY08 Accomplishments and Results

In FY08 we (1) completed a functioning projection micro-stereolithography system utilizing a liquid-crystal-on-silicon chip, having an ultraviolet light-emitting diode array as the light source, and controlled with a graphical interface; (2) began fabricating 3D components; (3) designed and fabricated a plasmonic superlens, began integrating it into the projection micro-stereolithography system, and began fabricating the first nanoscale features; and (4) completed a baseline optical-chemical model that can predict the depth and profile of photopolymerization.

Proposed Work for FY09

For FY09, we propose to (1) finish integrating the plasmonic superlens with the projection micro-stereolithography system, (2) provide a design for the integration of multiple light beams and interference patterns, (3) create a target design tool based on our model, and (4) fabricate structures relevant to laser targets.

Model-Based Flaw Localization from Perturbations in the Dynamic Response of Complex Mechanical Structures

David H. Chambers   08-ERD-063

Abstract

The objective of this project is to determine if a new method of structural flaw localization developed for simple shapes will work for complex mechanical structures. Changes in the dynamic response of a structure to induced vibrations will be used as inputs to a numerical model of the structure to localize the structural source of the changes. Our goal is to significantly reduce the need for disassembly to locate structural flaws in weapon systems. We will apply this new technique to simulated data created from a numerical model of a complex structure.

If successful, we will demonstrate localization of structural flaws in the numerical simulation of a complex structure as a precursor to actual experimental verification on real systems and will develop a prototype analysis system for stockpile stewardship. Our approach could significantly decrease the need for weapons disassembly to verify structural integrity.

Mission Relevance

This project supports the Laboratory's stockpile stewardship mission by developing the capability to computationally identify the location of structural flaws in mechanically complex weapons systems, thereby greatly reducing the need for actual disassembly.

FY08 Accomplishments and Results

In FY08 we (1) generated simulated vibration data using the Nike code for several variations of a model developed for structural analysis; (2) created artificial voids in the numerical models by setting the material density to zero in selected sets of structural elements, then used the Nike code to calculate changes in the structural response caused by the voids; and (3) demonstrated, with three increasingly complex structural models, that the voids can be located from the calculated differences in the vibrational response at a limited set of points. In summary, this project demonstrated that changes in vibrational response can be used to locate structural damage within a structure. This technique has potential applications in support of NNSA's Stockpile Stewardship Program.

Publications

Chambers, D. H., et al., 2008. "Flaw localization in a structure using model-based back propagation." *J. Acoust. Soc. Am.* **124**, 2. LLNL-ABS-404883.

Laboratory Directed Research and Development

Materials Science and Technology
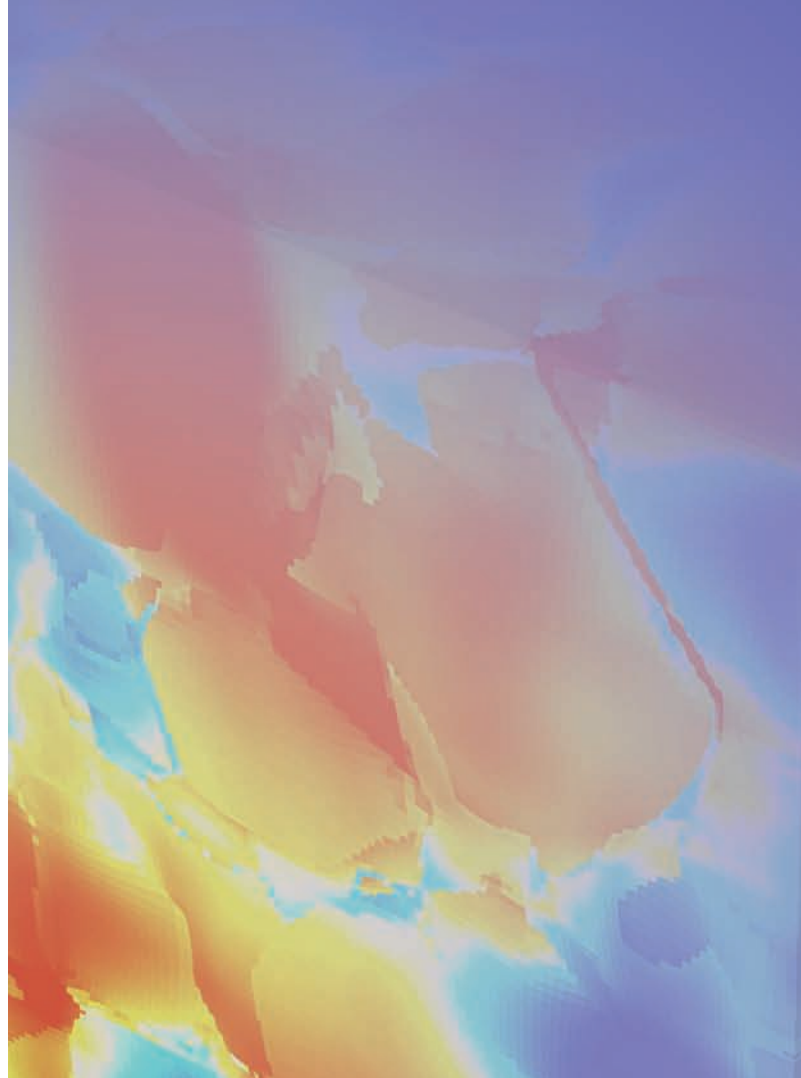
Transformational Materials Initiative

Robert S. Maxwell   **06-SI-005**

Abstract

The goal of this project is to provide the underlying science and technology for converting the U.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, and molecular design.

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.

FY08 Accomplishments and Results

In FY08 we made progress on reaching our research objectives in each of the four project areas: high explosives, multifunctional materials, metals, and sensing. Specifically, we (1) made major advances in energetic materials that demonstrated the ability to recycle historical supplies, with a demonstrated scale of up to 1 kg; (2) synthesized new complex hydrogen-catalyzing fillers; (3) parallelized our quality control codes and employed the codes for studying multivoid collapse; and (4) furthered our efforts to create prototypes of three novel sensors.

Proposed Work for FY09

In FY09, we will (1) complete research on the properties of an advanced high explosive; (2) make a final selection for synthesizing a candidate multifunctional material with hydrogen-acquiring capability and produce a prototype material; (3) demonstrate the feasibility of a large-scale production capability for the powder metallurgy material we developed; (4) integrate refined prototypes developed in FY08 into actual components (material and geometry), including combining the radiofrequency interrogation platform with the completed, curved-surface-contact stress sensor; and (5) build and demonstrate a prototype integrated hollow-fiber-based infrared and Raman system for detecting gas signatures in mixtures.

Publications

Armstrong, M., et al., 2008. "Ultrafast shock wave velocity measurement at high static pressure in a diamond anvil cell." *Appl. Phys. Lett.* **92**, 101930. UCRL-JRNL-232756.

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Maiti, A., et al., 2008. "Solvent screening for a hard-to-dissolve molecular crystal." *Phys. Chem. Chem. Phys.* **10**, 5050. UCRL-JRNL-233158.

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Critical Materials Issues for Generation IV Reactors

Magdalena A. Serrano De Caro   **06-ERD-005**

Abstract

In this project, we will develop predictive tools to calculate structural and mechanical properties of iron–chromium-based alloys, which form the base matrix of advanced ferritic/martensitic steels required for fuel cladding and structural components in Generation IV reactors. Using the paradigm of Multiscale Materials Modeling, we will develop the capability to predict hardening, swelling, and embrittlement. We will link approaches at atomistic and mesoscale levels to create an integrated modeling platform that relates dislocation dynamics to polycrystal plasticity. This will be used to develop engineering-scale materials strength models for irradiated alloys. For validation purposes, our physically based multiscale study will be compared with the existing experimental data over a range of length and time scales.

We expect to provide a detailed physical understanding of iron–chromium alloy behavior and predictions of its mechanical properties critical for resolving technological issues associated with future sources of nuclear energy. Progress in developing advanced reactor concepts is constrained by the behavior of materials under irradiation. Our methodology expands the limits of available science on the thermodynamic and mechanic behavior of metallic alloys. Our modeling results will contribute to an understanding of the performance of nuclear materials and development of new high-temperature, radiation-resistant materials.

Mission Relevance

This project supports Laboratory and DOE missions in long-term energy security by developing scalable materials-science codes to predict nuclear materials properties and their performance under extreme conditions. It will assist efforts to develop future reactor concepts such as the Advanced Burner Reactor envisioned by the DOE's Global Nuclear Energy Partnership initiative. In addition, materials properties codes developed in this project can be used to predict radiation damage to materials important for LLNL's stockpile stewardship mission.

FY08 Accomplishments and Results

We finished short-range order precipitation studies with iron-rich iron–chromium and made progress in determining the dislocation mobility in iron–chromium as a function of short-range order. In summary, this project developed a classical potential-based methodology that captures the essentials of the energetics and thermodynamics of the iron–chromium system using an innovative approach that allowed us to explain experimental findings at the atomic level in binary iron–chromium alloys. In addition, steps were successfully taken towards establishing the connection between atomistic and mesoscale modeling (i.e., dislocation dynamics). Work is already underway to extend these achievements to multicomponent materials and to enable further experimental comparison and validation.

Publications

Caro, M., P. Erhart, and A. Caro, 2007. "Precipitation, segregation and the origin of corrosion resistance of Fe–Cr alloys." Materials Research Society 2007 Fall Meeting, Boston, MA, Dec. 1–5, 2007. UCRL-PRES-237179.

Erhart, P., B. Sadigh, and A. Caro, 2008. "Are there stable long-range ordered $Fe_{1-x}Cr_x$ compounds?" *Appl. Phys. Lett.* **92**, 141904. UCRL-JRNL-236439.

Erhart, P. et al., 2008. "Short-range order and precipitation in Fe-rich Fe–Cr alloys." UCRL-JRNL-232916-DRAFT.

Martinez, E., et al. 2008. "A dislocation dynamics study of the strength of stacking fault tetrahedra. Part I: interactions with screw dislocations." *Philos. Mag.* **88**, 809. UCRL-JRNL-235520.

Fundamental Investigation of Laser-Induced Surface Damage in Optical Materials

Jeffrey D. Bude   06-ERD-035

Abstract

The objective of this research is to develop a fundamental understanding of laser-induced surface damage in optical materials—specifically, fused silica. Despite its excellent ultraviolet transparency, silica undergoes damage from high ultraviolet fluence. Although intrinsic bulk damage is relatively well understood, extrinsic surface damage, dominant in high-quality silica, is not. This work will develop a suite of high-resolution optical techniques and advanced computational models to help clarify the processes behind surface damage in fused silica.

We expect to (1) identify the defects that absorb sub-bandgap light and lead to surface damage, (2) develop methods to directly measure laser-energy absorption in the near-surface region of fused silica for fluences below the damage threshold, and (3) correlate energy absorption to damage probability. These tasks will help address major gaps in our understanding of the basic processes that lead to extrinsic surface damage: free-carrier generation by defects, free-carrier absorption in silica, and thermally induced runaway absorption.

Mission Relevance

This work directly addresses stockpile stewardship and laser fusion challenges by optimizing use of large fusion-class laser systems. It also will serve to establish science-based rules for optics reliability predictions, improve damage diagnostics, and suggest pathways to increase damage resistance in optical materials. By furthering the understanding of structural and electronic transitions in glasses and disordered materials—a frontier problem in condensed-matter physics—this project contributes to the Laboratory's mission in fundamental science and technology.

FY08 Accomplishments and Results

In FY08, we (1) performed lifetime-damage correlations to test the photoluminescence damage diagnostic and found good correlation with damage, which was critical in developing new damage-mitigation techniques; (2) designed and began testing a microdamage and photoluminescence capability; (3) performed surface and defect absorption simulations; (4) developed a direct surface temperature measurement technique accurate enough to eliminate the need for damage tests in a furnace; and (5) performed surface conditioning experiments and analyzed the results. This project made considerable progress towards developing a fundamental understanding of silica surface damage, provided promising new diagnostics for optical damage, and identified a novel near-metallic photoluminescence in fractured silica that may offer new insights into the electronic structure of dielectric surfaces. Results from this work will help develop more damage-resistant silica optics and new damage-mitigation techniques for fusion-class lasers.

Publications

Laurence, T. A., et al., in press. "Near-surface metallic-like photoluminescence and absorption in wide-band-gap materials." *Science*. LLNL-JRNL-407531.

Large-Aperture Optics Performance

Thomas G. Parham   06-ERD-054

Abstract

The performance of large-aperture optics has traditionally limited the maximum output of large fusion-class lasers. Prior work has not employed realistic testbeds that allow large-aperture optics to be studied in the same way they will actually be used in large laser systems. Especially important is the effect of unconverted 1ω and 2ω light on 3ω damage. Our project will evaluate large optics at full aperture with unconverted light present and with the statistical fluctuations that are typical of large-aperture lasers. Specialized optomechanical hardware that edge-illuminates optics will be coupled with extensive laser diagnostics in an existing large-aperture laser system, called the Precision Diagnostic System, to allow in situ analysis of damage initiation and growth.

Materials research that enhances our understanding of complex mechanisms involving the response of optical materials to intense laser irradiation will benefit the development of ever more powerful, fusion-class laser systems and allow such lasers to operate efficiently and reliably at or above their design specifications. Our modeling efforts will allow operators of fusion-class laser systems to predict the effects of experiments on the lifetime of optics and allow them to optimize experiments to minimize the costs of replacing optical components. In addition, this project will help ensure LLNL's continued leadership in the fields of optical materials science and laser technology.

Mission Relevance

This work will add substantially to the knowledge base of optical materials under the intense laser illumination of fusion-class lasers systems, and allow us to validate our theoretical and stochastic models. This work supports the Laboratory's mission in the national security area of stockpile stewardship, because safety and reliability of the nuclear stockpile in the absence of testing will rely heavily on experimental data from fusion-class laser systems to validate complex computer simulations.

FY08 Accomplishments and Results

In FY08, we (1) completed a final Precision Diagnostic System campaign and performed analyses; (2) demonstrated that damage to grating debris shields was caused by stimulated

Brillouin scattering pumped by higher diffractive orders of the grating and that it could be eliminated by modulating the main laser wavelength; (3) installed a new optics-damage inspection system, used it to monitor optics damage during 21 relevant shots on up to 20 beams/shot, and identified a new gravity-induced ghost damage on mirrors; (4) collected flaw metrology on a large number of final optics; and (5) mapped full-aperture damage versus local fluence to create high-quality initiation density versus fluence data, allowing improved prediction of damage initiation, which we subsequently implemented in a multi-beam damage prediction code. The successful conclusion of this project has demonstrated the importance of evaluating system-wide interactions to understand and minimize damage in large laser systems and has provided numerous tools to make this task easier to accomplish. The techniques established in this project may be applied on any large laser system and will form the future basis for controlling damage on National Ignition Facility optics, thus potentially improving the facility's operating cost.

Publications

Heestand, G. M., et al., 2008. "Demonstration of high-energy 2ω (526.5 nm) operation on the National Ignition Facility Laser System." *Appl. Optic.* **47**(19), 3494. UCRL-JRNL-237242.

Kinetics of Phase Evolution: Coupling Microstructure with Deformation

James F. 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 (MD) techniques for nucleation to hydrodynamic length and time scales. Phase and microstructure calculated by MD will serve as initial conditions for our continuum microstructure evolution model, whose dynamics will be validated with MD 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 solidification and solid–solid phase transformation under extreme conditions at relevant length and time scales—a prediction observable on emerging x-ray platforms such as the Linac Coherent Light Source at Stanford. This prediction is directly tied to MD simulations of nucleated microstructure using potentials applicable to metals and alloys of interest, and extends the MD results to hydrodynamic length and time scales. We will create the first phase-field modeling capability scalable to LLNL's high-performance computing resources. By using this microstructure to calculate material behavior, we will increase confidence in calculations at extreme conditions, for which experimental data are either obtained indirectly or entirely lacking.

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.

FY08 Accomplishments and Results

During FY08, we (1) extended our crystallographically aware adaptive-mesh phase-field code (AMPE) to include the physics of elasticity, grain boundaries, alloys, and thermal fluctuations, using overlapping MD simulations to parameterize these models; (2) coupled AMPE to the CALPHAD free-energy form to solve the concurrent diffusion of alloy content during phase transformation; (3) used the order parameter field from the MD simulation to initialize the phase-field code and to observe the formation of a grain size length-scale at the hydrodynamic time scale (the latter was made possible by implementing a new implicit time integration for long-time simulations); and (4) showed the code to be scalable to thousands of processors.

Proposed Work for FY09

In FY09 we will (1) simulate emerging experiments on fast x-ray and electron systems to both constrain our nucleation models and validate our simulations, (2) develop new numerical solutions of our coupled multiphysics models, (3) use the free-energy representation of multiphase equations of state to quantify the formation of microstructures under extreme conditions in metals and alloys, and (4) analyze the role of impurities such as helium on the formation of microstructures. Our goal is to implement anisotropic elasticity, which will make our AMPE code the most sophisticated phase-field code in existence, with the capability of modeling phase transformation and microstructure evolution in metals and alloys during finite deformation.

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.

Belak, J., et al., 2008. *Coupling of atomistic and meso-scale phase-field modeling of rapid solidification.* 4th Intl. Conf. Multiscale Materials Modeling, Tallahassee, FL, Oct. 27–31, 2008. LLNL-ABS-401826.

Belak, J., et al., 2008. *Molecular dynamics validation of phase field modeling.* 2008 TMS Ann. Mtg., New Orleans, LA, Mar. 9–13, 2008. LLNL-PRES-402132.

Dorr, M., et al., 2008. "The numerical solution of a crystallographically aware phase field model." *Proc. 2008 SIAM Conf. Mathematical Aspects of Materials Science.* LLNL-PRES-404101.

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

Vincenzo Lordi   07-ERD-013

Abstract

The nature of carrier dynamics and lifetimes in the complex semiconductors used in gamma-ray detection are 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 "toolbox" for predicting the structural, electronic, and transport properties of candidate semiconductor detector materials. For a given candidate material, the toolbox will help evaluate formation energies of defects and predict how carrier mobilities and lifetimes are determined by these defects. This fundamental understanding of the sensitivity of transport properties to material structure will help identify promising semiconductor materials.

This project will provide initial information on the nature of electron and hole states in semiconductor materials for gamma-ray detection 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.

FY08 Accomplishments and Results

We (1) determined the structures, relative equilibrium concentrations, and scattering rates of all native defects in cadmium telluride, finding cadmium vacancy to be an important, strong scattering defect and finding telluride interstitials to have high scattering rates but a low equilibrium concentration; (2) began kinetic Monte Carlo simulations of defect diffusion to study annealing dynamics; (3) implemented a cluster expansion code to treat alloy effects, enabling study of the effects of composition and structural order on transport properties as the basis for materials discovery efforts; and (4) implemented ab initio methods to calculate carrier trapping rates to predict carrier lifetimes.

Proposed Work for FY09

In FY09, we will focus on (1) calculating trapping lifetimes of the most relevant native and impurity defects in the materials of interest; (2) extend our work to cover additional materials systems, including gallium telluride and alloys such as cadmium–zinc–tellurium and aluminum–gallium–antimony; and (3) develop tools to enable computational combinatorial chemistry, in which we use these predictive techniques to identify new candidate semiconductor materials with enhanced performance characteristics.

Publications

Aberg, D., et al., 2007. *Effects of point defects on carrier transport in bulk Al–Sb.* 2007 IEEE Nuclear Science Symp. and Medical Imaging Conf., Honolulu, HI, Oct. 27–Nov. 3, 2007. UCRL-POST-234208.

Aberg, D., et al., 2008. "Intrinsic point defects in aluminum antimonide." *Phys. Rev. B* **77**, 165206. UCRL-JRNL-234774.

Erhart, P., et al., 2008. *Defect engineering of Al–Sb for improved room-temperature gamma radiation detection.* Nuclear Science Symposium, Dresden, Germany, Oct. 18–25, 2008. LLNL-ABS-403822.

Lordi, V., D. Aberg, and P. Erhart, 2008. *Effects of point defects on the electrical properties of aluminum antimonide—a first-principles investigation.* 2008 Symp. Radiation Measurements and Applications, Berkeley, CA, June 2–5, 2008. UCRL-ABS-236812.

Tringe, J. W., et al., in press. "Radiation effects on InGaN quantum wells and GaN simultaneously probed by ion beam-induced luminescence." *IEEE T. Nucl. Sci.* LLNL-JRNL-403115.

Vo, T. T. M., et al., 2008. "Atomistic design of thermoelectric properties of silicon nanowires." *Nano Lett.* **8**, 1111. LLNL-JRNL-408000.

Deformation of Low-Symmetry and Multiphase Materials

Nathan R. 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 constructing macroscale constitutive models. We are developing an approach that allows for explicit incorporation of microstructure and deformational heterogeneity in a framework appropriate

to use in analysis of engineering-scale components. In multiphase materials, microstructure influences yield stress, ductility, high- 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 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 effective treatment of deformational heterogeneities at the microstructural scale, and we will build on emerging technologies for effectively combining 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 both characterize and model 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 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 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 behavior of these materials is also critical to the Responsive Infrastructure initiative at NNSA and to industrial production of a vast range of consumer goods. Finally, it contributes to the Laboratory's mission in advancing basic materials and computational science.

FY08 Accomplishments and Results

For FY08, we (1) implemented and tested a new parameterized plastic-flow algorithm appropriate to embedding in deformation-driven fine-scale models; (2) explored various strategies for robust time integration; (3) performed finite-element calculations at the polycrystalline aggregate scale for both the Ti–6Al–4V alloy and $CaIrO_3$ post-perovskite and calculated sub-grain heterogeneities—calculations on $CaIrO_3$ demonstrate extensibility of the method to other low-symmetry materials; (4) developed methods for extracting salient features of the response, including distributions of strain energy; and (5) captured strain localization events at the coarse scale with simulations of integrated experiments such as Taylor cylinder impact and compression tests with frictional effects.

Proposed Work for FY09

Work in FY09 will focus on enabling the evolution of more detailed fine-scale state descriptors for our model, specifically including probability distribution functions for lattice orientation. In addition, we propose to enable mechanical deformation by twinning, a common deformation mechanism in low-symmetry materials that produces an abrupt change in lattice orientation. The new capabilities will be based on discrete harmonic expansion, with flexible, independent-control accuracy in initial-state representation and evolution of state. The material used will be alpha uranium. Accuracy will be assessed according to the order of expansion.

Publications

Barton, N. R., 2008. *Novel algorithms in computational materials science: Enabling adaptive sampling.* Advanced Scientific Computing Research Computer Science Research Principal Investigators Mtg., Denver, CO, Mar. 31–Apr. 2, 2008. LLNL-PRES-402559.

Barton, N. R., et al., in press. "Direct 3D simulation of plastic flow from EBSD data." *Electron Backscatter Diffraction in Materials Science.* 2nd Ed. Kluwer Academic/Plenum Publishers, New York. LLNL-JRNL-405176.

Barton, N. R., et al., 2008. "Embedded polycrystal plasticity and adaptive sampling." *Int. J. Plast.* **24**, 242. UCRL-JRNL-226715.

Bernier, J. V., N. R. Barton, and J. Knap, 2008. "Polycrystal plasticity based predictions of strain localization in metal forming." *J. Eng. Mater. Technol.* **130**(2), 021020. UCRL-JRNL-233796.

Bernier, J. V., et al., 2008. *Capturing strain localization via embedded polycrystal plasticity and in situ adaptive tabulation.* International Symp. Plasticity, Kona, HI, Jan. 3–8, 2008. LLNL-PRES-400081.

Knap, J., et al., 2008. "Adaptive sampling in hierarchical simulation." *Int. J. Numer. Meth. Eng.* **76**(4), 572. UCRL-JRNL-232594.

Plasticity at High Pressures and Strain Rates Using Oblique-Impact Isentropic-Compression Experiments

Jeffrey N. Florando   **07-ERD-034**

Abstract

Various aspects of the Laboratory's national security mission depend on accurate computer 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 rate, uncertainty still exists in understanding the strength of materials under conditions of 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 enhance the Laboratory's ability to develop predictive strength models for use in computer 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 that have never been explored. An understanding of the deformation mechanisms at work under these conditions will lead to development of more accurate strength models. An initial feasibility study using computer 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 be modified for fielding 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 an important component of the Stockpile Stewardship Program. This project supports the stockpile stewardship mission by providing previously unobtainable experimental data on materials strength under those conditions.

FY08 Accomplishments and Results

In FY08 we (1) tested vanadium samples at Brown University and achieved results that will aid in understanding strength under pressure—because of the need to perform additional scoping experiments, only low-pressure shots were performed; (2) discovered, after analyzing the data, that experiments with the 1-in. impactor had strain rates that allowed us to measure essential wave data; (3) characterized samples without having to use special soft-recovery experiments, because only low-pressure shots were performed; and (4) conducted a series of simulations to examine sensitivity of the technique to parameters such as strength, hardening, and friction, and to explore experimental designs.

Proposed Work for FY09

In FY09 we plan to (1) continue experiments on copper and vanadium at higher pressures (20–30 GPa) and velocities (300–700 m/s) with the larger gas gun to measure and understand strength under moderate pressure and strain rates, (2) use this information to refine and develop strength models, (3) explore designs to achieve even higher pressures (>50 GPa), and (4) publish our results in a peer-reviewed journal.

Investigation of the Double-C Behavior in the Plutonium–Gallium Time–Temperature–Transformation Diagram

Kerri Jayne M. 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 the transformation of these alloys has remained unsolved ever since. This project aims to study and explain this unusual behavior, which is important because it will help to connect 5f electronic structure to 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 the 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 whether 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.

FY08 Accomplishments and Results

We (1) collected optical micrographs in the upper and lower C curves, indicating that the alpha prime morphology is the same in the two C curves and that its formation is a function of ambient temperature conditioning; (2) formulated a plan for studying the double-C curve as a function of conditioning, hypothesizing that conditioning enables the lower C curve; (3) began mapping the time–temperature–transformation curves as a function of temperature; and (4) designed a sample holder and conducted x-ray diffraction experiments at the Advanced Photon Source.

Proposed Work for FY09

In FY09 we will complete the experimental work necessary to create a phenomenological model to explain the reason for double-C curve kinetics in the delta-to-alpha prime transformation in plutonium–gallium alloys. Because segregation of gallium to grain centers can occur in these materials, we will use differential scanning calorimetry and optical microscopy to assess the effects of gallium homogenization on double-C curve kinetics. With our understanding of the fundamental mechanisms responsible for the double-C curve kinetics, we will provide an assessment relevant to stockpile stewardship of how the phase transformation may change with age and how it occurs under pressure.

Publications

Blobaum, K. J. M., et al., 2008. *Enabling the double-C curve in Pu–Ga alloy time-temperature transformation diagrams: The importance of conditioning.* Plutonium Futures—The Science 2008, Dijon, France, July 7–11, 2008. LLNL-PRES-404831.

Jeffries, J. R., et al., 2008. *Ambient-temperature conditioning as a probe of double-C transformation mechanisms in Pu 2.0 at.% Ga.* American Physical Society March Meeting, New Orleans, LA, Mar. 10–14, 2008. LLNL-PRES-402042.

Jeffries, J. R., et al., 2008. "Ambient-temperature conditioning as a probe of double-C transformation mechanisms in Pu 2.0 at.% Ga." *Mater. Res. Soc. Proc.* **1104**, NN01. LLNL-PROC-402757.

Jeffries, J. R., et al., 2008. *Conditioning and its effects on the delta to alpha-prime isothermal martensite in Pu 2.0 at.% Ga.* Fundamental Plutonium Properties Workshop, Snezhinsk, Russia, Sept. 12–16, 2008. LLNL-POST-406541.

Jeffries, J. R., et al., 2008. *Conditioning and its effects on the delta to alpha-prime isothermal martensitic transformation in Pu–Ga.* Plutonium Futures—The Science 2008, Dijon, France, July 7–11, 2008. LLNL-POST-404840.

Jeffries, J. R., et al., 2008. *Enabling the double-C curve in the Pu–Ga time-temperature-transformation diagram.* Fundamental Plutonium Properties Workshop, Snezhinsk, Russia, Sept. 12–16, 2008. LLNL-PRES-406540.

Controlling the Structure of a Quantum Solid: Hydrogen

George H. 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 the nucleation and growth of crystalline films have shown that chemically patterned substrates can be used to direct the orientation, morphology, polymorph, and size of nucleating crystals. Moreover, use of amorphous materials to create smooth, homogeneous films is an area of active research. The purpose of this project is to explore two approaches to control the nucleation, growth, and defect population of hydrogen isotope crystals. The first is to develop templates that will provide preferential nucleation sites and set the orientation of the crystalline material. The second is to make the hydrogen lattice amorphous or fine-grained using particle bombardment. This project will combine atomistic simulations with experiments to better control the crystal structure.

Hydrogen isotopes provide a challenging but rich system for better understanding 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 the solid amorphous using particle radiation. The isotopes can be accurately modeled as computationally simple, point-interacting van der Waals molecules. Thus, this project's 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.

FY08 Accomplishments and Results

We (1) extended experiments on templates to include self-assembled monolayers and discovered a novel property that can be applied to enhancing single-crystal film growth in fusion target capsules; (2) conducted molecular dynamics simulations to elucidate the mechanism by which self-assembled monolayers inhibit the formation of dihydrogen, finding that the dihydrogen molecules penetrate the self-assembled monolayers, forming an amorphous mixture; (3) simulated the response of dihydrogen and dideuterium to strain fields, finding that film delamination occurs at strains of 7% and greater and determined that perfect dihydrogen and dideuterium single-crystal cylinders subjected to tensile stress can exhibit phase transformation from closely packed hexagonal to face-centered cubic; and (4) developed a powerful new technique based on exact path-integral formalism to improve the accuracy of our modeling of quantum effects.

Proposed Work for FY09

In FY09, we will modify our cryogenic stage to incorporate Raman spectroscopy for analyzing the structure and orientation of hydrogen crystals. Specifically, we will (1) use single-crystal gold templates with two different crystal orientations to study their epitaxial effects, along with nickel templates, on which hydrogen exhibits a very different adsorption behavior; (2) develop a novel large-scale molecular dynamics technique that includes higher-order quantum effects; (3) perform the first definitive calculations of the structure and energy of free surfaces and grain boundaries of a hydrogen crystal as a function of temperature and external stress, which is applicable to hydrogen solidification inside spheres; and (4) obtain atomic-scale data to determine the cause of stress development during hydrogen deposition.

Magnetism in Semiconductor Nanocrystals: New Physics at the Nanoscale

Robert W. Meulenberg   07-LW-041

Abstract

The novel magnetic effects that we recently discovered in cadmium selenide nanocrystals represent a new field of physics in nanoscience. This project aims to understand how these magnetic properties arise and how they can be manipulated. We will systematically tune particle size and surface functionality and explore their effect on the magnetic properties. In turn, we hope to formulate ways to optimize and control the strength of the magnetic effect. This work will lead to a model for how the surfaces of cadmium selenide nanocrystals influence their properties, and will have applications in a range of sensor applications.

We will look for a systematic relationship between surface termination, particle size, and magnetism in cadmium selenide nanocrystals. Measurements of x-ray magnetic circular dichroism (XMCD) at a synchrotron facility will enable us to identify the chemical source of the magnetism. In addition, more detailed magnetic measurements will provide insight into the

strength of magnetism in cadmium selenide samples. These studies represent very significant cutting-edge physics experiments. If initial measurements are confirmed, publication of these results in high-profile journals is very likely.

Mission Relevance

Cadmium selenide nanocrystals have potential applications in chemical sensors and bioassays based on magneto-optical effects. By establishing an understanding of how the surfaces influence the properties of these particles, this project supports the Laboratory's missions in homeland and national security through development of new sensors.

FY08 Accomplishments and Results

We (1) successfully performed XMCD studies of cadmium selenide nanoparticles at Argonne National Laboratory's Advanced Photon Source; (2) analyzed the XMCD data, compared it with superconducting quantum interference device studies, and thereby identified the mechanism by which changing the surface chemistry of the nanoparticles controls the degree of magnetization (we also filed a patent application based upon this research); and (3) built on work conducted in FY07 by experimentally identifying the size-dependent scaling of the exciton binding energy for cadmium selenide. The next step would be to measure the photoluminescence of cadmium selenide particles under intense magnetic fields to modify the light that is emitted. Coupling the light and magnetic field could result in very unique polarization effects, and such measurements would be the initial steps needed to fabricate devices based on these new physics discovered in this project.

Publications

Lee, J. R. I., et al., 2007. *Electronic structure studies of Cd–Se nanocrystals using synchrotron radiation.* 15th Intl. Conf. Crystal Growth, Salt Lake City, UT, Aug. 12–17, 2007. UCRL-PRES-224556.

Nanomaterials for Fusion Application Targets

Alex V. Hamza   08-SI-004

Abstract

Assembly of functional nanomaterials requires atomic-level control of the synthetic processes involved. Complex nuclear fusion laser targets for studying the mix in burning hydrogen plasmas, nuclear physics in high-neutron-brightness environments, and fast-ignition for inertial-confinement fusion (ICF) energy require precisely placing nanoporous materials and small quantities of dopants inside a target capsule. Innovative synthesis and manipulation 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 establishment of a capability for the 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, absorbtive, 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 weapons physics, (2) investigate the dynamics of nuclear excited states, (3) pursue ICF fast ignition, and (4) create new materials for catalysis, hydrogen storage, and self-healing nuclear reactor materials.

FY08 Accomplishments and Results

In FY08, we loaded an ICF capsule and cast nanoporous foam by spinning the precursor in 1-cm capsules to create nanoporous layers. Specifically, we (1) chemically blocked active sites on nanoporous materials to prevent atomic layer deposition—the sites are reactivated by thermal or oxygen plasma treatment, (2) used x-ray scattering to measure the effects of wetting of organic aerogels with liquid hydrogen—scattering changes are reversible upon removal of liquid hydrogen, and (3) used in situ stress monitoring to correlate a massive texture change in thick beryllium films with stress evolution. The texture change was induced by biasing the substrate, thereby changing the initial stress state from tensile to compressive.

Proposed Work for FY09

We will (1) create thin films of aerogels in target capsules—for example by growing cross-linkable polymer brushes; (2) use in situ x-ray techniques to study the effect of aerogel morphology on wetting with liquid hydrogen; (3) install an atomic-layer deposition system and develop novel deposition precursor chemistries for high atomic-number doping, including attempting area-selective doping through spatially selective modifications of the substrate; (4) add new functionalities to our nanomanipulator to measure thickness profiles from three-dimensional targets and to apply picoliter amounts of liquids; (5) continue to work on stress control in metal deposition and improve our predictive multiscale tools; and (6) model mixing at the interfaces between ablator and fuel and between doped and undoped fuel regions.

Publications

Detor, A. J., 2008. "Atomistic simulations of grain coalescence." *Phys. Rev. B* **78**(14), 144113. LLNL-JRNL-405099.

King, J. S., et al., 2008. "Ultralow loading Pt nanocatalysts prepared by atomic layer deposition on carbon aerogels." *Nano Lett.* **8**(8), 2405. LLNL-JRNL-403291.

Dynamics of Material Motion and Transformation Following Localized Laser-Energy Deposition in Transparent Dielectrics

Stavros G. 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 microshadowgraphy 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-class 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 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.

FY08 Accomplishments and Results

We (1) developed two portable diagnostic systems and performed detailed measurements through the entire timeline of dynamic events of bulk damage as well as surface damage for system characterization and optimization; (2) developed different approaches to image the formation of electronic excitations, crack propagation, material with transient absorption properties (an unexpected feature), melted regions, shock and stress waves, and ejecta; (3) used a probe laser with a 150-ps pulse length to achieve image resolution of dynamic events comparable to that of the static resolution of the imaging system of about 1 μm; and (4) explored hydrodynamic codes to model initial experimental observations.

Proposed Work for FY09

For FY09 we propose to (1) acquire 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) measure the kinetics of ejecta during surface damage initiation and growth; and (3) employ modeling tools to explain our experimental results. Our overall aim is to probe the sequence of events—including electronic excitations, material modifications, and pressure and shock wave propagation—that are responsible for energy deposition by the laser pulse to understand the physics that lead to the appearance of damage sites at different excitation conditions.

Publications

DeMange, P., et al. 2008. "The energy-coupling efficiency of multi-wavelength laser pulses to damage initiating defects in DKDP nonlinear crystals." *J. Appl. Phys.* **103**, 083122. UCRL-JRNL-234949.

Feit, M. D., et al., 2007. "Does complex absorption behavior leading to conditioning and damage in KDP/DKDP reflect the electronic structure of initiators?" *Proc. SPIE* **6720**, 672005. UCRL-PROC-236469.

Guss, G. M., et al., 2008. "In situ monitoring of surface post-processing in large-aperture fused-silica optics with optical coherence tomography." *Appl. Optic.* **47**, 4569. LLNL-JRNL-401368.

Negres, R. A., M. D. Feit, and S. G. Demos, 2007. "Pump and probe damage testing for investigation of transient material modifications associated with laser damage in optical materials." *Proc. SPIE* **6720**, 672019. UCRL-PROC-235690.

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 F. 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 on "Ceramic Laser Materials" (05-ERD-037) 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, which would remove preferential absorption near the edge during edge pumping or provide specified gain profiles. Another approach we will investigate is guiding pump light to optically active regions, hopefully resulting in a method in which different optically active ions are used in different regions to produce amplifier slabs that suppress amplified spontaneous emission, enabling much larger aperture slabs of high-gain materials. In addition, new ceramic laser materials we develop could provide, for example, long storage lifetimes while requiring significantly fewer laser diode arrays for inversion.

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 efficient laser geometries for applications in stockpile stewardship and fusion energy, in support of the Laboratory's national security and energy security missions.

FY08 Accomplishments and Results

During FY08, we (1) installed and tested the new hot isostatic press (HIP) and purchased and installed a new vacuum furnace for fabricating large parts; (2) pressed and sintered neodymium–YAG and undoped YAG-paired materials at various temperatures and times and characterized and modeled neodymium ion diffusion, which has implications for tailored parts; (3) developed the novel method of direct coagulation casting for creating large and tailored parts—parts fabricated using this new method were sintered with the HIP, yielding parts with high transparency; and (4) used this new method instead of tape casting or other casting methods to produce tailored-aperture ceramic laser parts, and have begun sintering large and tailored parts in the new vacuum furnace.

Proposed Work for FY09

In FY09 we will build on work accomplished in FY08 by (1) completing the small-scale transparent ceramic parts lab, including qualifying and operating our state-of-the-art tungsten sinter HIP and installing a large tungsten vacuum hot press to establish a capability to produce prototype parts; (2) modifying the process developed in FY08 to attempt to use our sinter HIP and slip-cast flame-sprayed powders to produce parts that are closer to those needed for eventual applications; (3) developing robust processes for producing composite preformed transparent ceramic parts and characterizing them; (4) developing improved methods for producing graded doping laser parts; (5) modeling the performance of lasers made from

composite ceramics, including beam quality and heat transfer; and (6) building on the previous five tasks to take a key step toward our final technical goal by fabricating small-scale lasers made of integral composite ceramics.

Publications

Kuntz, J., J. Hollingsworth, and T. Soules, 2007. *Transparent ceramics for lasers.* UCRL-JRNL-237245.

Soules, T., 2008. *Advanced transparent ceramics for lasers.* 4th Laser Ceramics Symp., Shanghai, China, Nov. 10–14, 2008. LLNL-PRES-408301.

Direct Continuum Simulation of Collective Void Nucleation and Growth in a Plastic Medium

Matthew J. Busche   08-ERD-029

Abstract

While spall has been investigated for nearly a century, details of spall evolution have been inaccessible experimentally, and models have been based on limited data and simplified micromechanical analyses. However, computational resources have now evolved to a state where simulation of the micromechanisms of spall failure (void nucleation, growth, and coalescence) is possible. With this project, we propose to investigate spall evolution using direct simulation of void processes within a continuum finite-element framework. These microscale simulations will provide a quantitative description of spall evolution. The data will be the basis for a macroscale, homogenized spall model that will capture the effects of microstructure statistics, material properties, and length scale.

A significant result of this project will be an homogenized macroscale spall model incorporating improved understanding of the dynamic processes involved in void nucleation, growth, and coalescence. The proposed methods will explicitly treat the effects of microstructure, material properties, and loading history. The improved model, implemented in ALE3D, will allow more accurate spall modeling in large-scale simulations. The improved understanding of the spall process will aid in quantifying uncertainties arising from changes in material or loading.

Mission Relevance

Spall frequently occurs when materials are driven by high explosives or subjected to high-speed impact. Modeling spall and the subsequent material behavior is necessary for high-fidelity simulation in many NNSA and defense applications in support of stockpile stewardship. Our proposed project will remove the empiricisms and heuristics from spall modeling and enable a truly predictive capability with reduced uncertainties in analyses.

FY08 Accomplishments and Results

In FY08 we (1) performed a literature review on analytical models and simulations of void growth and coalescence leading to ductile spall fracture; (2) identified various proposed spall models and began aggregating spall data generated at Livermore, Los Alamos National Laboratory, and other laboratories; and (3) ran preliminary two-dimensional calculations to gauge the computational expense of direct numerical simulation of spall and to develop a definitive plan for parameter studies.

Fundamental Mechanisms Driving the Amorphous-to-Crystalline Phase Transformation

Nigel D. 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 of transformation. However, by directly correlating experiments with theory on the same time and length scales, the mechanisms 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. Because of LLNL's advanced capabilities, our experiments and simulations will be able to cover the same spatiotemporal regime for the critical time scale of transition (10–100 ns) and the optimum volume of material transformed (~50 nm^3). The alloys we propose to investigate have tremendous technological potential as next-generation nonvolatile memory materials, with the potential to increase data storage density from gigabytes to terabytes per square centimeter.

The aim of this project is to understand the 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 with technological impact should result in highly cited papers published in leading journals.

Mission Relevance

This project supports LLNL's mission in stockpile stewardship because the experimental work will lead to new insights into the atomic-scale dynamics behind phase transformations while expanding the use of the 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.

FY08 Accomplishments and Results

In FY08, we (1) obtained $Ge_2Sb_2Te_5$ samples for TEM analysis; (2) measured images and diffraction patterns as a function of laser intensity and time; (3) determined that the process is growth-limited—the entire region transforms into nanocrystalline grains in 300 to 500 ns, which then grow on a microsecond scale; (4) captured images and diffraction patterns in aberration-corrected TEM—our results were hampered by difficulties in driving the process cyclically, but a new system (Sb_2Te_3) will overcome this; (5) developed empirical potentials for molecular dynamic simulations of the GeTe and GeSe alloys that show good agreement with first-principles studies; and (6) observed that the slow nucleation rate for these materials (~100 ns) limits comparison with experiments, but we are now developing a potential for $Ge_2Sb_2Te_5$ that will allow direct comparison.

Proposed Work for FY09

Because of its slower transformation rate, we will prepare Sb_2Te_3 on a support with higher thermal conductivity to allow the crystalline-to-amorphous transformation to be studied. This material ties in closely with theoretical models, facilitating the correlation between theory and experiment. The new sample will be cycled through the amorphous–crystalline transformation in the DTEM to determine the effect of cycling on transformation rate and grain growth. These samples will then be analyzed in the aberration-corrected TEM to systematically correlate the transformation rate with structure and composition of the amorphous and crystalline states.

Strain-Rate Effects on Plasticity and Defects

James A. Hawreliak   **08-ERD-033**

Abstract

This project will couple simulation and experiment to quantify the defect density and plastic response of dynamically compressed materials as a function of strain rate from the shock Hugoniot. 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 the three main accomplishments of (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—defect density during dynamic compression is expected to differ greatly from that seen in recovered samples, and 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 is central 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.

FY08 Accomplishments and Results

In FY08, we focused on large-scale molecular dynamics simulations of ramp-compressed single-crystal copper, successfully performing the first-ever molecular dynamics simulations of ramp compression using a 300-ps linear ramp in single-crystal copper to a peak pressure of 3 Mbar. We were able to follow the propagation of the compression wave through a 4-µm simulated sample until the loading profile steepened into a single shock, where shock melting occurred. Simulated x-ray diffraction patterns for ramp compression revealed large differences in the sample microstructure compared to single-shock loading.

Proposed Work for FY09

In FY09, we will build on the success of our first-year simulations by performing experiments on laser-based platforms using a temporally ramped laser profile to generate ramp compression. We will leverage techniques developed for the in situ probing of shock-compressed materials to determine the atomistic response of ramp-compressed materials. Using thin-tamped samples, we will look at the affective plastic relaxation as a function of strain rate. This will be the first study of material response at different strain rates at the atomic level.

New Physical Mechanisms for Next-Generation Fusion-Laser Dynamic Sensors and Diagnostics

Evan J. 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 propose to explore 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, shock-broken inversion symmetry, optically active phase transitions, dielectric breakdown, 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, including dynamic material strength measurement and spatially resolved dynamic strain measurements. We will closely couple theory and experimentation to examine this relatively unexplored regime of ultrafast processes.

Our primary result will be elucidating strain wave processes that can be discerned from the terahertz radiation emitted by the sensors, including the 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 high-visibility journals.

Mission Relevance

This work supports LLNL's missions in national security 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.

FY08 Accomplishments and Results

In FY08, we (1) successfully modified our existing experimental facilities to generate shocks and detect terahertz radiation; (2) extended our capabilities to generate shocks ablatively and use a single-shot terahertz detection scheme, a key requirement for future work; (3) determined the time resolution and amplitude characteristics of strain-transition radiation in gallium nitride-based nanostructures, concluding that polycrystalline effects and sample nonuniformity play roles in the observed shock rise times; (4) began to perform molecular dynamics simulations of our future cadmium selenide experiments that will guide our efforts to observe phase transformation in related materials; and (5) developed a new simulation methodology that will enable comparison to our experiments.

Proposed Work for FY09

In FY09, we plan to conduct experiments at much higher pressures (>10 GPa), most likely on LLNL's Europa laser, to improve the time resolution of strain-transition radiation in gallium nitride nanostructures. We will also perform molecular dynamics simulations of phase transformations in piezoelectric materials—including cadmium selenide and gallium nitride—to predict terahertz signals and to guide and interpret our experiments.

Publications

Reed, E. J., et al., 2008. "Atomic-scale time and space resolution of terahertz frequency acoustic waves." *Phys. Rev. Lett.* **101**, 014302. UCRL-JRNL-233178-DRAFT.

Do Brittle Metals Change Character Under Extreme Shock Conditions?

Damian C. 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 involving in situ deformation measurements and sample recovery. We will perform shock-loading experiments in the 10- to 100-GPa regime on microsecond and picosecond time scales—where different flow behavior may occur—using laser ablation and projectile impact. Imaging velocity and displacement histories will be obtained, along with x-ray scattering data. Molecular and continuum dynamics simulations will be performed to complement the experiments.

We will obtain systematic measurements of compressive and tensile strength from velocity histories and obtain defect densities from x-ray diffraction. Imaging records of velocity and displacement allow the response to be related to the microstructure. Comparison with molecular and continuum dynamics simulations will provide 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.

FY08 Accomplishments and Results

In FY08, we (1) performed simulations for laser-driven shock loading using ablators, as well as simulations for laser-driven ramp loading; (2) developed sample loading techniques with successful trial experiments at Livermore's Jupiter Laser Facility; (3) prepared and characterized magnesium crystals by microscopy and diffraction; (4) performed velocimetry measurements on beryllium foils, magnesium crystals and foils, and vanadium; and (5) performed scattering measurements on shock-loaded magnesium foils, and measurements of shock and ramp-loaded vanadium foils.

Proposed Work for FY09

In FY09, we will (1) use the crystal plasticity response calibrated in FY08 to study in detail the dynamic conditions needed for brittle-to-ductile transitions; (2) refine the design of the

dynamic loading experiments, including optimizations for x-ray diffraction and scattering to measure defect populations; (3) conduct further experiments at Janus and Los Alamos National Laboratory's Trident laser; and (4) use the resulting data as a "fine scan" of loading conditions, which we will compare with the "coarse scan" trial data obtained in FY08. One challenge will be to improve the spatial flatness of the laser drive to improve the accuracy of velocity and diffraction data.

Publications

Swift, D. C., and R. G. Kraus, 2008. "Properties of plastic ablators in laser-driven material dynamics experiments." *Phys. Rev. E* **77**(6), 066402. UCRL-JRNL-236641.

Swift, D. C., et al., 2008. *Shock formation and the ideal shape of ramp compression waves.* LLNL-JRNL-404275.

Chemical and Structural Modification and Figure Control during Glass Polishing

Tayyab I. Suratwala   08-ERD-055

Abstract

The chemistry and physics involved in the controlled removal of material from a surface remains poorly understood. Despite considerable empirical advances in the art of polishing, there is no coherent and complete understanding of the microphysical behavior of the material. The objective of our proposed study is to develop a fundamental scientific understanding of the chemical interactions that occur on a glass surface during polishing. In particular, we intend to pursue a systematic path that will allow us to develop an 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 the impurities and surface structural imperfections. The technical motivation for this project is, by understanding the genesis of these impurities and imperfections, to create more robust, deterministically fabricated optical surfaces. Such surfaces would possess considerably higher resistance to high-intensity laser light, reflect x-ray light with higher efficiency, and could enable significant advances in microfabrication and nanofabrication.

This project will provide a significant advance in 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 repeatable, less iterative, more economical, and 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 also be relevant to advances in fabrication of advanced x-ray diagnostics used throughout the Stockpile Stewardship Program.

FY08 Accomplishments and Results

In FY08 we (1) completed initial stages of the modeling effort needed to understand the kinematics of polishing, (2) established an experimental polishing setup and measured the removal rate and surface profile as a function of polishing time for various polishing parameters, (3) characterized and experimentally isolated several types of surface structural modification, (4) probed surfaces with laser beams to help quantify damage thresholds and to form a scientific-based physical picture relating surface modifications and laser damage, and (5) started developing several mitigation techniques to remove the newly identified absorbing species.

Proposed Work for FY09

For FY09, we will (1) extend our modeling efforts by including pressure distribution effects; (2) expand the experimental setup to include pitch and larger-size optics, and measure friction properties on pitch; (3) measure removal rate and surface profile as a function of polishing time and repeat the measurements as a function of polishing process parameters; (4) develop a code that combines physical models for material removal to predict surface shape as a function of polishing parameters; and (5) investigate various mitigation techniques for rendering surface fractures benign.

Physics of Local Reinitiation and Morphological Evolution of Mitigated Sites on Ultraviolet Optics

Manyalibo J. Matthews   08-ERD-057

Abstract

The objective of our proposed work is to develop a predictive, physics-based computational capability to accurately simulate energy deposition and transport as well as material hydrodynamics relevant to stress annealing and optics damage mitigation. 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 reinitiation, 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 current 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 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 approximate thermal diffusion models that provide only rough estimates of temperature and material evaporation rates. Present technology is limited in the size, shape, and ability to control residual stress of a mitigated site, which fundamentally impacts yield and performance. We expect to provide the background for an effective strategy to control morphology and conditions of the site resulting from the mitigation process.

Mission Relevance

High-energy laser systems are essential tools for the Stockpile Stewardship Program and other national security applications, as well as for 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.

FY08 Accomplishments and Results

We (1) continued work on heat deposition and transport in laser-heated silica, developing multiband (non-gray) diffusion approximation to radiation transport compatible with existing ALE3D multiphysics codes; (2) incorporated temperature-dependent capillary forces into ALE3D and began to elucidate subtle morphological features occurring near the ablation threshold of laser-heated silica; (3) achieved, for the first time (to our knowledge), the ability to map the real-time, approximately 300-ms morphological evolution of laser-heated surfaces using phase-shifting diffraction interferometry, revealing dynamic Marangoni-driven surface features; and (4) measured precise thermal gradients using the direct microthermography of about 500-μm irradiated regions using both mercury–cadmium–telluride and indium–antimony imaging systems.

Proposed Work for FY09

For FY09, we propose to (1) develop and improve the accuracy and resolution of thermal camera pyrometry and apply the technique to infrared laser-heated silica at size and temporal scales characteristic of mitigation techniques; (2) estimate the effective thermal conductivity of silica at temperatures, temperature gradients, and boundary conditions consistent with the carbon dioxide laser heating of silica surfaces; (3) determine the threshold surface temperatures for stress relaxation, viscous flow, and material evaporation for 4.6- and 10.6-μm laser irradiation and compare the results with thermal transport models; and (4) systematically evaluate the efficacy of improved surface temperature diagnostics and models to reduce surface modulation, improve the damage reinitiation threshold, and minimize damage growth associated with the infrared laser treatment of fused silica.

Kinetics of Weakly Fluctuating Crystal Surfaces: Beyond Classical Concepts

Luis A. 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 using 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 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 the 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 will have applicability in crystal growth and epitaxy, geochemistry, mineralogy, biomineralization, and materials science concerned with coarsening, phase transitions, and dislocation phenomena. We expect to publish our findings in high-profile journals.

Mission Relevance

This project supports stockpile science through predictive capabilities that apply to high-explosive materials; 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.

FY08 Accomplishments and Results

In FY08, we (1) created computational models that independently measure kink nucleation and propagation during growth; (2) used atomic force microscopy to directly observe single-kink sites on calcite surface steps; (3) found that the kink density from thermal fluctuations is far below that required to apply classical thermodynamic concepts such as the Gibbs–Thomson law and the theory of Burton, Cabrera, and Frank; (4) found that step fluctuations in low kink-

density systems is weak, and therefore the Burton, Cabrera, and Frank theory and corresponding impurity models that rely on the Gibbs–Thomson law fail to predict our results; and (5) showed by in situ atomic force microscopy studies and Monte Carlo simulations that impurities effects during growth are explained by a kink-limited mechanism that represents the opposite extreme of the Burton, Cabrera, and Frank model.

Proposed Work for FY09

In FY09, we will (1) perform atomic force microscopy studies of step structures, kink generation, and step-propagation rates; (2) study slightly soluble salts, brushite, and calcite in aqueous solutions; (3) investigate crystallites of the explosive triamino-trinitrobenzene in vapor to test the limitations of three-dimensional crystallite evaporation; and (4) modify the algorithms we developed in FY08 to allow us to compare kinetic Monte Carlo simulation results with experiments.

Confinement of Hydrogen in Multiwalled Carbon Nanotubes

David H. Lassila   08-FS-012

Abstract

We propose to study the feasibility of using multiwalled carbon nanotubes to confine hydrogen at high pressures. Bundles of nanotubes will be filled at pressures up to 0.2 GPa using a thermal charging technique, and experiments will then be performed on the charged nanotube samples to estimate hydrogen retained in the nanotubes' interior. Analyses of the nanotubes using scanning electron microscopy will be performed before and after all experimental procedures to assess any changes in tube structure. We believe that no experimental work has yet been performed to study the confinement of hydrogen in nanotubes, although some research has studied the confinement of other gases.

Our objective is to demonstrate the feasibility of systems using multiwalled carbon nanotubes to confine hydrogen at pressures on the order of 0.1 GPa. To do this, we will establish a methodology to cap the open ends of the nanotubes with palladium so the tube can be filled via a diffusion mechanism. This will yield the first information of its kind for the use of multiwalled carbon nanotubes in the confinement of hydrogen.

Mission Relevance

The proposed research will support the Laboratory's stockpile stewardship mission as well as efforts in energy and the environment. If we can confine hydrogen at high pressures in multiwalled carbon nanotubes, applications can be envisioned for hydrogen storage for use in a chemical power source as well as the study of hydrogen and hydrogen isotope states at high pressures such as in the creation of plasmas.

FY08 Accomplishments and Results

Because of unanticipated events, a decision was made to terminate this project before completing an assessment of the feasibility of the proposed concept.

Laboratory Directed Research and Development

Mathematics and Computing Sciences

LOCAL: Locality-Optimizing Caching Algorithms and Layouts

Peter G. Lindstrom   05-ERD-018

Abstract

This project is investigating layout and compression techniques for large, unstructured simulation data to reduce bandwidth requirements and latency for visualization and related tasks. Our goal is to eliminate the data-transfer bottleneck—for example, from disk to memory and from central processing unit to graphics processing unit—through cache-coherent data access and by trading underutilized computer power for bandwidth and storage. We will achieve this by designing algorithms that both enforce and exploit compactness and locality in unstructured data and by adapting offline computations to a novel stream-processing framework that supports pipelining and low-latency sequential access to compressed data. The scalable algorithms developed in this project will be able to run on both end-user desktops and dedicated visualization clusters.

We expect to achieve significant improvements in disk and memory usage, effective bandwidth, data-access latency, and cache reuse, which will result in more efficient random and sequential access to unstructured grid data. These improvements will enable management of larger data sets and storage of more complete simulation data dumps for post-analysis and visualization. They will additionally provide new capabilities and order-of-magnitude performance improvements in simulation setup, offline mesh processing, interactive data queries, and real-time paging and rendering. These bandwidth- and latency-efficient techniques will become increasingly valuable on next-generation computers as the gap in processor speed and input–output performance keeps widening.

Mission Relevance

Our research will serve as an important aid in managing and visualizing large data sets from scientific and engineering simulations by supporting analysis and interactive exploration of terascale data sets for the stockpile stewardship mission.

FY08 Accomplishments and Results

In FY08, we (1) designed a high-speed compressor for coding connectivity, geometry, and nodal data in unstructured hexahedral meshes, and helped integrate it with LLNL's Silo input–output library; (2) developed a framework for stream processing large data sets out-of-core and in parallel, including a method for parallel streaming ghost node and zone creation—we integrated this scheme with the VisIt parallel visualization and graphical analysis tool and demonstrated linear speedup when processing data sets of unprecedented scale on a small computer cluster with limited memory; and (3) designed a scheme for on-the-fly decoding and rendering of compressed triangle meshes on the graphics processing unit that reduces central processing unit to graphics processing unit memory traffic. Proposed work on parallel cache-oblivious layouts was eliminated because of loss of the project postdoctoral researcher. The successful conclusion of this project, however, enabled new, efficient out-of-core and parallel methods for

analyzing, processing, and visualizing unstructured data sets of unprecedented scale through order-of-magnitude reduction in memory and bandwidth use. Our techniques are being adopted by Laboratory programs via deployment to VisIt and Silo, and we expect continued research support from the DOE, industry, and a foreign academic institution.

Publications

Isenburg, M., P. Lindstrom, and H. Childs, in press. "Parallel and streaming generation of ghost data for structured grids." *IEEE Trans. Visual. Comp. Graph.* LLNL-TR-403175-DRAFT.

Lindstrom, P., and M. Isenburg, 2008. "Lossless compression of hexahedral meshes." *Proc. IEEE Data Compression Conf., Snowbird, UT, March 25-27, 2008*, p. 192. UCRL-CONF-236522.

A New Method for Wave Propagation in Elastic Media

Anders Petersson   05-ERD-079

Abstract

Simulation of elastic wave propagation is essential for monitoring nuclear explosions, predicting ground motion from earthquakes, and nondestructive evaluation of complex parts. We propose to develop significant improvements in the traditional finite-difference technique that will allow a fully second-order accurate treatment of boundary conditions in complex domains to handle topography and internal layers. Our improved technique will use local mesh refinement to avoid partial oversampling of the solution because of varying wave speeds.

This project will result in a verified, accurate, and efficient elastic Wave Propagation Project (WPP) code for numerical simulation in complex two- and three-dimensional (2D and 3D) media. This open-source code will be useful for many applications at Lawrence Livermore and in the scientific community. The computer software will support applications ranging from 2D simulations in nondestructive testing to 3D earthquake modeling using compute power ranging from desktop workstations (e.g., SUN, LINUX, and OSX platforms) to massively parallel high-performance machines (e.g., Zeus and Thunder). We plan to validate the code against benchmark problems relevant to LLNL program applications and publish our research in journals and conference proceedings.

Mission Relevance

Simulation of seismic-wave-propagation phenomena is essential for the success of many applications in support of Livermore's national security missions. This includes strong ground-motion prediction for the Enhanced Test Site Readiness Program and the Yucca Mountain Program, nuclear explosion monitoring and underground facilities characterization, and nondestructive testing for locating imperfections in critical components relevant to the Transformational Materials Initiative.

FY08 Accomplishments and Results

In FY08, we (1) performed a theoretical study of jump conditions together with internal mesh-refinement boundaries and devised an energy-conserving coupling technique; (2) implemented anelastic damping (visco-elastic attenuation) in the WPP code; and (3) developed and implemented an energy-absorbing far-field boundary condition based on the summation-by-parts principle, which, unlike the conventionally used perfectly matched layer technique, resulted in an energy-absorbing far-field boundary condition that is stable for heterogeneous elastic materials in the presence of free surfaces. In summary, this project has developed novel numerical techniques for elastic wave propagation which have been implemented in the open-source code WPP and applied in several large-scale earthquake modeling studies. The next step is to couple the WPP code to near-source nonlinear explosion simulations for nonproliferation applications.

Publications

Aagard B., et al., 2008. "Ground motion modeling of the 1906 San Francisco earthquake II: Ground motion estimates for the 1906 earthquake and scenario events." *Bull. Seism. Soc. Amer.* **98**, 1012. UCRL-JRNL-228005.

Appelo D., and N. A. Petersson, 2009. "A stable, finite-difference method for the elastic wave equation on complex geometries with free surfaces." *Comm. Comput. Phys.* **5**, 84. UCRL-JRNL-237329.

Rodgers, A., et al., 2008. "Broadband waveform modeling of moderate earthquakes in the San Francisco Bay Area and preliminary assessment of the USGS 3D seismic velocity model." *Bull. Seism. Soc. Amer.* **98**, 969. UCRL-JRNL-228251.

Sjogreen, B., and N. A. Petersson. "An energy-absorbing far-field boundary condition for the elastic wave equation." LLNL-JRNL-405423.

Predictive Knowledge Systems for Large, Complex Data Sources

James M. Brase   06-SI-006

Abstract

Nonproliferation, counterterrorism, and intelligence are primarily problems of information—sensors and data-collection systems can provide overwhelming quantities of data. Moreover, these data are often sparse, noisy, irrelevant, disjointed, and even intentionally misleading. The objective of this project is to discover complex patterns in large-scale, multisource data streams and to build predictive models based on these patterns. We will create algorithms and computations capabilities that allow analysts to extract knowledge from such data in a meaningful and timely way. To this end, we will pursue pattern discovery, learning and prediction, and data-intensive computational architectures. The project will focus on demonstrating applications in nonproliferation and homeland security.

We expect to develop (1) a technical base of algorithms and computational methods that will extend the frontiers of pattern recognition and stochastic predictive models, (2) confidence measures and performance metrics relevant to these tools, and (3) two demonstrations that apply these capabilities to important problems of nuclear nonproliferation and homeland security.

Mission Relevance

This project will enable accurate and relevant conclusions from a mix of complex data sources (e.g., imagery, sensor networks, semantic graphs, and relational databases) with unprecedented levels of performance in broad-area search and site-monitoring problems relevant to nonproliferation and homeland security. The central core of algorithms and computational methods developed will broadly support the LLNL mission in national security, particularly nonproliferation and homeland security.

FY08 Accomplishments and Results

In FY08, we (1) developed a graph-based analysis method that showed improved performance and is now in use in program applications; (2) optimized graph query retrieval with greater than tenfold increase in speed; (3) evaluated scaling of random tree models in program data sets, which enabled new capabilities; (4) successfully demonstrated the reconstruction of communication networks in signals intelligence data; (5) successfully demonstrated new algorithms for machine learning on semantic graphs with hierarchical structures and realistic dynamics, which was applied to computer-network monitoring data and has led to new approaches to cybersecurity behavioral monitoring; and (6) completed two demonstrations— linking image objects with signals intelligence activity and learning activity patterns in computer networks. Our predictive knowledge systems research has enabled a new set of capabilities for pattern discovery in multisource data sets such as imagery and signals intelligence and for analyzing patterns in relationships and dynamic behavior on large semantic graphs. The project has led to a new research partnership with the National Security Agency that is focused on applications of machine learning and large-scale graph analysis.

Publications

Gallagher, B., and T. Eliassi-Rad, 2007. *An examination of experimental methodology for classifiers of relational data.* IEEE Intl. Conf. Data Mining, Omaha, NE, Oct. 28–31, 2007. UCRL-CONF-233643.

Gallagher, B., and T. Elliasi-Rad, 2008. *Leveraging label-independent features for classification in sparsely labeled networks: An empirical study.* 2nd ACM Workshop on Social Network Mining and Analysis, Las Vegas, NV, Aug. 24–27, 2008. LLNL-CONF-405028.

Hatch, A. O., D. W. Paglieroni, and B. Y. Chen, 2008. *A road centrality function for tracking roads in overhead images.* IEEE Intl. Conf. Computer Vision and Pattern Recognition, Anchorage, AK, June 24–26, 2008. UCRL-CONF-237299.

Kaplan, I. L., et al., 2008. *Implementing graph pattern queries on a relational database.* LLNL-TR-400310.

Koutsourelakis, P. S., and T. Eliassi-Rad, 2008. *Finding mixed-memberships in social networks.* AAAI Spring Symp., Social Information Processing, Stanford, CA, Mar. 26–28, 2008. LLNL-CONF-400644.

Manay, S., and D. W. Paglieroni, 2008. *Detecting polygons of variable dimensions in overhead images with particle filters.* IEEE Intl. Conf. Image Processing, San Diego, CA, Oct. 12–15, 2008. LLNL-CONF-400576.

Paglieroni, D. W., and S. Manay, 2008. *Using particle filters to detect polygon structures of fixed shape in still images.* IEEE Intl. Conf. Computer Vision and Pattern Recognition, Anchorage, AK, June 24–26, 2008. UCRL-CONF-236941.

Sen, P., et al., 2008. "Collective classification in network data." *AI Mag.* **29**(3), 93. UCRL-JRNL-235753.

Sun, J., et al., 2008. "Two heads are better than one: Pattern discovery in time-evolving multi-aspect data." *Data Min. Knowl. Discov. J.* **17**(1), 111. LLNL-JRNL-407301.

Tong, H., et al., 2008. *Fast mining of complex time-stamped events.* ACM 17th Conf. Information and Knowledge Management, Napa Valley, CA, Oct. 26–30, 2008. LLNL-CONF-405539.

Scalable Data Management for Massive Semantic Graphs

Scott R. Kohn   **06-ERD-009**

Abstract

Semantic graphs are an important tool for the intelligence community and homeland security applications. However, current approaches do not address anticipated data sizes. We are investigating the scaling properties of semantic graphs using parallel databases running on multiple central processing units with storage arranged in an active-disk architecture. We believe that such approaches can support semantic graphs that are at least 100 times larger than currently possible. Our research focuses on the algorithms, architectures, and techniques necessary to support these massive, distributed semantic graphs.

The goal of this research is to understand how to use parallel active-disk architectures to support semantic graphs that are orders of magnitude larger than those possible using current technology. We expect this research to guide the development of next-generation semantic graph architectures. This size and scale are unmatched in the homeland security and intelligence community and would bring a unique analysis capability to Laboratory programs. We also will use results from our ongoing research to develop a system that identifies, for the analyst, sections of text that act as summaries of the data within a document set. This advance has the potential to reduce, by a factor of 10 or more, the amount of selected text that an analyst must work with. This project is also developing Laboratory expertise in the area of large-scale data management and analysis.

Mission Relevance

Increasingly massive data sets collected for nonproliferation, intelligence, and military applications require new technologies to query and analyze these data. By furthering understanding the performance characteristics of a cluster architecture on data-intensive semantic graph applications, this project supports the large-scale data management and analysis needs of the Laboratory's homeland and national security missions.

FY08 Accomplishments and Results

We (1) developed new semantic graph pattern-matching approaches that run orders of magnitude faster than those previously used in production systems; (2) evaluated Map-Reduce, the LexisNexis Enterprise Data Fusion System, and Violin Memory technologies for large semantic graph algorithms and compared the results to previous benchmarks on Netezza and relational databases; (3) developed new approaches for solving the "random walk with restart" equations on large graphs that are four to seven times faster than standard methods; and (4) developed new text triage approaches using faceted searching, which significantly reduced— from months to hours—the amount of time needed to triage documents.

In summary, this project has developed novel algorithms for analyzing and querying large semantic graphs, determined hardware and software characteristics necessary for the successful analysis of large graphs, and developed a new text analysis approach that significantly reduces triage time for important documents. The research on graph algorithms and architectures is being integrated into existing global security-related efforts, and the text triage work is being pursued by multiple U.S. government agencies.

Publications

Kaplan, I., et al., 2008. *Implementing graph pattern queries on a relational database.* LLNL-TR-400310.

A Predictive Model of Fragmentation Using Adaptive Mesh Refinement and Hierarchical Material Models

Alice E. Koniges   06-ERD-036

Abstract

Fragmentation naturally spans microscopic to macroscopic scales. Recent advances in algorithms and computer power enable us to connect the continuum to microstructural regimes in a real simulation through a heterogeneous multiscale mathematical model. We will develop a mathematical framework using an innovative combination of hierarchical material models (HMM) and adaptive mesh refinement (AMR) and apply it to a problem that can be verified experimentally and computationally in a scalable parallel simulation. The unique AMR

formulation allows us to model different scales at different AMR levels. We will guide and benchmark these simulations with dedicated laser experiments on thin foils, the size of which allows for full-scale simulation and microstructural analysis.

This project will culminate with a verifiable simulation that connects the continuum to microstructural regimes through a heterogeneous multiscale AMR model. We will leverage the Structured Adaptive Mesh Refinement Application Infrastructure (SAMRAI) library and the methods developed by the "Petascale Simulation Initiative" (LDRD project 04-ERD-102). Our experimentally verified simulation provides a path forward for a design tool for future fusion-class lasers, a basic understanding of ductile failure, and new AMR algorithms, such as partitioning field variables in mixed zones that aid other AMR-based research efforts. The predictive model developed will yield an increased understanding of fragmentation, which will have impact in many different fields, from fusion-class lasers to weapons systems to space shuttle re-entry.

Mission Relevance

This research has direct relevance to national security as well as to breakthroughs in fundamental science and technology. Benefits include significant enhancement and broadening of our expertise in computational solid mechanics and advancement of the application base for our AMR framework. A significantly improved capability to predict fragmentation will find application in fusion-class laser experiments in support of the stockpile stewardship mission.

FY08 Accomplishments and Results

For FY08, we (1) implemented a flexible material modeling framework that allows for integration of a hierarchical material model; (2) implemented a laser deposition package consistent with the hierarchy of grids and implemented the Poisson solver for conduction; (3) tested the simulations on available systems of up to 512 processors, which is our largest available allocated number; (4) tested the models against experimental fragmentation data and determined how to overcome difficulties associated with different degrees of refinement; and (5) fully connected the code to the libraries that were an integral part of the "Petascale Simulation Initiative." Our code has been adopted by the National Ignition Facility as a primary tool for debris and shrapnel analysis. Additionally, we have targeted several areas where our code may prove useful, including the study of warm dense matter, astrophysics, and material science.

Publications

Koniges, A., et al., 2008. "Experiments for the validation of debris and shrapnel calculations." *J. Phys. Conf.* **112**, 032072. UCRL-CONF-234490.

Masters, N. D., et al., 2008. "Interface reconstruction in two-and three-dimensional arbitrary Lagrangian–Eulerian adaptive mesh refinement simulations." *J. Phys. Conf.* **112**, 022017. UCRL-CONF-234452.

Eder, D., et al., 2008. "Debris and shrapnel mitigation procedure for NIF experiments." *J. Phys. Conf.* **112**, 032023. UCRL-CONF-234490.

Fisher, A., et al., 2008. "Hierarchical material models for fragmentation modeling in NIF-ALE-AMR." *J. Phys. Conf.* **112**, 032072. UCRL-CONF-234451.

Benson, D., et al., in press. *Hierarchical material models for modeling fragmentation of targets in inertial confinement fusion research.* International Symposium on Structures under Earthquake, Impact, and Blast Loading, Osaka, Japan, Oct. 10–11, 2008. LLNL-CONF-406899.

A Novel Structure-Driven Approach to Sequence Pattern Definition for Remote Homology Detection

Adam T. Zemla   **06-ERD-059**

Abstract

We propose to 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. We will devise sequence patterns representing structure fragments and test if 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 the 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.

FY08 Accomplishments and Results

In FY08, we (1) developed an algorithm that defines sequence patterns from a set of structurally related proteins (results are output in the format of a position-specific scoring matrix and tested on the set of nonredundant protein sequences); (2) continued developing an algorithm for defining substitution matrices (i.e., allowed position mutations); (3) tested our clustering algorithm on

a set of 11,800 protein domains from over 50 folds in the Structural Classification of Proteins database; (4) developed domain-fusion protein and homology search algorithms to help functional assignments and reconstruct links between interacting partners from the *Y. pestis* quorum-sensing network; and (5) began to experimentally validate created computational predictions, confirming one interaction (between proteins ypo0407 and ypo0408) before year's end.

Proposed Work for FY09

Building on our FY08 results, which indicate that the initial version of our structure-driven system for distant homology detection and domain fusion-based prediction is capable of making previously difficult-to-identify links between proteins (interacting partners), we will (1) complete algorithm development, (2) construct structure-driven patterns code (profiles and scoring matrices) for given proteins, (3) perform pattern-based homology searches, and (4) reconstruct links between interacting partners from the *Y. pestis* autoinducer quorum-sensing network using our novel domain fusion-based approaches. The goal is to elucidate the mechanism by which cell–cell communication via signaling molecules regulates virulence factor gene expression during host invasion.

Publications

Cosman, M., et al., 2008. "Identification of a thermo-regulated glutamine-binding protein from *Yersinia pestis*." *Protein Peptide Lett.* **15**, 887. UCRL-JRNL-213767.

Gryshuk, A., et al., 2008. *Structure-driven approach to detection and characterization of virulence proteins*. 11th Ann. Bay Area Microbial Pathogenesis Symp., San Francisco, CA, Mar. 29, 2008. UCRL-POST-216262.

Singer, S. W., et al., 2008. "Characterization of cytochrome 579, an unusual cytochrome isolated from an iron-oxidizing microbial community." *Appl. Environ. Microb.* **74**, 4454. UCRL-JRNL-216376.

Knowledge-Based Coreference Resolution

David J. Buttler   **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 ADVISE semantic graphs 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.

FY08 Accomplishment and Results

We (1) improved the results from our baseline system from an f-measure of 62 to 70% and expanded the system to run on arbitrary corpora; (2) developed methods (about which two papers were published) to identify relevant articles in background text from which signatures can be obtained; (3) developed automated, unsupervised coreference annotation software to create feature vectors for training our coreference resolver from domain-specific background text; and (4) began creating our own semantic graph from text (because we can no longer assume that we will have existing semantic graphs to leverage) using a system to extract local relationships between entities.

Proposed Work for FY09

For FY09, we propose to (1) extend entity signature development; (2) explore bootstrapping for automated annotation of training and test sets and knowledge acquisition, with emphasis on domain independence; (3) continue development of new algorithms to acquire external semantic knowledge about coreference relations from the Web; (4) extend our application-programming interface and documentation in a manner suitable for specific mission-critical applications at LLNL; and (5) publish papers about external knowledge-base contributions for improved coreference resolution.

Publications

Buttler, D., 2008. "Java metadata facility." *Encyclopedia of Database Systems*. Springer, Secaucus, NJ. LLNL-JRNL-402071.

Pon, R., and D. Buttler, in press. "Metadata registry, ISO/IEC 11179." *Encyclopedia of Database Systems*. Springer, Secaucus, NJ. LLNL-JRNL-400269.

Pon, R., A. Cardenas, and D. Buttler, 2008. *Improving naive Bayes with online feature selection for quick adaptation to evolving feature usefulness*. 8th SIAM Intl. Conf. Data Mining, Atlanta, GA, Apr. 24–26, 2008. LLNL-CONF-400048.

Pon, R., A. Cardenas, and D. Buttler, 2008. "Measuring the interestingness of news articles." *Encyclopedia of Data Warehousing and Mining.* Vol. III. Information Science Reference, Pennsylvania. UCRL-JRNL-235441.

Pon, R., A. Cardenas, and D. Buttler, 2008. *Online selection of parameters in the Rocchio algorithm for identifying interesting news articles.* ACM 17th Conf. Information and Knowledge Management, Napa Valley, CA, Oct. 26–30, 2008. LLNL-CONF-405224.

Advanced Computational Techniques for Uncertainty Quantification

Charles H. 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 LLNL simulation-based applications, as well as new initiatives such as the DOE Global Nuclear Energy Partnership (GNEP) 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 will result in software tools and published journal and conference proceedings papers. The developed software will find immediate application to Laboratory applications as well as to the broad scientific community.

Mission Relevance

Our project aligns well with the Laboratory 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 new DOE GNEP initiative and will help support LLNL'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.

FY08 Accomplishments and Results

In FY08, we (1) enhanced and implemented a response surface methodology using derivative information in the PSUADE software library; (2) performed a comparison of Bayesian versus our enhanced sensitivity analysis methods on a hydrodynamics simulation problem, which motivated a follow-on multi-algorithmic sensitivity analysis approach; (3) incorporated a suite of variance-based sensitivity analysis methods into PSUADE (publicly released in version 1.1); and (4) applied an initial demonstration of our uncertainty quantification methodology to a two-dimensional soil–structure interaction model.

Proposed Work for FY09

In FY09 we plan to (1) complete development of a mathematical framework for intelligent sampling with application to fast-response surface methods based on geometric refinement versus importance sampling and efficient Bayesian and frequentist risk analysis, (2) develop these tools within the PSUADE software package and publish our results, and (3) use all of the uncertainty quantification capabilities we have developed to study a three-dimensional soil–foundation structure interaction system.

Publications

Tong, C., 2008. *An adaptive derivative-based method for function approximation.* LLNL-TR-408156.

Tong, C., 2008. *Quantifying uncertainties of a soil-foundation structure-interaction system under seismic excitation*. LLNL-TR-402883.

VidCharts: Real-Time Algorithms for Large-Scale Video Analysis, Compression, and Visualization

Mark A. 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 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 a prototype visual indexing system for huge video streams, including scene segmentation, pan/zoom/mover analysis, space–time drill-down, visualization of complex movers 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 thousandfold 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.

FY08 Accomplishments and Results

In FY08 we (1) made excellent progress in producing 3D models using video cameras that move over a scene, including novel camera parameter estimation and error-analysis techniques; (2) conducted initial studies on applying scalar field topology to video; (3) increased the scalability of the scale-invariant feature-transform algorithm and extended it from still images to video; (4) performed experiments on using selective refinement to adapt large-format video to moving objects; (5) made major progress in devising sensor artifact correction at both fine and coarse scales; and (6) leveraged graphics processing units to scale many video processing core operations, including those for resolution enhancement using multiple video frames.

Proposed Work for FY09

Our proposed goals for FY09 include (1) generating super-resolution movies from conventional video feeds in real time, with potential integration in the interactive mosaic generation; (2) improving 3D extraction through per-pixel neighborhood-mapping sensitivity analysis and background and foreground unmixing estimation; (3) enabling streaming 3D model estimation and resolution and accuracy enhancement as stereo depth estimates are produced; and (4) creating an initial experimental nonlinear video visualization system with semi-automated analysis of scene changes and graph structure and the visual abstraction of moving objects or exceptions to the summaries.

Software Security Analysis

Daniel J. Quinlan   07-ERD-057

Abstract

The DOE obtains software from a wide variety of sources, both as binaries and source code. Currently, Lawrence Livermore has limited ability to determine if such software is free from 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—something not possible with any existing security analysis capability of which we are aware.

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 the compilation and analysis of LLNL's largest-scale Advanced Simulation and Computing applications.

Mission Relevance

The 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 build a significant level of internal expertise in software security analysis.

FY08 Accomplishments and Results

We developed both source code and binary analysis capabilities and tools using the ROSE source-to-source compiler infrastructure. These capabilities support a custom analysis of binaries, including disassembly of instructions for instruction sets and analysis of control flow and data flow programs. We focused on the development of individual tools, including analysis of binary clones and visualization on the binary clone database. We also demonstrated the first-ever parallel forms of program analysis for source code allowing large-scale software to be quickly analyzed using distributed memory parallel computers. Parallelism with up to 512 processors was demonstrated.

Proposed Work for FY09

In FY09 we will expand the capabilities of our Compass tool, focusing on the applicability of the tool to Laboratory missions, and improve our performance speed on binary analysis for several heterogeneous architectures.

Publications

Panas, T., 2008. "Signature visualization of software binaries." *Proc. 4th ACM Symp. Software Visualization.* LLNL-CONF-403008-DRAFT.

Quinlan, D., G. Barany, and T. Panas, 2008. *Shared and distributed memory parallel security analysis of large-scale source code and binary analysis.* Dagstuhl Conf. on Scalable Program Analysis, Dagstuhl, Germany, Apr. 13–18, 2008. LLNL-POST-403615.

Verification and Validation of Radiation Hydrodynamics for Astrophysical Applications

Louis H. 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 analytical solutions that will be used to determine the accuracy of 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 the 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.

FY08 Accomplishments and Results

In FY08 we (1) ran nine gray and multigroup radiation problems, testing different aspects of solver performance; (2) added new comparison software and automated test scripts; (3) completed verification work on the radiation-hydrodynamics solver; (4) identified the associated astrophysical environments; (5) began assembly of the necessary modules for the requisite physics; (6) performed preliminary calculations using pure hydrodynamic solvers; and (7) incorporated a multigroup light-front problem and a partial completion of the radiating sphere test into our test suite.

Proposed Work for FY09

In FY09, we will (1) continue to expand our verification test suite with problems involving multigroup radiation and coupled radiation and hydrodynamics problems; (2) perform tests on prompt radiation from a radiating sphere, on the crooked-pipe problem, and on radiation damping of acoustic waves; and (3) perform validation calculations for one or more astrophysical problems involving real material properties and radiating shocks and compare the results against data from observations or experiments.

Storage-Intensive Supercomputing

Maya B. 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 (SISC) 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 SISC in partnership with industry collaborators; and (4) enable an order-of-magnitude improvement in price and performance over today's data-intensive 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.

FY08 Accomplishments and Results

In FY08 we (1) tested the Hadoop framework for graph processing on cluster architectures; (2) evaluated large memory systems; (3) developed a benchmark generator that mimics the input–output activity of SISC applications with an error of less than 10%, along with a suite of microbenchmarks to study input–output performance; (4) developed a checkpoint file system with twofold scaling; (5) began building a metadata-rich file system; and (6) collaborated with the manufacturer of a 336-processor system on a chip to map two data- and computation-intensive kernels onto a chip, achieving a tenfold performance increase over a typical workstation.

Proposed Work for FY09

In FY09 we will (1) continue to collaborate with industrial partners to develop SISC system architectures that are flexible, scalable, robust, and cost effective; (2) address the difficulty of

programming scalable applications software with file systems and programming models focused on data-intensive problems; (3) create software tools for performance measurement; and (4) develop new approaches for mapping algorithms and applications onto SISC architectures.

Publications

Damkroger, P., et al., 2008. *Rethinking supercomputing for data-intensive problems.* Intl. Supercomputing Conf. 2008, Dresden, Germany, June 17–20, 2008. LLNL-CONF-401367.

Gokhale, M. B., et al., 2008. "Hardware technologies for high-performance data-intensive computing." *IEEE Comput.* **41**, 4. UCRL-JRNL-235506.

Gokhale, M. B., et al., 2008. *Storage-intensive supercomputing benchmark study.* UCRL-TR-236179.

Ulmer, C., and M. B. Gokhale, 2008. *Threading opportunities in high-performance flash-memory storage.* High-Performance Embedded Computing 12th Ann. Workshop, Lexington, MA, Sept. 23–25, 2008. LLNL-ABS-409960.

Probabilistic Inference of Metabolic Pathways from Metagenomic Sequence Data

Patrik M. D'Haeseleer   08-ERD-011

Abstract

Metagenomic "shotgun" sequencing of microbial communities has the potential to revolutionize microbial ecology, yet the complexity and scrambled nature of the data poses a tremendous challenge. We propose to develop a set of novel metagenomic sequence analysis tools, including a binning method to group sequences by species, probabilistic inference of metabolic pathways, and extraction of coarse-grained flux models. We will collaborate with the DOE Joint Genome Institute and Stanford Research institutes in an analysis of a hydrogen-producing layered cyanobacterial mat. Results will be cross-validated with simulated metagenomic data using a testing platform developed at the Joint Genome Institute.

Success in this endeavor will enable researchers to truly understand microbial communities via their metagenome sequence, just as the availability of whole genome sequences has allowed the scientific community to make a quantum leap in understanding single organisms. Given the intense amount of interest in metagenomics at the moment, this could potentially provide the Laboratory with high visibility and a reputation as a leader in this field.

Mission Relevance

This work is highly relevant to a number of Laboratory initiatives in biological, chemical, and computational science and supports its mission in breakthrough science and in homeland security by helping to identify and characterize biological systems, as well as enable

fundamental understanding of energy metabolism in microbes and microbial communities. Furthermore, our work also is well-aligned with efforts of the DOE's Genomics:GTL program and the Joint BioEnergy Institute collaboration of national laboratories, industry, universities, and federal agencies to help ensure energy security and long-term energy needs.

FY08 Accomplishments and Results

In FY08, we (1) continued integration of the microbial genotype and phenotype database, (2) constructed a prototype of a phenotype prediction pipeline from a known genome sequence, (3) began developing a phylogenomic algorithm for pathway prediction, and (4) began designing a stand-alone, Web-based tool. The next step would be to build on these foundations at institutions such as the Joint Genome Institute and Stanford Research institutes, both of which have expressed interest in this work.

New Algorithms to Scale Domain Decomposition Up to BlueGene Architectures

Gary K. Kumfert   **08-ERD-014**

Abstract

We propose to develop novel mesh-partitioning algorithms and software that is more scalable (>100,000 processors) and delivers higher-quality results than the current state of the art. 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. Because no known high-quality partitioner scales above 16,000 processors in BlueGene/L (only one-eighth of the available processors), simulations are slowed by a factor of two or more simply from load imbalance and communication. The key element of 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.

We expect to deliver production-quality code that produces higher-quality domain decompositions for applications of Laboratory relevance that are scalable to the full BlueGene/L machine. High-quality domain decompositions 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 the maximum number of neighboring domains possible. 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 Livermore's sustained preeminence in the field of stockpile stewardship simulations.

FY08 Accomplishments and Results

In FY08, we (1) completed all basic infrastructure code for the foundation of our new multiblock partitioners; (2) integrated our foundational code with the Zoltan software package from Sandia National Laboratory, which is used to manage communication and query functions, and implemented the code for our algorithms; (3) characterized the effect of our new partitioning scheme on production codes; and (4) devised a method for evaluating proposed algorithms in serial, which gives us the capability of evaluating the advantages and trade-offs of various approaches independent of full implementation.

Proposed Work for FY09

In FY09, we will (1) begin developing adaptive repartitioning capabilities in our code—our primary FY09 milestone will be to perform adaptive repartitioning in the limited case of pure multiblock meshes without degenerate zones or unstructured regions, (2) demonstrate adaptive repartitioning capability on test cases, and (3) continue scaling our static partitioning capability to the full BlueGene/L machine and refine the figures of merit we use to quantify the quality of a domain decomposition and validate them against full simulations.

Robust Ensemble Classifier Methods for Detection Problems with Unequal and Evolving Error Costs

Barry Y. Chen   08-ERD-022

Abstract

In computer and electronic detection applications involving counterterrorism or nonproliferation, signature patterns are often deliberately camouflaged, hence the need to solve detection problems having unequal and evolving costs (i.e., consequences) for false alarms and missed detections or having an imbalance in training examples. In this project we will generalize individual cost-sensitive classifiers to cost-sensitive ensemble classifiers, combining the strengths of both cost-sensitive and ensemble-classification methods. We will jointly optimize the key ensemble design factors via a novel global cost-minimization approach to deliver a hitherto unachievable robust, high-performance, and easy-to-use solution to counterterrorism and nonproliferation detection problems.

We will develop and demonstrate a methodology for building cost-sensitive ensemble classifiers, globally optimized over key design factors and capable of delivering robust, high-performance, easy-to-use solutions to detection problems involving (1) large data sets, (2) high feature dimensionality, (3) unequal or evolving misclassification costs, and (4) unbalanced training data. The resulting methodology will be the first to address all of these challenges simultaneously and significantly advance the state of the art in classifier technology, in terms of both performance and insight into the effects of, and interactions between, design factors.

The capability to solve detection problems of this type has broad applicability to many mission-relevant fields.

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 (1) hidden signals in intelligence data, (2) radiological sources in low-intensity spectral signatures, (3) attack signatures for site-protection applications, (4) failing components in weapons systems, (5) nefarious activities on computer networks, and (6) clandestine underground nuclear explosions.

FY08 Accomplishments and Results

In FY08 we (1) developed a methodology to minimize the expected total cost of ensemble classifiers with respect to their design factors, (2) analyzed interactions among these design factors, and (3) investigated linear and hierarchical combination methods for combining classifiers. This work led to the development of several ground-breaking ensemble classifiers, two peer-reviewed publications, and one provisional patent. Our novel, cost-sensitive random-subspace support vector classifier, discriminant random forest, and cost-sensitive discriminant random forest all outperform existing ensembles on our primary application for hidden signal detection, in which false alarms are extremely costly. Our methods significantly reduce the false alarm rate while maintaining 65% detection.

Proposed Work for FY09

Our three main goals for FY09 are to (1) develop combination architectures (e.g., hierarchical and staged) that can adapt to changing costs and data distributions without completely retraining the cost-sensitive ensemble classifiers, (2) extend homogeneous cost-sensitive ensemble classifiers developed in FY08 to heterogeneous ensembles composed of different base classifiers, and (3) adapt and apply developed technologies to program applications burdened by imbalanced training data and unequal misclassification costs. The final deliverables in FY09 will be software implementations of our novel classifiers, a users manual enabling technology transfer, two peer-reviewed publications, and a full patent on at least one of our new algorithms.

Publications

Lemmond, T. D., et al., 2008. "An Extended Study of Discriminant Random Forests." *Annals of Information Systems, Special Issue on Data Mining*, Springer, New York. LLNL-JRNL-407403.

Lemmond, T. D., et al., 2008. *Discriminant Random Forests.* KDD08 14th ACM SIGKDD Intl. Conf. Knowledge Discovery and Data Mining, Las Vegas, NV, Aug. 24–27, 2008. LLNL-CONF-401701.

Enhanced Event Extraction from Text Via Error-Driven Aggregation Methodologies

Tracy D. Lemmond   08-ERD-023

Abstract

Knowledge discovery systems construct massive data repositories via the extraction of events from text, and are prone to event extraction errors. We propose to enhance performance of the data-ingestion process via an aggregated extraction framework, leading to reliable downstream inference in support of Livermore's counterterrorism and nonproliferation efforts, and more generally, to a critical breakthrough in the natural language processing and knowledge discovery fields. 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 with respect to the underlying error processes.

Our research will yield a novel methodology for probabilistically characterizing the error processes underlying knowledge discovery, providing valuable insight into the expected reliability of knowledge discovery systems. This will serve as the foundation for development of the aggregate meta-extractor, which we expect to substantially improve the 60% accuracy rate of current state-of-the-art methods. These systems demand higher-quality data ingestion, along with a more complete understanding of their reliability. In addition, because our approach incorporates existing tools, we can leverage the investments made in the commercial and academic 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.

FY08 Accomplishments and Results

In FY08, we analyzed the impact of event extraction error processes on queries and downstream inference. Specifically, we (1) modeled five common extraction errors—missing events, missing entities, misidentified entities, pronoun resolution failure, and false entities; (2) performed formal statistical experiments to analyze the effects of these errors and their interactions on queries, revealing critical insights into the relative ranking of their impact on inference; and (3) conducted a parallel-entity meta-extraction effort, in which we defined seven distinct and disjoint error types and developed a probabilistic aggregation approach that we applied to three extractors—SNER, GATE, and LingPipe. Our approach achieved a more than 15% error reduction over the best of the three.

Proposed Work for FY09

In FY09, we will complete our error analysis framework. We will leverage the error analysis and ranking produced via our methodologies to characterize the performance of existing extractors by (1) emphasizing errors having the most significant impact on extracted events and downstream inference; (2) accounting for variation across domains, ontologies, data, and user-specified relevance; and (3) assessing extractor dependencies. Development of the probabilistic meta-extraction system will proceed concurrently.

Scalable Methods for Discrete-Ordinate Transport Algorithms on Massively Parallel Architectures

Robert D. Falgout   08-ERD-026

Abstract

We propose to develop parallel multilevel solutions for the mono-energetic Boltzmann transport equations on inner neutron iteration and lambda iteration for x-rays. 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.

FY08 Accomplishments and Results

In FY08, we (1) developed a multigrid method for discrete-ordinate transport that is robust and optimal across a wide range of parameters including spatial resolution, scattering ratios, jump coefficients, diamond difference, corner balance, the Petrov–Galerkin finite element methods, and discontinuous Galerkin method; (2) derived a performance model for the minimum stages possible in a sweep algorithm and demonstrated an algorithm that achieves this minimum; and

(3) performed scaling tests to verify the theory and showed that sweeps can scale well to huge processor counts.

Proposed Work for FY09

In FY09, we will extend our FY08 results to the particular needs of the codes AMTRAN and Kull. Specifically, we will (1) extend our multigrid algorithm to the unstructured grid setting and modify the algorithm so that it does not require user-given coarse grids and coarse-grid discretizations, (2) examine other anisotropic scattering kernels and explore methods for solving the full multiple-energy-group Boltzmann transport equations, and (3) extend our parallel sweep algorithm and parallel performance models to structured adaptive mesh-refinement grids.

Publications

Lee, B., 2008. *A novel multigrid method for Sn discretizations of the mono-energetic Boltzmann transport equation in the optically thick and thin regimes with anisotropic scattering, part I.* LLNL-JRNL-409949.

Lee, B., 2008. *A novel multigrid method for Sn discretizations of the mono-energetic Boltzmann transport equation in the optically thick and thin regimes with anisotropic scattering, part II.* LLNL-JRNL-409967.

Lee, B., 2008. *Improved multiple-coarsening methods for Sn discretizations of the Boltzmann equation.* LLNL-TR-409109.

Image Segmentation and Feature Quantification for Advanced Radiography and Tomography

Peer-Timo Bremer   **08-ERD-028**

Abstract

Bringing together expertise from across the Laboratory and academia, we propose to address outstanding issues related to the quantitative analysis of digital radiography and tomography for both weapons and medical applications. Specifically, we will leverage LLNL's investments in visualization capabilities to develop user-guided segmentation techniques that will lead to robust, quantitative feature extraction for a broad range of high-energy imaging modalities. Our expertise and background in statistical methods, biomedical imaging, and the topology-based simplification of complex, three-dimensional (3D) imagery will allow us to advance the state of the art in segmentation, in which quantitative analysis is currently limited to a few specific problems.

We propose to combine LLNL's investment in advanced visualization tools with our team's expertise in medical imaging, Bayesian statistical methods, and topology-based simplification of 3D data structures to develop a truly revolutionary image segmentation and quantitative

feature capability. We envision a suite of tools allowing the user to easily manipulate data, identify a region, and initiate segmentation of features. The results would include a quantitative assessment of characteristics such as volume, shape, density, heterogeneity, and their associated uncertainties. By not requiring problem-specific models (as current methods do), this capability will enable advances in inspection and surveillance for stockpile stewardship, as well as patient diagnosis and treatment and drug and therapy development.

Mission Relevance

This project directly supports LLNL's national security mission by delivering a new capability for stockpile stewardship that will enable the robust, quantitative analysis of digital x-ray radiography and tomography. The algorithms and techniques we develop will also support the Laboratory's mission in bioscience to improve human health by providing new methods and tools for imaging disease and quantifying the efficacy of treatment.

FY08 Accomplishments and Results

After some initial testing in FY08, we (1) implemented a new visualization platform using the new ViSUS 2.0 code-base, allowing users to browse extensive 3D image data—our prototype allows an arbitrary number of slice planes with varying color maps as well as data probes and annotations; (2) developed a new topology-based method for segmenting features of interest; (3) tested our new methods with images from the National Ignition Facility target data set, and found that our method automatically detected boundaries of inner and outer laser target shells and created statistics indicating shell alignment by computing and sub-selecting contours—a primary problem posted by users; and (4) adapted new filtering techniques based on nonlocal means, and for the first time were able to partially segment the known defect in the target data set.

Efficient Numerical Algorithms for Vlasov Simulation of Laser–Plasma Interactions

Jeffrey A. 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 hour runs on 128 processors) and ground-breaking 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.

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.

FY08 Accomplishments and Results

In FY08, we (1) created an AMR testbed code based on the Structured Adaptive Mesh Refinement Application Infrastructure (SAMRAI) code, (2) documented test problems for laser–plasma interaction applications, (3) developed an AMR Poisson solver, (4) devised and documented B-spline AMR extensions to a semi-Lagrangian Vlasov scheme, (5) documented the SAPRISTI 2D Vlasov laser–plasma interaction code—the basis for this project—in detail for reference, and (6) began to create AMR extensions for the Maxwell equations.

Proposed Work for FY09

For FY09, we expect to demonstrate increased AMR speed using semi-Lagrangian methods and finite-volume methods on a realistic 4D laser–plasma interaction problem. To achieve this, we will continue to (1) develop a testbed code based on our SAMRAI code library; (2) develop efficient AMR extensions to the Vlasov standard semi-Lagrangian discretization; (3) develop AMR extensions using fast adaptive-composite and multigrid methods for a subset of Maxwell equations; (4) develop a multidimensional, fourth-order, finite-volume discretization of the Vlasov simulation; and (5) verify our method for use with the coupled Vlasov–Maxwell system.

Publications

Cohen, B. I., et al., in press. "Stimulated Brillouin backscattering and ion acoustic wave secondary instability." *Phys. Plasma.* LLNL-JRNL-407238.

Understanding Viral Quasispecies Evolution Through Computation and Experiment

Tanya V. Vassilevska   08-ERD-036

Abstract

Understanding how viruses evolve is a major scientific goal of LLNL's biodefense efforts. This understanding will lead to predictive pathogen science and lay the foundations for computationally guided design of therapeutics, diagnostics, and detection reagents. We propose to develop a predictive approach that combines novel multiscale modeling and simulation and bioinformatics analysis. Our results will enable the development of new biodefense technologies by providing key insight into how viruses mutate, adapt, and evolve under different selective pressures. The models we develop will include the first-ever computational model of the evolution of a quasispecies at cellular and multicellular scales of organization. Fed and calibrated with data from standard and novel biological assays, these models will be used for simulation and hypotheses testing, and will be a first step toward a full model of quasispecies evolution from the cellular to the population scale.

We intend to develop a computational model for simulating quasispecies evolution and for hypothesis testing and use the model to conduct simulations that will bring new scientific insights into virus evolution.

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.

FY08 Accomplishments and Results

In FY08, we worked to develop a computational framework to enable simulation of many viral families. Specifically, we (1) completed a comprehensive review of the quasispecies model and biological literature; (2) completed a conceptual framework model representing the common features of positive-sense, single-stranded viral replication strategies; (3) developed a novel algorithm, STRALSV, to identify regions of sequence variability; and (4) initiated construction of a database of locations of functional genome and proteome regions.

Proposed Work for FY09

In FY09 we will (1) complete the implementation, verification, calibration, and sensitivity and scalability analysis of the in-cell virus replication model; (2) complete our design of the cell culture (cell-to-cell infection) model; (3) continue the research, design, and development of our bioinformatics tools: the Web-based structure-alignment–based sequence variability tool and the functional annotation of the genome database; (4) collaborate with the University of California

at San Francisco on areas of common interest; and (5) submit journal articles that describe the in-cell model with simulations and bioinformatics approaches to evaluation of genome variability and fitness.

Hierarchical Vehicle Activity Models for Site Security

Douglas N. 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 vehicle activity detection scenarios—repeated surveillance and a coordinated attack—that are not addressed by current surveillance systems and which 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).

FY08 Accomplishments and Results

For FY08, we (1) acquired the components for and began installing our video tracking system, including bringing the surveillance video server online and resolving various configuration issues; (2) performed initial work on vehicle tracking and feature extraction under various camera and environmental conditions; (3) developed the requisite traffic-modeling data structures and a simulation capability; and (4) began planning rigorous experiments to test the overall system.

Proposed Work for FY09

For FY09, we will (1) develop and implement individual vehicle activity models—data structures and learning algorithms—as a hierarchical dynamic Bayesian network under our dynamic tracking and modeling software architecture; (2) perform testing with individual vehicles to verify our sensor error models, architecture, and learning algorithms; (3) iterate the feature extraction, vehicle identification, and model learning parameters and algorithms and characterize activity model accuracy and behavioral complexity; (4) implement an anomaly-detection algorithm for individual vehicles; (5) define and procure the testbed; and (6) define specific anomaly scenarios of interest and the initial approach for collective activity models.

Modeling Threat Mitigation of Cyber and Information Operation for the Space Intelligence, Surveillance, and Reconnaissance Infrastructure

Deborah W. May   08-FS-002

Abstract

The objective of this study is to determine if a modeling and simulation framework can be used to identify and mitigate cyber and information operation threats to the space community's intelligence, surveillance, and reconnaissance infrastructure. We also will explore incorporating cyber and information operation situational awareness into the larger space situational awareness system. Current models don't include cyber and information operation components. We will examine existing threat models to perform a gap analysis of existing capabilities compared to space awareness model data and the integration requirements. This will tell us if integration is feasible and, if so, what research and development is required to augment and integrate cyber and information operation models into space situational models.

Working closely with appropriate government stakeholders, we plan to establish a set of input requirements that a modeling and simulation framework would need to effectively incorporate cyber and information operation strategies into the larger framework. In addition, we will recommend technology that would help close the gap between current cyber and information operation awareness and that required by space situational awareness frameworks. Information and communication systems are an integral part of today's space architecture. A comprehensive space awareness framework should include cyber and information operation situational awareness. Understanding what the feasible approaches are to achieving that goal is a major part of the design of next-generation space situational awareness systems.

Mission Relevance

The U.S. space assets and supporting infrastructure are critical to national defense and intelligence efforts. Maintaining an awareness of threats to these systems and quickly evaluating strategies and response options to those threats are a key focus of the Department of Defense community responsible for the next-generation systems that will support their mission.

FY08 Accomplishments and Results

Based on changes in participation of the appropriate government partners for this project, we based our work on available all-source data. Specifically, in FY08 we (1) researched, documented, and summarized current models and approaches and determined that very little information is available; (2) analyzed and documented the information requirements for conducting a more realistic study—for example, what level of detail about network configurations would be required, or details as to the information processing pipeline and data ownership handoffs along that pipeline; and (3) classified threat types and mapped in the cyber component of those threats, including indicators. Overall, this project successfully analyzed and documented the information and partnership requirements necessary to develop a full-scoped space situational awareness model that includes the cyber component. We anticipate our results will be folded into a more comprehensive space situational awareness effort at Lawrence Livermore.

Fast-Running Tools for Explosions in Urban Environments

Charles R. Noble   08-FS-003

Abstract

The goal of this project is to determine the feasibility of a fast-running blast-structure analysis tool that would use simplified engineering models, advanced statistical techniques, and empirical data on blast pressures and structural damage to determine the probabilities of damage from explosions in urban environments. The defense community currently uses fast-running computational tools such as the Joint Munitions Effectiveness Manual for military applications, but the need exists for fast-running tools for analysis in support of domestic infrastructure protection. We will leverage LLNL's expertise in engineering models, state-of-the-art finite element tools, advanced stochastic techniques, and advanced computation to create a powerful tool for homeland security applications.

In short, our deliverable would be a framework for using simple engineering models and advanced stochastic techniques to create a fast-running blast effect tool that is more advanced than any currently available. This is important not only because of the need for such tools, but also because of the fundamental limitations of current tools that preclude their use for explosives of the most immediate interest.

Mission Relevance

This work supports LLNL's mission in homeland security by building on the Laboratory's expertise in fully coupled blast effects simulations, critical infrastructure modeling, advanced stochastic techniques, and supercomputing to lay the foundations for a tool for supporting the protection of domestic infrastructure.

FY08 Accomplishments and Results

In FY08, we (1) obtained empirical data on air blast pressures; (2) applied the data to improved fast-running models of canonical steel moment-resisting frame buildings (e.g., from 3- to 40-story buildings); (3) determined that it was feasible to produce damage maps for the building types and validated building response with historical data; (4) calculated probabilities of damage of a 3-story steel structure using a logistic regression model based on 10,000 simulations, varying the charge weight, standoff, yield stress, tangent modulus, and damping factor; and (5) integrated these achievements into a tool framework. In summary, this project created the framework for a fast-running blast-structure analysis tool for explosions in urban environments. The Department of Homeland Security has expressed interest in pursuing this technology further.

A Posteriori Error Calculation of Hydrodynamics Simulations Using Adjoint Methodologies

Carol S. Woodward   08-FS-005

Abstract

A new approach for estimating discretization errors in computed solutions to multiphysics simulations employs adjoint operators formed and solved for each component in addition to time-splitting operators. Such methodologies represent a powerful new tool for quantifying uncertainty because of discretization error in a given calculation without the strong assumptions required by current methods. However, little work has been done on applying adjoint methodologies to the explicit hydrodynamic systems that are relevant to stockpile stewardship and fusion energy because of the nonlinearities of the problems and the discretization methods applied to solve them. We propose to investigate whether adjoint methodologies can be developed and implemented for the estimation of numerical discretization error within explicit hydrodynamic simulations. We will start with simpler parabolic hydrodynamics and then broaden to hyperbolic hydrodynamic systems.

This project will determine the feasibility of estimating discretization error for multiphysics calculations, such as those used in stockpile stewardship and inertial-confinement fusion. The area with least prior work in adjoint formulation is hyperbolic hydrodynamics, and adjoints for this component must be understood before error estimates of the full multiphysics system can be developed.

Mission Relevance

Numerical discretization error is a poorly understood error in stockpile stewardship and fusion calculations used by NNSA's Advanced Simulation and Computing Campaign. Current methods for estimating this error rely on unrealistic assumptions about calculations. This work supports LLNL's national security mission by investigating an alternate strategy that promises to be more flexible but is currently limited in its maturity for stockpile stewardship applications.

FY08 Accomplishments and Results

We (1) developed a preliminary error analysis for the Lax–Friedrichs scheme using the adjoint of the modified equation applied to the parabolic viscous Burger's equation, a scalar hydrodynamic model; (2) developed an a posteriori error estimate of the marker-and-cell scheme for the incompressible Navier–Stokes parabolic hydrodynamic system in two dimensions, then began implementing the adjoint solution for testing; and (3) developed a preliminary analysis of the Lax–Friedrichs scheme for the hyperbolic inviscid Burger's equation and began developing an implementation for testing. This project determined that in the short term, it is not yet feasible to apply adjoint methods to hydrodynamic systems emitting discontinuities such as those used in inertial-confinement fusion. Further work is required to develop mature tools such as modified equation analysis, variational forms, and viscous solutions for use in a posteriori error analysis for discretizations of hydrodynamic systems emitting discontinuities.

Distributed Data Flow for In Situ Visualization and Analysis at the Petascale

Daniel E. Laney   08-FS-006

Abstract

Existing computational tools are known to fail at the petascale. Rather than discarding these tools, we propose to examine a computer architecture that allows processing pipelines to be automatically distributed across multiple machines. Distributed data flow is a crucial technology to ensure that applications such as the VisIt parallel visualization and graphical analysis tool can provide in situ data analysis and post-processing for simulations on petascale machines. This project will enable us to understand if petascale applications are possible, taking into account trade-offs between stability, load balancing, and remote streaming when performing visualization operations with a combination of light-weight kernel compute assets and dedicated post-processing cluster nodes.

This work would establish the fundamental feasibility of constructing visualization platforms that would work at the petascale by distributing data flow across a heterogeneous network of systems, enabling more efficient use of available resources. The results will determine the feasibility of moving this class of tools into the petascale regime, where it is likely that some combination of in situ processing and post-processing on compute nodes will be required. We expect that our research will have broad impact across a number of communities of future petascale users.

Mission Relevance

This project will contribute to developing petascale analysis and post-processing capabilities for NNSA and LLNL users and will establish the feasibility of building capabilities to perform visualization and analysis tasks on datasets within the current high-performance computing

environment at LLNL. High-performance computing at Livermore is crucial to scientific and engineering simulations in support of the stockpile stewardship mission as well as breakthroughs in fundamental science research.

FY08 Accomplishments and Results

Our research has resulted in a prototype version of the VisIt tool that allows distributed data flow across multiple machines. In FY08, we (1) focused on distributing data when memory requirements are exceeded on compute hardware, (2) simulated this configuration with a runtime parameter, (3) determined our system allows a set of master compute engines to communicate to a set of slave engines running on post-processing resources, and (4) modified a small set of filters to estimate the memory required by their output. If this estimate was larger than the available memory, the filter sent data to a slave engine instead of continuing on the master engine. The successful conclusion of this project will help enable efficient in situ analysis and visualization on petascale systems. We expect support from Livermore's Advanced Simulation and Computing Program to perform scaling studies of the system, and components of the prototype (including the socket communication infrastructure) may be introduced into the main VisIt distribution.

Internet Protocol Profiling Through Network Service Cluster Membership

Anthony Bartoletti   **08-FS-007**

Abstract

This project seeks to demonstrate the feasibility of utilizing compact Internet Protocol behavioral profiles as a robust means for detecting compromised systems, illicit data exfiltration, and related abuse. The profiles would reflect the degree and variability in which individual client machines engage in various forms of Internet traffic, as determined by several terabytes of historical LLNL session summaries. We will establish this feasibility by determining characteristic classes of network service usage and then defining client profiles in terms of their degree of activity in these classes. Onset of system compromise is expected to reveal unusual directions of deviation from profile and could thus provide an effective new approach to thwarting cyber-security attacks.

We will gain an understanding of what would be necessary to build a robust and enduring capability to identify anomalous system behaviors—often associated with system subversion and related misuse—in the absence of knowledge of specific a priori behavioral features. This capability would be significant, given that modern adversary activities avoid fixed detection signatures and present only statistical features by which characterizations may be made. The space and time resources necessary for profile maintenance and ongoing detection activity will be provided, given the Internet Protocol population and foreseeable rates of network traffic capture.

Mission Relevance

All national defense and infrastructure protection missions and related scientific endeavors rely upon secured computing and communications resources. State-sponsored adversaries display considerable sophistication in conducting hostile and stealthy system intrusion. A broad-scale means for detecting and mitigating pre-characterized changes in system-specific traffic behaviors will provide network security operators valuable indicators of suspect activities, in support of the Laboratory's homeland security mission.

FY08 Accomplishments and Results

We determined stable service cluster solutions for sessions in the seven most common network services in LLNL boundary traffic, which were migrated daily via Hungarian matching and exponential decay. Sessions for three services not subject to boundary proxy were partitioned by client–host, and the resulting cluster membership vectors were used as compact profiling instruments. In particular, File Transfer Protocol traffic data yielded strong scores (such as the area under the receiver operating characteristic curve) for distinguishing clients from neighbors, along with a visual trace of cluster membership vector movement, and provided a marked ability to depict departures from routine behaviors. We surmised that pre-proxied Web traffic would exhibit similar utility for detection. Finally, commodity hardware proved easily able to supply the requisite performance. In summary, this project successfully established the feasibility of employing and migrating stable clustering solutions of network service traffic as a basis for characterizing and tracking the behaviors of client systems by their fractional membership in the identified clusters. The next step will be to expand these results to pre-proxied traffic and refine the measures for use in detecting malicious or suspect network events.

Large-Scale Epidemiological Model of Human Diseases

Matthew J. Dombroski   08-FS-008

Abstract

We propose to explore and determine the feasibility of extending the current Multiscale Epidemiological/Economic Simulation and Analysis (MESA) epidemiological software developed by Lawrence Livermore to model the spread of human communicable diseases and the impact of countermeasure systems such as quarantine rules and vaccination strategies. Currently, MESA is being developed to model animal diseases not present in the U.S. This effort will explore the applicability of some of the MESA constructs to the simulation of human communicable diseases at a national scale. MESA algorithms have demonstrated national scalability for processes and phenomena related to foreign animal diseases.

The proposed project will determine the feasibility of extending MESA to develop an accurate and computationally efficient human epidemiological simulation model that incorporates detection events and countermeasures in a meaningful and realistic way. The enhanced MESA

model may provide a more efficient and accurate human infectious disease model than existing capabilities at other laboratories.

Mission Relevance

There is a critical national need for a real-time epidemiology tool that will predict the spatiotemporal spread of emerging human infections and assess the effectiveness of various countermeasure strategies. This project will enable the Laboratory to help counter infectious disease propagation in support of both homeland security and human health missions.

FY08 Accomplishments and Results

In FY08, MESA was applied to human epidemiology by (1) loading 2000 U.S. Census data, populating the susceptible-exposed-infectious-recovered model with influenza spread parameters; (2) implementing four different spread methods of schools, workplaces, households, and air travel; (3) developing a baseline scenario that simulated an index influenza case in a Queens, New York school, which appears to conform to historical influenza data from Centers for Disease Control and Prevention—the majority of influenza outbreaks are limited to local or regional outbreaks, but periodically a pandemic occurs; and (4) examining several different types of countermeasures including restricting air travel, establishing surveillance zones and quarantines, and reducing contact between infected and uninfected zones. The successful application of the MESA model to human epidemiology is a first step to enabling a new capability for modeling nationwide spread of contagious diseases and biological threat agents, as well as countermeasures to contain them.

Publications

Dombroski, M., et al., 2008. *Simulating nationwide pandemics: Applying the multi-scale epidemiologic simulation and analysis system to human infectious diseases.* LLNL-TR-407672.

Computational Biology for Target Discovery and Characterization

Carol E. Zhou   08-FS-009

Abstract

We propose to determine the feasibility of extending current LLNL capabilities to produce a high-throughput system bioinformatics capability for identifying and characterizing putative interacting protein partners within known or suspected networks. These codes will be applicable to pathogen or host protein interaction networks and will also establish an important capability for identifying useful drug targets. If successful, we will lay the groundwork for an important component of a high-throughput systems approach for the computational design of therapeutics

against known pathogens and for the rapid development of vaccines and therapeutics as countermeasures for known and emerging or engineered organisms.

Mission Relevance

This project seeks to leverage LLNL's strengths in biodefense, computational biology, bioinformatics, and pathogen detection to help devise a high-throughput systems approach for the computational design of therapeutics against various pathogens—including potential bioterror pathogens—in support of the Laboratory's missions in biodefense and improving human health.

FY08 Accomplishments and Results

We accomplished our main goal of extending current codes to produce a high-throughput capability for identifying and characterizing putative interacting protein partners within small networks (of two to ten proteins) and also to determine how interacting partners could best be detected starting with an arbitrarily large set of proteins. Specifically, we (1) devised a method for detecting high-order domain fusion linkages, (2) devised a method to structurally and functionally tag linkages to cluster results, and (3) determined that the most feasible method to identify domain fusion linkages, given an arbitrarily large input set, would require a database of domain–domain linkages generated by domain-splitting all structures in the Protein Data Bank database and by binary domain fusion analysis across all domains. In summary, this project furthered the detection of the interacting protein partners of pathogens of interest in biodefense. These codes are applicable to current efforts in the biodefense community to identify and structurally and functionally characterize therapeutic targets.

Feasibility of *n*-Gram Data Structures for Next-Generation Pathogen Signature Design

Shea N. Gardner   08-FS-014

Abstract

We propose a feasibility study to determine the most appropriate data structure for handling *n*-gram probabilistic models for predicting the next item in a sequence, which will be used in string comparisons and storage for genomic sequence data. The critical application will be in pathogen detection to guide design of the next-generation system for computational signature prediction. We will work with the storage-intensive supercomputer team to evaluate memory requirements and speed of candidate data structures and algorithms on a board with 128 GB of memory, to determine a hardware and software combination that will facilitate our sequence comparison needs and scale with sequence databases that double in size every 16 months.

Livermore bioinformatics has advanced to the forefront of pathogen signature design. However, the current Laboratory-developed computational DNA signature design system, KPATH, was designed years ago prior to the data explosion resulting from new sequencing technologies. Although still useful, KPATH is now severely challenged by data scaling and the advent of novel assay platforms. Collaboration between bioinformatic and computer science experts will enable us to determine which approach should be employed in the next-generation KPATH for signature prediction. If a feasible design for the system is ascertained, it will enable the design of higher quality signatures, to keep up with ever-expanding sequence databases, and to respond more quickly to signature design requests on novel assay platforms.

Mission Relevance

Our project is crucial for maintaining Livermore as a leader in pathogen detection because it will guide the design of the next-generation bioinformatics system for computational signature prediction. This research supports the Laboratory's mission in homeland security, as well as efforts to improve human health.

FY08 Accomplishments and Results

For the k-mer analysis of specific n-grams of nucleic or amino acid sequences for gene prediction, suffix arrays are preferred because of increased memory efficiency and speed over other (e.g., various hashing) methods. A subset of the k-mers based on frequency characteristics can be stored and manipulated in a hash for downstream tasks such as signature prediction or functional correlations. In FY08, we provided test code for performing suffix array computations to storage-intensive supercomputing collaborators for benchmarking on different machines, including SiCortex, a Violin flash-disk system, and a 500-GB Silicon Graphics workstation. These benchmarks were useful in LLNL evaluation of various large memory systems, and contributed to the decision of which large memory nodes the Laboratory would purchase. We determined the data structures that would be most useful for k-mer computations. The results of this study will be applied to federal agency-sponsored work on advanced threat detection as well as LDRD-supported research on a viral discovery platform.

Multiscale, Multiphysics Membranes Technology

William D. Henshaw   08-FS-016

Abstract

We propose to investigate the mathematical feasibility of a general-purpose interface technology called "membranes" to couple two different physics solvers. This would enable multiphysics simulations that couple a gas-phase physics solver to a deforming-solid physics solver to solve

difficult multiphase, multiscale problems of critical interest to Laboratory efforts. The objective of this study is to develop a theoretical understanding of the mathematical and numerical issues involved in this type of interface coupling. Our approach will involve mathematical and numerical analysis as well as computational studies.

This study will lead to an improved understanding of the mathematical and numerical issues involved in the coupling of interfaces of different physics solvers, thereby laying the groundwork for future work in the effective coupling of large physics packages to solve difficult multiphase problems.

Mission Relevance

Many important multiphysics problems require the simulation of a gas or fluid interacting with the motion of deforming solids. Our project supports multiple Laboratory missions. For national security, membranes technology will have applications in weapons effects, insensitive munitions, warhead design, composite armor, and earth penetration. For energy security, it will benefit studies of vibrations in reactor fuel rods for the Global Nuclear Energy Partnership, as well as laser hohlraum targets. For homeland security, the technology will be used in threat assessments and neutralization, and for breakthrough science there will be applications in ablation, fluidized beds, combustion, and pharmaceutical research.

FY08 Accomplishments and Results

In FY08 we (1) developed a numerical approach for modeling fluid–structure problems and began development of a software infrastructure for modeling multiphysics, multidomain problems; (2) analyzed the problem of a planar interface between a compressible fluid and elastic solid; (3) computed the solution to this problem with our new approach, and used the exact solution to measure the error; (4) demonstrated our approach for solving an elastic cylinder embedded in a fluid; and (5) analyzed the numerical stability and accuracy of a new centered-interface approximation for the jumps in temperature and heat flux at the fluid–solid interface and submitted a paper describing this approach. This feasibility study has been successful in determining a mathematical and numerical understanding of, and in beginning development of, a new multidomain approach for simulating fluid–structure problems. We plan to continue to develop this approach with support from the DOE Office of Science.

Publications

Henshaw, W. D., and K. K. Chand, in press. "A composite grid solver for conjugate heat transfer in fluid–structure systems." *J. Comp Phys*. LLNL-JRNL-407079.

Laboratory Directed Research and Development

Nuclear Science and Engineering

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

James V. Candy   07-ERD-019

Abstract

The detection of special nuclear material 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 on-line, real-time operation. This project is focused on the detection, classification, and estimation of illicit special nuclear material from highly uncertain, low-count radionuclide measurements using a statistical approach based on Bayesian inference and physics-based signal processing.

We expect to develop solutions for the detection, classification, and estimation of a moving special nuclear material 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 special nuclear material 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.

FY08 Accomplishments and Results

In FY08 we (1) developed the full-physics simulation and validation on controlled experimental data, (2) developed a novel point-to-point signal processing model capable of being incorporated into a Bayesian processor to identify Compton scattered photons, (3) developed (and patented) a distributed parallel solution to the radionuclide detection problem capable of extension to moving sources, (4) developed a solid design for classification of special nuclear material detected, (5) demonstrated the feasibility of our classification approach by applying it to both simulated and controlled experimental data, (6) completed experimental runs for both germanium and sodium iodide detector materials, and (7) discussed collaboration and licensing with potential industrial partners for implementation.

Proposed Work for FY09

For FY09, we propose to (1) complete performance evaluation of the Bayesian detection scheme using both simulated and experimental data, (2) continue development of the simplified signal-processing model—which is based on point-to-point modeling of the transport process—by incorporating additional transport physics and validating the results with full-physics simulations and experiments, (3) use our signal-processing model to investigate solutions to the Compton inversion problem of source determination, (4) begin solving the classification problem using Bayesian processors, and (5) begin efforts to solve the nonstationary source problem for time-varying statistics.

Publications

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 J. 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 alternative 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 Lawrence Livermore's 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 for strontium-90. This capability 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. Additionally, 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.

FY08 Accomplishments and Results

A majority of the effort in FY08 was devoted to development of sample preparation methods for real matrices. Specifically, we (1) discovered that most methods utilizing commercial extraction chromatography columns do not effectively remove zirconium-90 (which interferes with the accelerator mass spectrometry measurement of strontium-90) and necessitated a modification of our scope of work, (2) investigated alternative methods using these columns and found that addition of oxalate to the eluting solution dramatically improved the suppression of zirconium-90, and (3) designed and constructed a new detector that improved the resolving power between strontium-90 and zirconium-90 by a factor of 100.

Proposed Work for FY09

The major effort in FY09 will be continuing the development of chemical protocols for preparation of real samples. Specifically, we will (1) investigate suitable methods for removing bulk quantities of calcium from real sample matrices, (2) research chemical purification procedures to eliminate zirconium-90 interference, (3) validate our sample-preparation protocols by measuring strontium-90 in standard reference materials, and (4) demonstrate our strontium-90 capabilities by participating in round-robin exercises (e.g., DOE's Laboratory Accreditation Program).

Publications

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.

Shock Ignition: A New Approach to High Gain and Yield Targets for Stockpile and Energy Applications

L. John Perkins   08-ERD-050

Abstract

We propose to evaluate shock ignition, a new concept for igniting and burning inertial-confinement fusion targets at high gains and yields. Employed on fusion-class lasers following indirect-drive ignition, such targets potentially offer high fusion yield (>200 MJ) for stockpile stewardship needs, high reactor yields for fusion energy, and high gain at low laser drive energies. We will first conduct one-dimensional studies with radiation-hydrodynamic burn codes, then investigate laser–plasma instabilities, two-dimensional stability and symmetry, and the fusion-laser power and rise time needed to drive such targets. This project will establish the technical basis for advanced stockpile- and reactor-relevant targets fielded on fusion-class lasers and will position the Laboratory for leadership in inertial-confinement fusion energy.

We intend to produce the technical basis and credible designs for shock-ignited targets such as: (1) a high-fusion-yield target for stockpile stewardship; (2) a fully fusion-reactor-relevant target testable on a single-shot basis—if repetition-rated at 6 Hz on a future reactor facility, it would yield a fusion power of approximately 1200 MWt or about 500 MWe; (3) targets with appreciable gain at low laser drive energies—for example, a gain of about 50 at approximately 150 kJ of laser energy, which mitigates the risk that optics damage may preclude high laser energy; and (4) a simple, noncryogenic (room-temperature) single-shell gas target, instead of expensive and complex cryogenically frozen deuterium–tritium targets, that may enable fusion ignition and burn.

Mission Relevance

By delivering technically credible designs for advanced stockpile- and reactor-relevant targets that can be fielded on fusion-class lasers, this projects supports Lawrence Livermore's missions in national and energy security.

FY08 Accomplishments and Results

In FY08, we evaluated shock ignition as an option for high gain and yield targets for future fusion-class lasers. Our results indicate that approximately 200-MJ yields may be achievable with drive energies of about 1.5 MJ, while tenfold gains may only be possible for drives around 200 kJ. Linear analysis indicated that laser backscatter via stimulated Brillouin scattering is low.

Moreover, because the high laser intensity is not applied until late time, the dense imploding shell is capable of absorbing Raman-generated electrons up to at least 100 keV, making it feasible to drive this class of targets with green laser light. This will enable us to exploit higher damage thresholds in advanced laser optics through higher drive energies and greater shot budgets. We hope to continue our research with support from a joint DOE/NNSA program in high-energy-density laboratory plasmas to extend this exploratory assessment to full fusion-class laser target designs.

Publications

Perkins, L. J., 2008. *Advanced target design for ICF/IFE and the physics of high gain.* High Energy-Density Laboratory Plasmas, Fusion Energy Science Advisory Committee Subpanel Workshop, Washington, D.C., Aug. 25, 2008. LLNL-PRES-405463.

Perkins, L. J., et al., 2008. *Shock-ignited targets for the National Ignition Facility.* 35th European Physical Society on Plasma Physics, Hersonissos, Greece, June 9–13, 2008. LLNL-ABS-401585.

LaFortune, K. N., and L. J. Perkins, 2008. *Shock-ignited sub-MJ green-light ICF targets potentially fieldable on the NIF.* 50th Ann. Mtg. Division of Plasma Physics, Dallas, Texas, Nov. 17–21, 2008. LLNL-ABS-405465.

Perkins, L. J., et al., 2008. *Shock ignition: A new approach to high gain targets for the National Ignition Facility.* 50th Ann. Mtg. Division of Plasma Physics, Dallas, Texas, Nov. 17–21, 2008. LLNL-ABS-408694.

Laboratory Directed Research and Development

Physics
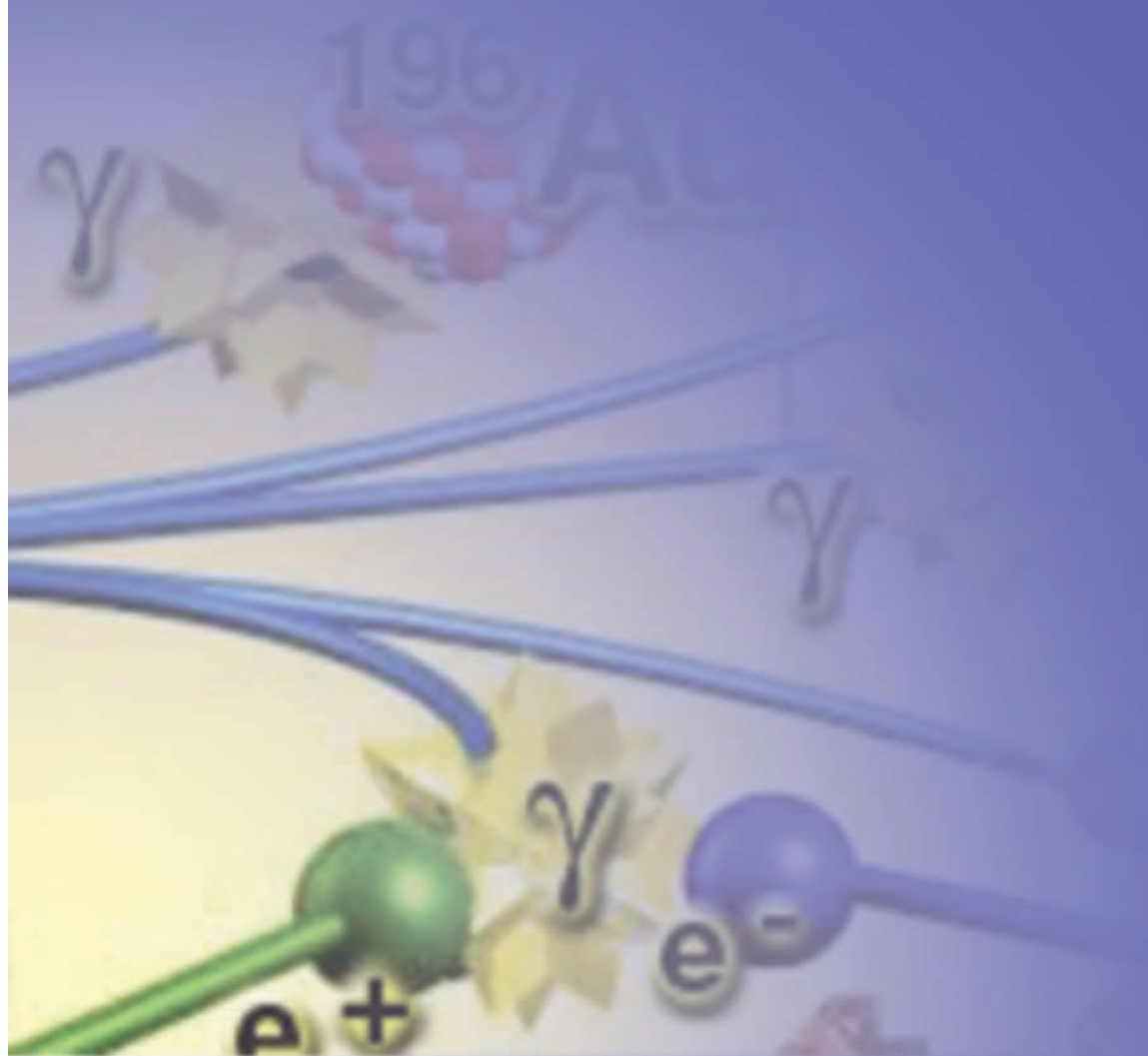
Biological Imaging with Fourth-Generation Light Sources

Henry N. Chapman   05-SI-003

Abstract

We propose to develop capabilities to carry out single-molecule, atomic-resolution imaging at future x-ray free-electron laser (XFEL) facilities. Our goal is to perform groundbreaking experiments at new and existing sources to test the key concepts of single-molecule XFEL imaging, including measurement of the Coulomb explosion of particles in intense, ultrashort x-ray beams; lensless x-ray imaging beyond the radiation-damage limit; and manipulation and orientation of single particles in space and time to interact with XFEL pulses. We will compare experiments with high-fidelity modeling to understand the new abilities that the XFEL will bring to biological imaging. These capabilities will allow us to determine the atomic structure of any protein.

Each of our experiments, which will be a world first and a major new result in x-ray science in every case, will (1) determine the duration and fluence of XFEL pulses required for single-molecule imaging, (2) demonstrate reconstruction methods, and (3) demonstrate ultrahigh-resolution, three-dimensional imaging of container-free particles, for which new technologies in biological sample preparation will be developed. Together, these experiments will demonstrate the extraordinary science achievable with XFELs and the impact they will have on structural determination of biological macromolecules, protein complexes, viruses, and spores.

Mission Relevance

Improved tomography algorithms will benefit stockpile stewardship. As a specific example, diffraction imaging techniques can be applied to the study of warm dense matter, a critical regime of weapons physics. Single-molecule imaging will allow us to determine the structure of virtually any macromolecule, protein, or virus, which furthers Lawrence Livermore missions in both biodefense and bioscience to improve human health. Our research also enhances the capabilities of the Linac Coherent Light Source (LCLS), a high-priority project of the DOE Office of Science, in support of LLNL's mission in breakthrough science and technology.

FY08 Accomplishments and Results

In FY08 we (1) imaged hydrated cells "on the fly" by injecting them into the XFEL beam using an x-ray dose well above the radiation damage limit; (2) imaged three-dimensional structures with the XFEL beam on the fly, then analyzed and classified their orientation; (3) used tampers to mitigate radiation damage in experiments, clearly demonstrating their efficacy in containing particle explosion at nanometer scales; and (4) developed an experimental plan for future work at the LCLS. In summary, this project has culminated in over 8 proposals for using the first beam at the LCLS in 2009 and has produced over 25 high-profile publications, many in prestigious journals such as *Nature* and *Physical Review Letters*. This project also established LLNL as a worldwide leader in ultrafast x-ray imaging, spawned an entirely new field of femtosecond diffractive imaging, and opened the doors to a wealth of new science opportunities using fourth-generation x-ray sources. Follow-on work will be supported by the University of California,

Stanford Linear Accelerator Center, and Italy's Sincrotrone Trieste. We are also pursuing the possibility of establishing, with university collaborators, a National Science Foundation center devoted to femtosecond diffractive imaging.

Publications

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Barty, A., and H. Chapman, 2007. *Imaging without lenses: X-ray snapshots with nanometer spatial and femtosecond temporal resolution*. UCRL-ABS-235770.

Barty, A., H. Chapman, and S. Hau-Riege, 2008. "Femtosecond coherent imaging with a free electron laser: X-ray snapshots of nanoscale transient phenomena." *Proc. SPIE* **7005**, 7005-5. UCRL-ABS-236138.

Barty, A., et al., 2008. "Three-dimensional coherent x-ray diffraction imaging of a ceramic nanofoam: Determination of structural deformation mechanisms." *Phys. Rev. Lett.* **101**(5). UCRL-JRNL-231416.

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Advanced Studies of Hydrogen at High Pressures and Temperatures

William J. Evans   **05-ERD-036**

Abstract

The goal of this project is to study hydrogen at high pressures (megabars) and temperatures (thousands of kelvin). Properties of high-pressure hydrogen in this regime are important to a range of basic and applied sciences, including condensed-matter theory, modeling efforts, planetary science, and hydrogen energy storage. High-pressure hydrogen is the subject of intensive theoretical and experimental studies, both static and dynamic. Our proposed high-pressure and high-temperature experiments bridge the gap between static and dynamic experiments. We propose to apply state-of-the-art high-pressure, x-ray, laser, and spectroscopic capabilities. These studies address important issues such as the equation of state at high pressures and temperatures, phase lines, and novel phase transitions.

The rich physics in the regime between dynamic and static studies are targeted by our project. Shockwave studies at 150 GPa and 3000 K reveal a liquid metallic phase, while static work at 300 GPa and 77 K has identified only solid insulating states. The goal is to find the pressure and temperature states bridging these regimes that contain transitions in properties to reconcile these disparate results; that is, the phase lines for melting, metallization, and dissociation. Further, we seek to measure the melt line, liquid–liquid (molecular–nonmolecular) transition, and the metallic fluid state predicted by theory. Such discoveries in hydrogen would impact our understanding for defense applications, Jovian planets, and hydrogen energy storage.

Mission Relevance

The project deliverables of equation of state and phase transitions of high-pressure and high-temperature hydrogen directly address needs in stockpile stewardship (specifically, the extreme dynamics of materials) and hydrogen energy storage, in support of LLNL's national and energy security missions.

FY08 Accomplishments and Results

In FY08, we found that determining the reactivity of hydrogen—particularly at extreme conditions of melt—was a major challenge, even at moderate pressures. Our results, however, proved to be consistent with previous measurements. While achieving successes in measuring the hydrogen melt curve, we also used our measurements to develop insights regarding discrepancies in widely used in situ high-pressure sensor calibrations, and our results were summarized in the *Journal of Applied Physics*. The successes of this project have enhanced our fundamental understanding of hydrogen—specifically the band gap at high pressure and the existence of a new high-pressure and high-temperature phase. We developed crucial expertise, capabilities, and infrastructure that we hope will be of interest to the DOE's Hydrogen Fuel Initiative for the development of novel hydrogen fuel-storage materials using high-pressure approaches.

Publications

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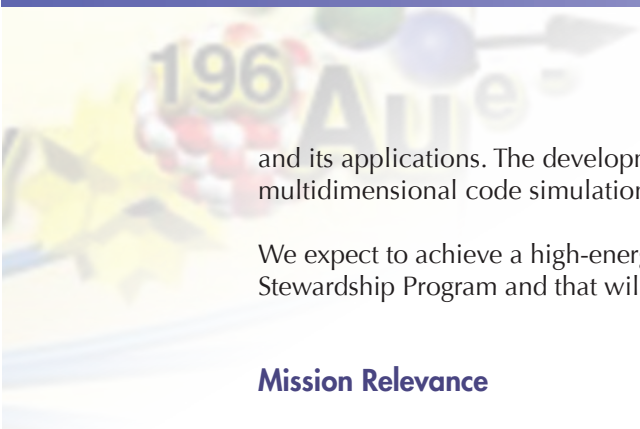
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Novel High-Energy-Density Source

James H. Hammer   **06-SI-001**

Abstract

With this project, our objective is to develop a novel high-energy-density source of higher quality than 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 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.

FY08 Accomplishments and Results

In FY08, we (1) continued source development, output characterization, and development of a stable, reproducible platform for high-energy-density experiments; (2) made further improvements in predictive capability by detailed comparisons of calculational models with data; (3) designed and experimentally tested an innovative variation on the core concept, achieving good agreement with models; and (4) used the improved models to evaluate the potential of the original and improved concepts for future applications.

Proposed Work for FY09

In FY09, we propose to (1) fabricate and test a series of targets to complete the work of this project, (2) continue modeling these and earlier targets as preparation for follow-on efforts to apply the design principles and physics developed through our research, and (3) document the results achieved in this project.

Publications

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Active Detection and Imaging of Nuclear Materials with High-Brightness Gamma Rays

Christopher P. Barty   06-SI-002

Abstract

This proposal leverages LLNL's world-leading capabilities in laser science, x-ray source development, nuclear science, and detector technology to enable a new class of active

interrogation techniques. We propose to demonstrate the use of new linear accelerator and laser-based gamma-ray sources for isotopic imaging of well-shielded objects, and thus provide an effective means of detecting concealed highly enriched uranium, including uranium-235. Isotopic selectivity of the detection scheme is based on nuclear resonance fluorescence from target nuclei. Specifically, our efforts will include (1) determining the location and width of nuclear resonance fluorescence transitions in uranium-235 and plutonium-239; (2) developing, modeling, and demonstrating linear accelerator and laser-based high-brightness x-ray generation; (3) demonstrating nuclear resonance fluorescence detection of uranium-238; (4) developing modeling tools for optimizing nuclear resonance fluorescence-based detection and imaging; and (5) using this new light source to perform inverse radiography on a broad array of targets.

If successful, this project will create the world's highest-brightness gamma-ray source and enable, for the first time, an effective detection modality for hidden highly enriched uranium. This detection capability could launch "nuclear photo science" as a new field of study and result in numerous follow-on applications.

Mission Relevance

The ability to detect and image highly enriched uranium would support LLNL's national security mission, specifically homeland security and counterproliferation. Furthermore, the picosecond, high-spatial-resolution, tunable, megaelectronvolt source capability developed as part of this proposal would also impact a wide range of applications of importance to stockpile stewardship in support of national security, and high-energy-density science and technology in support of national and energy security.

FY08 Accomplishments and Results

The last year of our project has seen success on many fronts. Specifically, (1) the Thomson-radiated extreme x-ray system (T-REX) achieved first light early in the calendar year; (2) high-energy x rays and gamma rays were generated at 776 keV and at approximately 500 keV, which in this spectral regime is believed to be the highest peak-brightness photon source in the world; (3) near-record emittance and charge electron bunches were also created; (4) tuning of the T-REX beam enabled excitation and observation of nuclear resonance fluorescence from lithium-7; (5) a new technique for detection and use of T-REX–like sources was invented, and a record of invention was filed; and (6) modeling efforts identified four high-profile potential NNSA relevant applications of T-REX isotope imaging. The NNSA, SLAC National Accelerator Laboratory, and Department of Homeland Security will collaborate to create a compact mono-energetic gamma-ray capability in the 1- to 3-MeV range for isotope imaging applications.

Publications

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The Ultrafast Lattice Response of the Shocked Solid

Hector E. Lorenzana   **06-SI-004**

Abstract

Our goal is to perform the first studies exploiting the new generation of bright, ultrafast x-ray sources to investigate real-time dynamics of shocked materials at characteristic temporal and

spatial scales of the controlling physical phenomena. We will measure the microscopic state of the materials and their evolution under shock loading by a combination of dynamic x-ray diffraction and scattering. We will characterize, in situ, two phenomena: condensed matter phase transformations and damage. We will couple our experimental results with state-of-the-art simulations which, for the first time, will match the length and time scales of the experiments. These results will lay the foundation for physics-based models of macroscopic material behavior under extreme conditions.

We expect to perform the first comprehensive real-time, in situ study of the lattice response under shock loading, a problem of great scientific importance. Properties of solids undergoing phase transitions, plastic deformation, or void growth during a shock are largely unknown, yet this information is crucial to predictively understand material response and failure. Success in this endeavor through laser and synchrotron-based experiments coupled with simulations will position LLNL at the forefront of a new field, high-energy-density materials science. The close coupling of experiment and theory will validate existing modeling at the atomistic, mesoscopic, and continuum scales, and spur the development of new models.

Mission Relevance

Success in stockpile stewardship, high-energy-density science, and other national security mission areas demand a fundamental understanding of dynamic materials behavior. The expertise developed in this project will further current and future research in support of stockpile stewardship at facilities such as the Joint Actinide Shock Physics Experimental Research (JASPER) gas gun at the Nevada Test Site, and basic science facilities such as the Linac Coherent Light Source at Stanford. This work will drive development of computational tools for predicting performance, safety, and reliability of nuclear weapons, as well as for high-power laser research.

FY08 Accomplishments and Results

In FY08, we (1) studied shock loading along different crystallographic directions in single-crystal iron and observed corresponding differences in the high-pressure structure; (2) measured phase transformation in a polycrystal material for the first time under shock compression; (3) studied the one- and three-dimensional lattice relaxation in several materials, which has provided an estimate of dynamic yield stress in both single crystals and polycrystals; and (4) successfully measured incipient spall in aluminum under shock at a synchrotron light source. This project has been very successful in demonstrating the feasibility of in situ studies of materials properties under dynamic compression. These developments have been transitioned to a high-energy-density program being pursued at the National Ignition Facility, and some of the unresolved basic science is currently being pursued under a new LDRD Strategic Initiative project.

Publications

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Laser-Driven Dynamic Hohlraums

Sharon G. Glendinning   **06-ERD-017**

Abstract

With this project, we propose to use experiments and simulations to explore the laser-driven dynamic hohlraum (LDDH), a laser-driven analog to the dynamic hohlraum used at the Sandia Z machine, as an ignition target for future fusion-class lasers. The project will investigate the neutron production history of capsules driven with an LDDH, determine radiation production during an implosion, use "polar" direct drive on the Omega laser, and optimize the LDDH as a

potential bright x-ray source. Experiments will be fielded on the Omega laser to test simulations of the LDDH addressing each of these points.

We expect to demonstrate the feasibility of the LDDH as a candidate for an ignition target, for x-ray source development, and for diverse high-energy-density physics experiments in regimes not otherwise achievable. A noncryogenic ignition option could allow for more ignition experiments at lower cost than currently feasible, making possible more experiments on the effects and uses of ignition.

Mission Relevance

The LDDH, once demonstrated, could become a platform for a variety of high-energy-density physics experiments that support Lawrence Livermore's stockpile stewardship mission. Radiatively driven shocks are also of great interest in basic science, especially astrophysics, and thus this project supports the Laboratory's mission in breakthrough science.

FY08 Accomplishments and Results
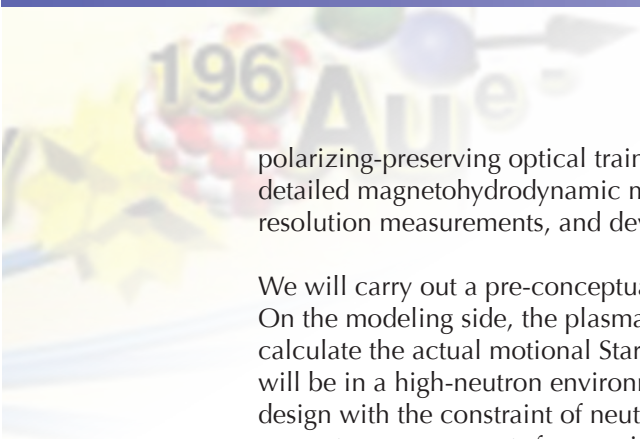
In FY08 we (1) conducted experiments on the Omega laser to test an LDDH backlighter, successfully demonstrating bright emission between 4.5 and 9 keV (a factor-of-1.6 increase in the spectral range for opacity experiments) and also measuring the absorption and emission of plastic-tamped, heated iron samples; (2) conducted detailed simulations of the proposed higher-Z capsules, showing that the improved coupling to drive would not result in an observable signal given the degradation of yield caused by mixing between the shells; and (3) successfully fielded experiments designed to improve our understanding of the effect of mixing in the LDDH capsules. This project's achievements have enabled opacity experiments in previously inaccessible energy regimes on the Omega and fusion-class lasers through the novel x-ray sources created, and have also increased our understanding of the issues involved with achieving noncryogenic ignition with LDDH targets.

Measurements to Facilitate Advanced Tokamak Science in Burning Plasma Experiments

Steven L. Allen   06-ERD-024

Abstract

The presently envisioned method of measuring the plasma current profile in advanced tokamaks is based on the motional Stark effect. When a high-energy neutral beam interacts with the plasma in a magnetic field, the motional Stark effect results in a polarized photon that can be used to measure the local plasma current and electric field. This project will investigate the possibility of making high-resolution measurements of the plasma current profile in a burning plasma environment. This will include modeling the spectrum and propagation through a

polarizing-preserving optical train, detecting the full modulated-intensity spectrum, making detailed magnetohydrodynamic measurements with appropriate processing of the high-time-resolution measurements, and developing system-calibration techniques.

We will carry out a pre-conceptual study of a motional Stark effect diagnostic on several levels. On the modeling side, the plasma code CORSICA will be upgraded with synthetic diagnostics to calculate the actual motional Stark effect signals in a burning plasma. Because the measurement will be in a high-neutron environment, we will develop the capability to optimize the optical design with the constraint of neutron shielding. Adequate shielding favors multiple mirrors, but accurate measurements favor a simple, no-mirror system. We will characterize prototypical optics and model their polarization performance. Polarization-sensitive optics may be degraded by plasma exposure, and we will start these measurements in existing devices.

Mission Relevance

This project will contribute to burning plasma fusion research, an important step in achieving fusion power for the country's long-term energy needs. The combined development of a new diagnostic tool and a new predictive code for International Thermonuclear Experimental Reactor scenarios will advance plasma physics research, in support of LLNL and DOE's missions in fundamental science and energy security.

FY08 Accomplishments and Results

In FY08, we (1) established a new collaboration with the University of Arizona and measured the Mueller matrix of several optical components, including dielectric and rhodium mirrors; (2) used a new in situ polarization generator to determine the Mueller matrix of three different polarimeter systems in the existing DIII-D tokamak (with plasma exposure), which resulted in an improved in situ polarization calibration technique; (3) completed installation of a new system that permits processing of the full temporal spectrum of a typical system, allowing magnetohydrodynamic and polarization response; and (4) developed improved calculations of the motional Stark effect spectrum (beam into gas). This project established a new collaboration with the University of Arizona Optical Science Lab, and helped resolve key issues of fielding a motional Stark effect measurement of the plasma current profile on a burning plasma device. Our work will help position the Laboratory to provide plasma science on future burning plasma machines such as the International Thermonuclear Experimental Reactor.

Publications

Gu, M. F., et al., 2008. "Atomic models for motional Stark diagnostics." *J. Phys. B: At. Mol. Opt. Phys.* **41**, 95701. UCRL-JRNL-233134.

Investigating New Regimes of Material Strength at Ultrahigh Strain Rates and Pressures

Stephen M. Pollaine   06-ERD-027

Abstract

In this project, we propose to measure material strength of metals at high pressures greater than 1 Mbar and strain rates up to 10^8/s by developing the following three new Velocity Interferometer System for Any Reflector (VISAR) techniques: (1) compression wave reverberations in foil, (2) hysteresis between loading and unloading waves in foil, and (3) use of multi-stepped targets to measure equation of state and strength simultaneously. We also will develop a new hohlraum isentropic compression experiment (ICE) drive that will serve as a platform for these techniques on fusion-class lasers. This new technology will test various models of material strength, such as the Preston–Tonks–Wallace model, and will provide parameters for those models. We will be exploring new regimes never before measured, where current models of strength differ dramatically from each other.

We will develop three new experimental techniques for measuring strength and a new hohlraum–ICE drive that will deliver larger, more uniform loading than is currently possible. These will be the first strength measurements to span a factor of 1000 in strain rate across different regimes. We intend to perform the first-ever, time-resolved measurements of the strength of nanocrystalline materials at ultrahigh strain rates. Also, our work will contribute to understanding the effect of strength on the shock processing of interstellar dust grains, which affects the size distribution of the grains and, indirectly, the rate of star formation. We expect our results will be submitted for publication in peer-reviewed physics and materials science journals.

Mission Relevance

The three new VISAR techniques we develop will make it possible to measure the strength of materials important for stockpile stewardship on existing facilities, while the development of the hohlraum–ICE drive is a critical advance for stockpile stewardship experiments on fusion-class lasers. Investigating new regimes of material strength at high strain rates and pressures also contributes to LLNL's mission to advance fundamental science.

FY08 Accomplishments and Results

Using the VISAR techniques, we performed a total of eight shots on the Omega laser to measure the strength of aluminum at pressures ranging from 150 to 700 kbar, determining that reservoirs with polyimide vapor-deposited onto aluminum perform much better than reservoirs with polyimide glued to aluminum. We also proved the technique of using laser-irradiated hohlraums to drive an ICE package to measure material strength using a ramp wave. This project has set

the stage for measuring the strength of any material using Omega to illuminate halfraums that drive the target. The next step would be to extend the technique from aluminum to nanograined tantalum metals and other materials of interest.

The Properties of Confined Water and Fluid Flow at the Nanoscale

Eric R. Schwegler   06-ERD-039

Abstract

The properties of confined water affect a wide range of scientific and technological areas of interest, including protein folding, cell-membrane flow, materials properties in confined media, and nanofluidic devices. We propose to develop accurate computational tools to study fluids in confined, nanoscale geometries, and to apply these techniques to probe the structural and electronic properties of water confined between hydrophilic and hydrophobic substrates, including the presence of simple ions at the interfaces. In particular, we will use a series of ab initio molecular dynamics simulations to build an understanding of how hydrogen bonding and solvation are modified at the nanoscale.

The primary results of this research project will be threefold: (1) a first-principles-based computational framework for investigating and characterizing liquids that are confined at the nanoscale, (2) a better understanding of how the properties of water change upon nanoscale confinement by hydrophobic and hydrophilic surfaces, and (3) a suitable empirical model that can be used to describe the flow of water in confined media.

Mission Relevance

This project will contribute to a detailed understanding of how the structural, electronic, and dynamical properties of water are modified upon nanoscale confinement, which is relevant to the development of nanoscale-material sensor technologies for national security missions in nonproliferation and counterproliferation, as well as for homeland security missions in counterterrorism.

FY08 Accomplishments and Results

In FY08, we (1) completed first-principles molecular dynamics simulations of sodium chloride sodium bromide in water-filled carbon nanotubes and carried out a preliminary comparison between the simulation data and experimental x-ray absorption measurements, (2) evaluated the use of five different empirical water models—two of which include polarization effects—for water confined in carbon nanotubes, (3) developed a fluidized piston model for fluid-flow simulations, (4) determined the spectroscopic signature of confined water by computing the

proton nuclear magnetic resonance chemical shielding tensors and infrared spectra of water-filled carbon nanotubes and water confined by graphene sheets, and (5) completed the use of x-ray absorption calculations to examine ion solvation properties for simulations of magnesium chloride and calcium chloride in bulk liquid water. In summary, this project developed a first-principles computational framework for investigating and characterizing liquids confined at the nanoscale and identified a suitable empirical model for describing the flow of water in confined media. The Scientific Discovery through Advanced Computing Program in DOE is continuing the development of this project's quantum simulation tools.

Publications

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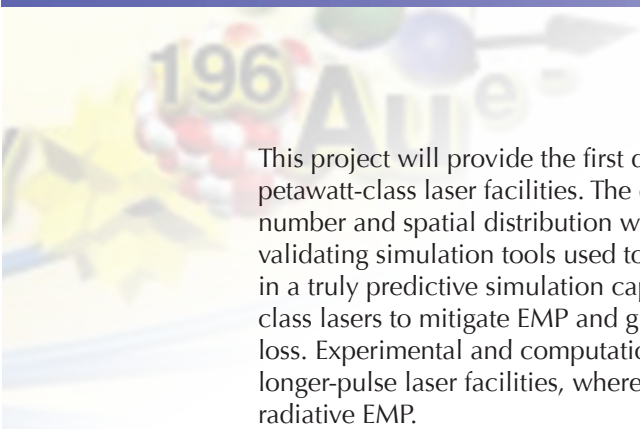
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Mitigation of Electromagnetic Pulse Effects from Short-Pulse Lasers and Fusion Neutrons

David C. Eder   06-ERD-055

Abstract

The main source of damaging electromagnetic pulses (EMP) at petawatt-class laser facilities is believed to be the small fraction of electrons that escape the target. This project is exploring this theory at the new Titan petawatt-class laser facility, where we will measure the number and spatial distribution of escaping electrons as well as the resulting transient currents and EMP. The electron properties will be used in three-dimensional (3D) electromagnetic simulations of the Titan chamber. Radiation measurements will be used to calculate the system-generated EMP (SGEMP) and results compared to data from coaxial cables. The EMP simulations will provide a quantitative understanding of the relationship between escaping electrons and EMP. We hope to develop ways to reduce EMP by controlling the escaping electrons and the structures that the electrons strike.

This project will provide the first quantitative understanding of EMP, including SGEMP, in petawatt-class laser facilities. The data obtained on the dependence of escaping electron number and spatial distribution with laser and target conditions will greatly benefit research by validating simulation tools used to predict these quantities. Success of this project will result in a truly predictive simulation capability that can be applied to existing and future petawatt-class lasers to mitigate EMP and greatly reduce the occurrence of diagnostic damage and data loss. Experimental and computational techniques that we develop will be applicable to EMP at longer-pulse laser facilities, where hot electrons from laser–plasma interactions are the source of radiative EMP.

Mission Relevance

The work supports stockpile stewardship in two ways. First, knowledge of EMP and system response is critical for the reliable operation of facilities used to validate ignition simulations and simulate weapons effects. Second, possible future underground experiments require knowledge of SGEMP on components that did not exist during earlier testing. This work on EMP mitigation techniques also will apply to short-pulse lasers for fast ignition, in support of Lawrence Livermore's energy security mission.

FY08 Accomplishments and Results

In FY08, we (1) developed an EMP predictive capability and mitigation approaches based on an improved understanding of the underlying mechanisms in the Titan chamber, (2) measured spatial distributions of escaping electrons that were used in 3D electromagnetic simulations to obtain improved predictions of radiative EMP, (3) conducted additional measurements of radiative EMP and SGEMP—using a range of target and laser conditions—to determine optimum shielding methods, (4) refined modeling and empirical scaling laws to allow predication of EMP on other high-power lasers, and (5) evaluated mitigation approaches on Titan, for potential use at other facilities. Overall, this project produced an EMP measurement and predictive capability and appropriate mitigation approaches for high-power laser facilities. These measurement techniques and simulation capability can be used at fusion-class lasers to mitigate the impact of EMP.

Publications

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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 radically change the size and configuration of the ion accelerator, enabling a palm-sized neutron source. Thus, this project could have broad impact on weapons science, nuclear physics, and homeland security applications.
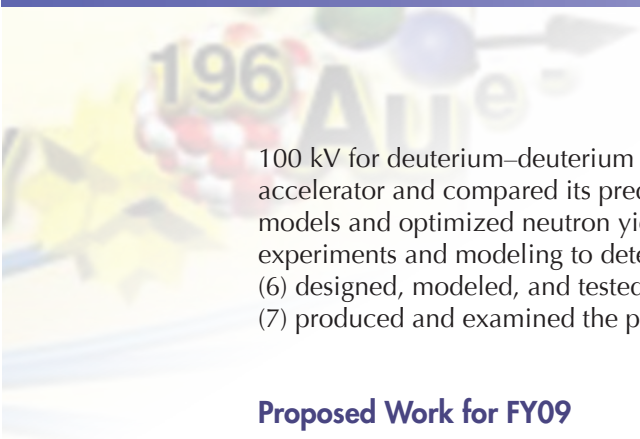
We will quantitatively determine the potential for scaling pyroelectric-crystal-driven ion and neutron sources to fluxes of 10^6 n/s or higher. Our technical approach is to (1) complete a modeling study of the crystal-based neutron source; (2) demonstrate experimental scaling— that is, neutron output up to three orders of magnitude greater than the initial results; and (3) test and evaluate the neutron source in actual applications. We plan to investigate a new source approach that will further intensify the ion beam, enabling both pulsed and continuous operation.

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.

FY08 Accomplishments and Results

In FY08 we (1) demonstrated the integration of a user-controlled ion source with a negative high-voltage crystal target and produced pulsed neutrons with peak rates greater than 10^{10} n/s, exceeding our FY08 milestone; (2) demonstrated the generation of ion beams in excess of

100 kV for deuterium–deuterium fusion reactions; (3) completed a preliminary model of the accelerator and compared its predictions with experimental results; (4) studied ion trajectory models and optimized neutron yields using a negative-voltage crystal target; (5) conducted experiments and modeling to determine optimal thermal cycles for maximum acceleration; (6) designed, modeled, and tested new nanotube ion sources for neutron production; and (7) produced and examined the physics of the first-ever liquid-driven pyroelectric accelerator.

Proposed Work for FY09

For FY09, we propose to establish the technology and science basis for a non-isotopic, palm-size, highly mobile crystal neutron source that can be used to detect special nuclear materials. Specifically, we will (1) continue efforts on coupling or integrating crystals with an independent ion source such as a gated nanotip ion source, which will allow higher pulsed and controlled neutron production; (2) continue to study voltage-holding strategies for a negative target terminal or crystal; (3) continue studying options for pulsed neutron production with a positive crystal; (4) demonstrate pulsed neutron production using a crystal high-voltage source; and (5) develop preliminary models of scenarios in which a palm-size mobile source is used to detect special nuclear materials.

Publications

Tang, V., et al., in press. "Crystal-driven neutron source: A new paradigm for miniature neutron sources." *Proc. 20th Intl. Conf. Application of Accelerators in Research and Industry.* LLNL-PROC-406224.

Tang, V., et al., 2008. *Intense pulsed neutron emission from a compact pyroelectric-driven accelerator.* LLNL-JRNL-407763.

Tang, V., et al., in press. "Experimental investigation and simulations of liquid driven pyroelectric voltage sources for compact accelerators." *Proc. 20th Intl. Conf. Application of Accelerators in Research and Industry.* LLNL-ABS-403201.

Tang, V., et al., in press. "Nanostructure ion sources for neutron production." *Proc. 20th Intl. Conf. Application of Accelerators in Research and Industry.* LLNL-ABS-403195.

Tang, V., et al., 2008. "Neutron production from feedback-controlled thermal cycling of a pyroelectric crystal." *Rev. Sci. Instrum.* **78**, 123504. UCRL-JRNL-233604.

Observation of Coherent Terahertz-Frequency Emission from Shocked Polarizable Materials

Evan J. Reed   06-LW-063

Abstract

We recently predicted that coherent electromagnetic radiation (1–100 THz) can be generated in crystalline materials when subjected to a shock wave. This phenomenon represents a fundamentally new form of coherent optical radiation. The predicted coherent emission contains information regarding shock speed, the lattice and atomic structure of the crystal, and shock-front rise time, suggesting this effect represents a new experimental probe. In this project, we propose to perform the first-ever experimental measurements of terahertz emission from shocked materials and determine the ultrafast dynamical processes responsible for this emission. The experiments will utilize ultrafast laser-driven shock waves in ionic crystals, coupled with a theoretical effort for guidance and interpretation.

We expect to make the first observation of terahertz radiation from a shocked crystal in search of our predicted emission of coherent photons. We will extract the information contained in observed coherent or other emission regarding shock-front rise time, picosecond-timescale shock-speed history, and crystal lattice constant. If successful, this will result in a paper reporting the observation of a fundamentally new source of coherent optical radiation or a measurement of the rise time of an elastic shock wave. We will assess the utility of terahertz emission as a fundamentally new general probe into dynamical processes in shock waves. Our results will be submitted for publication in peer-reviewed journals.

Mission Relevance

New tools for understanding shock wave properties and materials phenomena are central to mission needs in stockpile stewardship. This work will provide fundamentally new insight into shock wave properties and phenomena in materials. It also provides a new source of terahertz radiation with unique properties, which can be used for applications in defending against explosives and chemical and biological threats, in support of the Laboratory's missions in national security and homeland security.

FY08 Accomplishments and Results

In FY08, we (1) maximized the emission frequency and amplitude of the observed coherent radiation; (2) used experimentation to achieve strain frequencies up to a few hundred gigahertz and electric field amplitudes greater than 1 V/cm at our detector; (3) observed and characterized terahertz radiation from other processes, including long-lived sample-bound modes excited by the shock wave; and (4) assessed the utility of using terahertz emission spectra as a fundamentally new general probe into dynamical processes in shock waves and found that our new technique has great applicability to probe a wide variety of processes. Overall, this project

has enabled a fundamentally new class of shock and strain wave probes to measure previously unobservable ultrafast phenomena. The next step is to develop these techniques for use with shock- and ramp-wave experiments at higher pressures.

Publications

Armstrong, M. R., et al., 2008. *Ultrafast strain gauge: Observation of terahertz radiation coherently generated by strain waves.* LLNL-JRNL-407104.

Multipulse, High-Energy Backlighting for a Compton-Radiography Ignition Diagnostic for High-Power Lasers

Riccardo Tommasini   07-ERD-004

Abstract

We plan to develop the capability for multipulse Compton radiography over an approximate 0.1-ns interval using 80-keV x-rays to obtain an ultrahigh-speed movie of the compressed deuterium–tritium (DT) fuel in ignition capsules during high-power laser experiments. We will develop the ability to produce multiple radiographs at 40 kV 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 for extracting maximum experimental information from each laser shot, thereby decreasing the number of laser shots required to achieve a given scientific result.

We expect to develop a K-alpha backlighter with a high signal-to-noise ratio at about 80 keV for Compton radiography, and at about 40 keV for high-energy-density physics experiments. These 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 about 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 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, and a multipulse, high-energy radiography capability, applicable to a wide range of experiments. The Compton radiography diagnostic will greatly improve our ability to understand ignition experiments on fusion-class lasers in an efficient manner by giving a time sequence of two-dimensional images of the compressed DT fuel.

FY08 Accomplishments and Results

In FY08, we (1) measured conversion efficiencies into x-ray photons in the 100- to 200-keV spectral range in experiments at the Titan laser facility using pulses with intensities of 10^{18} W/cm^2 focused on 10-μm-thick gold foils; (2) demonstrated source sizes of 10 μm using 10-μm-diameter gold wires as backlighters with photon energies around and above 100 keV; (3) developed, after achieving high conversion efficiencies for continuum backlighters, K-alpha uranium sources; (4) succeeded, using special double-wire backlighters, in demonstrating collimation techniques for multipulse capabilities on short time interframes; and (5) designed a detector that mitigates background issues and optimizes the signal-to-noise ratio.

Proposed Work for FY09

In FY09 we propose to (1) measure the conversion efficiency of gold microwires, (2) demonstrate source sizes of less than 10 μm for x-ray photon energies greater than 100 keV using thinner foils and wires, (3) demonstrate radiographs based on Compton scattering using static objects, (4) replicate Titan experiments on the Omega Extended Performance laser to conduct measurements at higher energies and intensities, (5) demonstrate Compton radiography on laser-driven targets at the Omega Extended Performance laser, (6) finalize the design of backlighter targets and shielding, and (7) predict Compton radiography performance as a function of implosion yield and associated background.

Publications

Tommasini, R. D., 2008. *Development of backlighting sources for a Compton radiography diagnostic of inertial confinement fusion targets.* 17th Ann. High-Temperature Plasma Diagnostics, Albuquerque, NM, May 11, 2008. LLNL-ABS-401425.
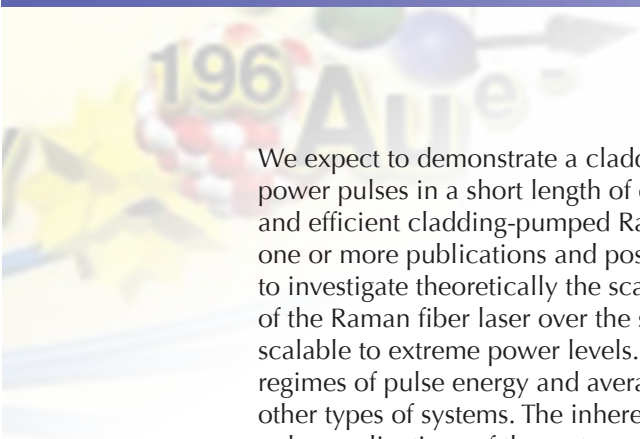
Tommasini, R., et al., in press. "Development of backlighting sources for a Compton radiography diagnostic of inertial confinement fusion targets." *Rev. Sci. Instrum.* LLNL-CONF-403746.

Cladding-Pumped Raman Fiber Lasers

Jay W. 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. The project will result in one or more publications and possibly some significant intellectual property. We further expect to investigate theoretically the scaling properties of such a laser. The lower quantum defect of the Raman fiber laser over the standard ytterbium fiber laser suggests these lasers may be scalable to extreme power levels. 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.

FY08 Accomplishments and Results

Using pulsed light and a single-mode–multiple-mode pump combiner, we demonstrated gains of up to 300 times with conversion efficiencies of 40% and brightness enhancements of greater than 1000 times. Our demonstration was the first to show significant brightness enhancements and the first to convincingly demonstrate the clad-pumping effect. We also developed a comprehensive model of the effect, and with it developed a new scheme to use wavelength-dependent loss to suppress higher-order Stokes cascade, thus greatly increasing the utility of cladding-pumped Raman fiber amplifiers. Our model also showed that above a clad-to-core diameter ratio of around two to three, the conversion efficiency into the first Stokes wavelength decreases dramatically because of cascade energy transfer to longer-wavelength Stokes lines. Incomplete pump depletion caps the brightness enhancement to 10 to 40 times, which would not be competitive with other schemes. This issue will be addressed in FY09.

Proposed Work for FY09

In FY09, we (1) intend to suppress the onset of cascade energy transfer by using a specially designed fiber that provides a differential loss between the first and second Stokes lines of the Raman process, (2) fabricate and implement a new fiber design, and (3) achieve brightness enhancement factors greater than 1000 times by exploiting the fact that enhancement is proportional to the ratio of the cladding to core areas.

Maximizing the Science from Astrophysical, Time-Domain Surveys: Targeted Follow-Up

Kem H. Cook   07-ERD-014

Abstract

We are developing approaches to maximize data from astrophysical, time-domain surveys that will produce significant science on issues ranging from new exoplanets to a better understanding of dark energy. Lawrence Livermore participates in many ongoing wide-field, time-domain surveys such as the Super Massively Compact Halo Object (SuperMACHO), Equation of State: Supernovae Trace Cosmic Expansion (ESSENCE), and the Lowell Observatory Near-Earth Object Search (LONEOS), and is uniquely positioned to mine the data coming from these surveys. Using time-domain data either in place at the Laboratory and/or publicly available (for example, the Optical Gravitational Lensing Experiment and Microlensing Observations in Astrophysics data sets) with data-management experience from the Large Synoptic Survey Telescope (LSST) precursor projects, we will perform new studies and identify follow-up observations (at Boyden, Keck, and Gemini observatories, for example) that will supplement and leverage the survey data to produce exciting new science. We also will share our data and data-mining tools on a public portal for time-domain astronomy.

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 (e.g., 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 will 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 LSST (a part of the Laboratory's science and technology plan) can greatly enhance its scientific payoff.

FY08 Accomplishments and Results

In FY08 we (1) completed the efficiency analysis of SuperMACHO data and collected the final SuperMACHO Hubble Space Telescope data, (2) observed and published the first spectrum of an ancient supernova in the Large Magellanic Cloud, (3) discovered light echo systems for both Tycho and Cas A with our survey for Milky Way historical supernova light echos, (4) published four significant papers on our MACHO data mining, (5) discovered an analogue to our solar system with the Probing Lensing Anomalies Network (PLANET) survey, (6) determined the best limits on the population of small Kuiper Belt objects from the Taiwanese American Occultation Survey, and (7) reduced LONEOS data that indicated presence of two Milky Way halo populations, and collected additional spectra.

Proposed Work for FY09

In FY09 we will (1) pursue our search for light echoes from historical supernovae in the Milky Way and conduct spectroscopic follow-up observations of those found; (2) publish our first two data-mining papers from the SuperMACHO survey on delta Scuti variables in the Large Magellanic Cloud and the active galactic nuclei behind the Large Magellanic Cloud; (3) complete follow-up spectroscopy and Hubble Space Telescope imaging analysis of SuperMACHO microlensing candidates, which will allow us to estimate the baryonic content of the Milky Way's halo; (4) continue analysis and follow-up of the PLANET exoplanet discoveries and microlensing events; (5) finish LONEOS follow-up observations to probe the Milky Way's halo; and (6) complete a comparative study of long-period variables in the Small Magellanic Cloud, Large Magellanic Cloud, and Milky Way from the MACHO project.

Publications

Faccioli, L., et al., 2007. "Eclipsing binary stars in the Large and Small Magellanic Clouds from the MACHO project: The sample." *Astron. J.* **134**, 1963. UCRL-JRNL-236835.

Faccioli, L., et al., 2008. "Post main sequence orbital circularization of binary stars in the Large and Small Magellanic Clouds." *Astrophys. J.* **672**, 604. UCRL-JRNL-236706.

Fraser, O., S. Hawley, and K. H. Cook, 2008. "The properties of long period variables in the LMC from MACHO." *Astron. J.* **136**, 1242. LLNL-JRNL-405328.

Gaudi, B. S. et al., 2008. "Discovery of a Jupiter/Saturn analog with gravitational microlensing." *Science* **319**(5865), 927. UCRL-JRNL-236568.

Kubas, D., et al., 2008. "Limits on further planetary companions to OGLE 2005–BLG–390L." *Astron. Astrophys.* **483**(1), 317. UCRL-JRNL-236565.

Kunder, A., et al., 2008. "The extinction toward the Galactic bulge from RR Lyrae stars." *Astron. J.* **135**, 631. UCRL-JRNL-236566.

Rest, A., et al., 2008. "Scattered-light echoes from the historical Galactic supernovae Cassiopeia A and Tycho (SN 1572)." *Astrophys. J.* **681**(2), L81. LLNL-JRNL-403751.

Rest, A., et al., 2008. "Spectral identification of an ancient supernova using light echoes in the Large Magellanic Cloud." *Astrophys. J.* **680**(2), 1137. LLNL-JRNL-401204.

Wang, J. H., et al., 2008. "Early optical brightening in the GRB 071010B." *Astrophys. J.* **679**(1), L5. LLNL-JRNL-403007.

Zhang, Z.-W., et al., 2008. "First results from the Taiwanese-American Occultation Survey (TAOS)." *Astrophys. J.* **685**(2), L157. LLNL-JRNL-406655.

Discovery of a Light Higgs Boson with b Quarks

David J. Lange   07-ERD-015

Abstract

A new era in particle physics will begin when the Large Hadron Collider (LHC) comes fully online in 2008 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 required particle-identification techniques, trigger algorithms, and analysis codes to search for the Higgs boson in its dominant decay mode. By the end of this project, we will complete the first-ever analysis of this 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. 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.

FY08 Accomplishments and Results

We (1) helped commission the Compact Muon Solenoid high-level trigger, in collaboration with colleagues at the LHC; (2) used our completed detector and cosmic-ray data to integrate a wide range of algorithms in the data-acquisition system; (3) successfully developed a configuration-tracking database; and (4) developed an analysis to study the dominant source of LHC background in our Higgs analysis—a Z boson accompanied by jets.

Proposed Work for FY09

During FY09, we will focus on the initial Compact Muon Solenoid data, using it to analyze a Z boson produced with two or more particle jets. The initial data will be sufficient to measure the kinematic distributions of these events and their total cross-section, which will not only pin down our Higgs background but also test our theory at a significantly advanced center-of-mass energy. As such, these measurements will test for possible processes beyond our standard theories and, as one of the first LHC measurements, should result in a publication in a premier journal, most likely *Physical Review Letters*.

A New Approach to Simulating Inhomogeneous Plasmas for Inertial Fusion Energy and Other Applications

David P. 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.

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 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. While development of this method for the latter application is beyond the scope of this proposal, this work would enable the Laboratory to assess its feasibility.

Mission Relevance

This project is designed to strengthen LLNL's capabilities in modeling inhomogeneous plasmas for high-energy-density science and 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.

FY08 Accomplishments and Results

In FY08, we (1) completed development of the implicit electrostatic version of the drift-Lorentz mover, implemented it in the Warp code, and verified it with tests of single-particle orbits and of the self-consistent capability with the magnetized Buneman instability; (2) developed an improvement to the Langevin collision operator that ensures conservation of energy and momentum, accommodating relativistic, multispecies systems; and (3) implemented the improved Langevin collision operator in the Large Scale Plasma (LSP) code and verified it on temperature equilibration in two-species plasmas.

Proposed Work for FY09

Having focused on developing algorithms for the adaptation of the drift-Lorentz mover in the first two years of this project, in FY09 we propose to (1) implement the electromagnetic implicit drift-Lorentz model in LSP, (2) test the implicit drift-Lorentz model with the Langevin collision operator in LSP, and (3) apply the new algorithms to Weibel or Titan/Omega electron-transport experiments. The new capabilities will be immediately available for fast ignition work, improving accuracy and efficiency of the LSP code.

A Novel Method for Extracting Signals from Noisy Broadband Data Using Poynting Vector Measurements

Charles R. Carrigan   07-ERD-018

Abstract

We will explore and develop techniques for exploiting electric and magnetic field measurements in noisy electromagnetic environments in conjunction with developing a novel method using the Poynting vector to extract low-level signals. We will develop a method to identify unknown signals and increase the signal-to-noise ratio in an omnidirectional signal-acquisition system by tagging the frequency spectrum of a broadband signal. A combination of laboratory experiments and analysis will be used to accomplish this goal.

If successful, we will develop a new method that allows for reconstructing an electromagnetic signal of interest from a noisy broadband data stream acquired from an omnidirectional acquisition system with only knowledge of the signal direction. With minimal information about a signal of interest, we also will be able to determine the direction of its source. In principle, this allows us to reconstruct signals from facilities and other electromagnetic sources of interest, or to determine the direction to such facilities and sources if we have knowledge about the signal. Analysis applications that associate a collection of signals or harmonics with activities at predetermined standoff locations will benefit considerably from this technique.

Mission Relevance

This project is consistent with the Laboratory's commitment to exploring innovative system concepts to develop novel approaches for national security issues including homeland security, nonproliferation, and counterterrorism. Specific relevant challenges include information processing to yield enhanced detection and characterization requiring recovery of sparse, noisy measurements relating to proliferation detection; tagging, tracking, and locating high-value objects; and predictive simulation and modeling approaches for optimization of sensor and data-collection system performance.

FY08 Accomplishments and Results

In FY08 we described the possible applications of this novel technology involving use of triaxial electric and magnetic field data to locate and characterize sources of unintended radiated emissions. This project has resulted in a patent issued in October 2008, and the filing for another has been completed. With the aid of the Industrial Partnerships Office at Livermore, we are pursuing collaborations with industry to more fully develop this technology.

Techniques for Supernova Cosmology with the Large Synoptic Survey Telescope

Scot S. 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 in 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.

FY08 Accomplishments and Results

In FY08, we (1) continued investigations into the accuracy of redshift estimates from supernova light curves (photometric redshifts) and propagated errors to measurements of cosmological parameters, (2) completed the performance analysis of the LSST wavefront sensing and reconstruction system, and (3) analyzed observations of supernovae to quantify intrinsic variability in spectral evolution.

Proposed Work for FY09

In FY09, we plan to (1) continue investigating the accuracy of redshift estimates from photometric redshifts and the resulting accuracy of measurements of cosmological parameters, and define the baseline LSST capability for supernova cosmology; (2) expand our efforts to evaluate the effect of optical errors in the LSST design on the photometric accuracy of measurements of supernovae—and thus better define the connection between LSST engineering design and performance for supernova cosmology; (3) analyze observations of supernovae to quantify the characteristics that limit their accuracy as standard candles to identify fundamental limitations; and (4) accelerate our efforts to incorporate models of supernovae into the comprehensive LSST data management, simulation, and visualization framework.

Publications

Olivier, S., et al., 2008. *Supernova science and cosmology with the LSST*. 211th Mtg. American Astronomical Society, Austin, TX, Jan. 7–11, 2008. LLNL-POST-401134.

Electronic Anomalies in Ordered and Disordered Cerium at High Pressures and Temperatures

Magnus J. 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 limited 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.

This project will increase our understanding of the behavior of cerium, including if (1) its anomalous transition is not isostructural but rather a second-order transition extending from the critical point to the melt-line minimum, (2) a remnant of this transition continues into the melt and separate liquids of different density, and (3) the change in entropy across the transition is because of electrons alone, which is an assumption recently challenged on the basis of 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 stockpile stewardship. Such research will provide crucial data in support of the Laboratory's national security and stockpile stewardship missions.

FY08 Accomplishments and Results

In FY08 we (1) manufactured the large-volume diamond-anvil cell and conducted a safety evaluation of key parts, (2) used the cell in an x-ray scattering investigation of cerium melt, (3) measured susceptibility in the alpha phase, and (4) disseminated key findings at two conferences and published in the prestigious journal *Physical Review Letters*.

Proposed Work for FY09

In FY09, we will (1) conduct x-ray emission experiments to investigate the magnetic moment of cerium at high pressure and temperature to complement our previous structural studies, (2) perform x-ray scattering measurements of the structure and equation of state of liquid cerium, (3) perform analogous measurements of the f-electron prototype actinide curium, (4) begin pressure-dependent magnetic susceptibility measurements of cerium and curium using

designer anvils and a large-volume pressure cell to increase signal strength, and (5) publish results of this work in peer-reviewed journals.

Publications

Lipp, M. J., 2007. *The volume collapse (VC) in cerium revisited.* Computational Materials Science Network: Predictive Capability for Strongly Correlated Systems Fall 2007 Coordination Mtg., Davis, CA, Sept. 15–16, 2007. LLNL-PRES-234630.

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Lipp, M. J., et al., 2008. *Thermal signatures of the volume collapse in cerium.* International Alloy Conf. V, Munich, Germany, Sept. 11–14, 2008. LLNL-PRES-406657.

Molecular Dynamics Simulations of Hot, Radiative Plasmas

Frank R. Graziani   **07-ERD-044**
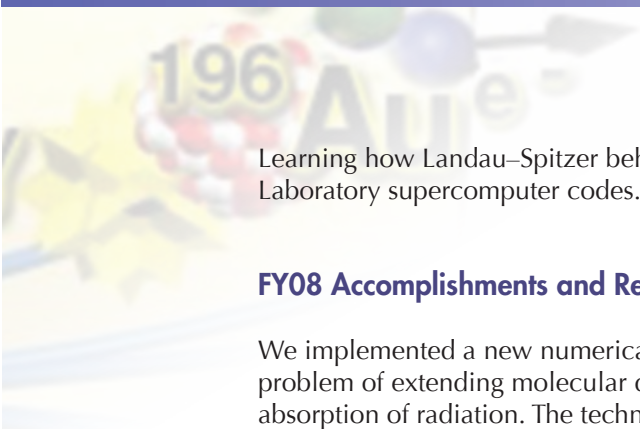
Abstract

Applications as varied in scale as inertial-confinement fusion and the physics of stars involve understanding the complex processes present in hot, dense radiative plasmas. Processes interact with each other in highly nonlinear ways, and hence uncertainties in the physics can be amplified exponentially. Recent theoretical investigations of dense plasmas have been performed but are controversial because of the approximations made in these analyses. Direct numerical simulation of the complex interactions in plasmas offer an alternative, but they either rely on the collision-less approximation or ignore radiation. We propose to develop a new numerical simulation capability that addresses a currently unsolved problem—the extension of molecular dynamics to collisional plasmas where radiation is present.

The particular application of this new code will be to the thermalization problem. That is, given two species of plasma, each with its own temperature, what is the rate at which they relax to a common temperature because of the exchange of momentum and energy? This is the classic problem solved by Landau and Spitzer for Coulombic systems. We will consider single-species hot plasmas with varying ion atomic numbers, and investigate the effects of radiation on thermalization rates. Our final applications will be to multispecie, hot, dense radiative plasmas. Learning how the Landau–Spitzer model behaves in radiative plasmas could have significant impacts on Livermore's supercomputing codes.

Mission Relevance

This project supports the Laboratory's work in advanced computer simulations, especially as they relate to stockpile stewardship and energy security. This simulation capability will be the first for a microphysical (molecular dynamics) description of a plasma with radiation present.

Learning how Landau–Spitzer behaves in radiative plasmas could have large impacts on Laboratory supercomputer codes.

FY08 Accomplishments and Results

We implemented a new numerical simulation technique to address the currently unsolved problem of extending molecular dynamics to collisional plasmas, including emission and absorption of radiation. The technique passes a key test: it relaxes to a blackbody spectrum for a plasma in local thermodynamic equilibrium. This new tool also provides a method for assessing the accuracy of energy and momentum-exchange models in hot dense plasmas. For example, we simulated the evolution of nonequilibrium electron, ion, and radiation temperatures for a hydrogen plasma and compared the results to a radiation-transport code. The temperature evolution between the two codes agreed and the time evolution of the spectrum was consistent with free–free transitions in the plasma. The successful conclusion of this project also includes the effects of high atomic-number dopants and enables evaluation of the effects of mixed plasmas on energy exchange rates and transport properties.

Publications

Glosli, J., et al., in press. "Radiation in molecular dynamic simulations." *J. Phys. A.* LLNL-JRNL-407813.

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Quantum Properties of Plutonium and Plutonium Compounds

Michael J. Fluss   07-ERD-048

Abstract

The anomalous properties of plutonium and plutonium compounds arise from electronic correlation effects, but the nature, the organizing principle, and the order parameter is unknown. In addition to ongoing negative-pressure tuning with americium, we are exploiting physical property measurements of plutonium at very low temperatures using low-specific-activity plutonium-244 and characterizing plutonium superconductivity to understand the element's ground state. We are using the 300-keV transmission electron microscope for atomic-scale characterization, which should lead to an understanding of structure property aspects of the superconducting $PuCoGa_5$. The 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 creates important new skills and knowledge for LLNL 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 of 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 impossible any other way. 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.

FY08 Accomplishments and Results

For FY08, we (1) completed magnetic measurements of negative-pressure–tuned plutonium–americium and found that expanding the lattice increases magnetic susceptibility, and discovered a temperature dependence indicative of spin-wave behavior; (2) completed electrical transport–damage annealing measurements on defects in delta plutonium; (3) designed a low-temperature specific-heat sample holder for use with low-activity plutonium—we will use plutonium-242 to reach a temperature of about 1 K; and (4) reported theoretical results, using dynamical mean field theory, for the physical properties of delta plutonium as a function of lattice expansion, which are consistent with our experimental observations. This has led us to shift our focus to the plutonium–americium alloys in the final year, and design experiments to test for spin fluctuations.

Proposed Work for FY09

In FY09 we will (1) measure the specific heat of plutonium at low temperatures using plutonium-244 as a function of field; (2) complete resistivity, magnetoresistivity, and Hall measurements on plutonium and plutonium–americium alloys, exploiting magnetoresistivity to investigate the electron-pairing mechanism, spin-orbit coupling, and radiation self-damage to probe for Kondo screening; (3) extend recent dynamical mean field theory results on delta plutonium to impurities (gallium, americium, and vacancies) and determine the total energy as a function of volume and temperature (i.e., the free energy); and (4) apply dynamical mean field theory to alpha plutonium with its eight unique atomic sites. This work will be conducted in collaboration with Los Alamos National Laboratory and the French Atomic Energy Commission.

Publications

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Chapline, G. F., in press. "Quantum criticality and the alpha/delta puzzle." *Phil Mag.* LLNL-JRNL-407700.

Marianetti, C. A., 2008. *Electronic coherence in delta-Pu: A DMFT study.* Fundamental Plutonium Properties, Snezhinsk, Russia, Sept. 8–12, 2008. LLNL-ABS-401407.

Marianetti, C. A., 2008. *Electronic coherence in delta-Pu: A DMFT study.* Plutonium Futures "The Science" 2008, Dijon, France, July 7–11, 2008. LLNL-ABS-401407.

Marianetti, C. A., et al., 2008. "Electronic coherence in delta-Pu: A dynamical mean-field theory study." *Phys. Rev. Lett.* **101**(5), 056403. LLNL-JRNL-403401.

McCall, S. K., M. J. Fluss, and B. W. Chung, 2008. *Evidence for spin fluctuations in plutonium americium alloys.* Fundamental Plutonium Properties, Snezhinsk, Russia, Sept. 8–12, 2008. LLNL-ABS-405527.

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McCall, S. K., et al., 2008. *Probing disorder in Pu(Am) alloys.* Plutonium Futures "The Science" 2008, Dijon, France, July 7–11, 2008. LLNL-ABS-401309.

Finding and Characterizing Rare Events in Two Next-Generation Particle Astrophysics Experiments

Adam Bernstein   **07-ERD-056**

Abstract

We propose to participate in two fundamental physics experiments. The goal of one is direct detection of dark matter using dual-phase xenon detectors. The goal of the other is to measure the neutrino oscillation parameter theta 13 using large liquid scintillator detectors. These efforts are widely acknowledged to be among the most important in particle astrophysics for the coming decades. We will build detectors with unprecedented levels of sensitivity for the dark-matter search and detectors with record low levels of systematic error for the theta 13 measurement.

If successful, we will be key collaborators in first-ever direct detection, or stringent constraint, on the existence of dark-matter particles and will play a major role in first-ever measurement of theta 13. The detection of dark matter is one of the most important scientific questions

in the 21st century, and measurement of the neutrino oscillation parameter has nearly the same level of scientific significance. This project is already attracting top scientists to the Laboratory, with technical skills that are directly relevant to immediate needs in LLNL radiation-detection programs.

Mission Relevance

This project will help fulfill LLNL's mission of breakthrough fundamental science and technology. The skills being developed here also have direct relevance to Laboratory missions in national and homeland security, as well as nonproliferation efforts. In particular, the advanced simulation capabilities, event-selection algorithms, and analog electronics have immediate relevance to ongoing reactor monitoring and active interrogation efforts by the DOE and Department of Homeland Security. Additionally, it has been realized that neutrinos are a potentially very valuable signature for reactor monitoring and treaty verification. This project helps develop our growing competency in neutrino detection, and is being concurrently applied to nonproliferation efforts and basic science research.

FY08 Accomplishments and Results

In FY08, we (1) participated in two major experiments—the Large Underground Xenon (LUX) experiment at the Homestake gold mine in South Dakota and the Double Chooz antineutrino detector at the Chooz nuclear power station in France; (2) hired two top post-doctoral researchers; (3) tested the 40-kg liquid and gas-phase xenon detector; (4) created a standard simulation framework for the detector, and designed, built, and installed essential subsystems including analog electronics; (5) designed and built a gadolinium-doped water detector and demonstrated first-ever detection of neutrons, which proves neutron sensitivity of the 2-m diameter LUX detector; and (6) improved simulations of neutron response, and continued radioactivity screening and evaluation of the Double Chooz detector components. Overall, our project met all of its goals, and we anticipate DOE funding for additional experiments including those at the Deep Underground Science and Engineering Laboratory at Homestake.

Publications

Goldstein, W. H., et al., 2008. "Neutrinos, dark matter and nuclear detection." *Prevention, Detection and Response to Nuclear and Radiological Threats*, Springer Netherlands, Dordrecht, Netherlands, p. 117. UCRL-CONF-231454.

Kazkaz, K., et al., 2007. "Reducing neutron backgrounds in dark matter detectors with doped water shields." *American Physical Society April Meeting, April 14–17, 2007*, C16.008. UCRL-ABS-227279.

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, which builds on recent successes with the Janus laser. The goal is to demonstrate pulse compression that will allow existing laser facilities to operate with as much as 1000 times higher output powers than 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 to the zettawatt realm, and has broad application in inertial fusion, radiation sources, and particle accelerators, and will also provide critical data on the saturation of stimulated Raman scattering.

We expect that experiments with the 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 will 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.

FY08 Accomplishments and Results

In FY08 we studied focal spot quality after increasing the plasma interaction length to greater than about 3 mm using an exact counter-propagating geometry. Results showed that beam forward scatter was reduced to less than 1° when the pump intensity was less than 2×10^{14} W/cm^2, enabling a dramatic improvement in the focal spot quality. We increased the seed energy by a factor of five to 1.5 mJ , which showed that the focal spot quality of a 500-µm spot could be maintained with a ninefold amplification and output energy of 13 mJ. Varying seed intensity showed output increasing with input energy, with some evidence of wave saturation. This data and the benchmarked simulations support the attempt at pulse compression with optimized conditions and higher seed energies in FY09.

Proposed Work for FY09

In FY09, we will complete experiments to demonstrate the compression of a 20- to 30-ps portion of a nanosecond pulse to less than 1-ps duration in a plasma optimized for focal spot quality and efficiency. This will be the first demonstration of pulse compression in such a plasma. These results will build on our FY07 and FY08 results in large-scale plasmas with long interaction times. We will also carry out studies of pump beam combination by ion waves with the available resources to facilitate application of plasma pulse compression to large lasers with multiple beams.

Publications

Kirkwood, R. K., et al., 2007. "Amplification of an ultra short pulse laser by stimulated Raman scattering of a 1 ns pump pulse in a low density plasma." *Phys. Plasmas* **14**(11), 113109. UCRL-JRNL-235750.

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Helium Burning in Steady-State and Explosive Nucleosynthesis

Jason T. Burke   07-LW-006

Abstract

We propose a project involving helium burning in stellar environments using the STARS/LIBERACE detector system developed in collaboration with Lawrence Berkeley National Laboratory. We will perform a triple-alpha experiment to measure the radiative width of the Hoyle resonance to a precision better than 5%. The experiment makes use of the highly segmented large-area silicon detector in the STARS system. A second experiment measures a key cross section in a supernova, the reaction of calcium-40 with an alpha particle, producing titanium-44 in an excited state. The decay of titanium-44 is a signature of the dynamics of explosive helium burning in supernova remnants such as Cassiopeia A. This experiment will use two methods to determine the cross section below 4 MeV—an in-beam measurement followed by a low-background count of the activation product.

We expect to produce, for the first time, a high-precision single measurement of the triple-alpha radiative width. The result will be used as a critical input to stellar modeling codes used by the astrophysics community. The cross section for the production of titanium-44 from the reaction described above currently has an uncertainty of a factor of 2 or more. Our self-consistent, independent determinations of the cross section should provide an absolute value with an uncertainty on the order of 5%. This would have direct impact on the interpretation of supernova remnant Cassiopeia A. Both results will be submitted to highly regarded journals such as *Nature* and *Physical Review Letters*.

Mission Relevance

Exploring stellar thermonuclear phenomena similar to those in man-made nuclear explosions benefits fundamental research used in stockpile assessment and in thermonuclear experiments at future, fusion-class lasers, in support of the Laboratory's national security mission. Specifically, this project explores the ability to measure low-yield cross sections through direct (in-beam) and activation methods, which is of high scientific value to the nuclear and astrophysics community. Our experiments in cross-section measurements, particle detection, gamma-ray spectroscopy, nuclear physics, and astrophysics will benefit Laboratory efforts in fundamental science and technology breakthroughs, as well as attract talented student and postdoctoral researchers.

FY08 Accomplishments and Results

In FY08, we (1) performed an experiment at Livermore's Center for Accelerator Mass Spectrometry and measured the prompt gamma-ray spectrum from the reaction of alpha particles on calcium-40 at alpha beam energies of 4.1, 4.5, and 5.3 MeV; (2) analyzed the data and found agreement with prior experiments dating back to the 1970s; (3) performed low background counting and found the results to agree within statistical uncertainties with the prompt online results; and (4) prepared research results for publication in a peer-reviewed journal.

Uncovering Supersymmetric Leptons at the Large Hadron Collider

Jeffrey B. Gronberg   07-LW-037

Abstract

A new era in particle physics will begin when the Large Hadron Collider (LHC) comes fully online in 2008. The LHC will be the first collider to reach the energy regime where current theory predicts a completely new realm of particle physics. Although expected to discover new fundamental particles, the LHC will be blind to an entire class of new particles, supersymmetric leptons (sleptons). We propose to develop a novel triggering technique based on exploiting photon–photon interactions of beam protons, which would allow these particles to be discovered. 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 the fundamental physics occurring at the teraelectronvolt scale. To complete that picture, experiments will need to have 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 physics program of the LHC, 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.

FY08 Accomplishments and Results

In FY08 we used Monte Carlo techniques to evaluate our proposed measurement of gamma–gamma-to-dilepton events and to evaluate the kinematic information available to separate slepton events from backgrounds. The Standard Model background of W boson pair production was shown to be manageable as long as the slepton did not have the same mass as the W boson. However, we determined that the dominant background would be from random triple coincidences of forward protons with dileptons at the design luminosity.

Proposed Work for FY09

For FY09, we propose to (1) analyze the first data set to measure the photon–photon production of Standard Model dimuons in events in which the proton remains intact (exclusive) and events in which the proton disintegrates (inclusive), (2) analyze the initial sample of dimuon detections to determine our ability to maximize the slepton signal and minimize background in a future high-luminosity large data set, and (3) make an initial search for slepton events if the forward proton detectors at 220 m in the Total Elastic and Diffractive Cross-Section Measurement experiment have been connected to the Compact Muon Solenoid experiment at the LHC.

Publications

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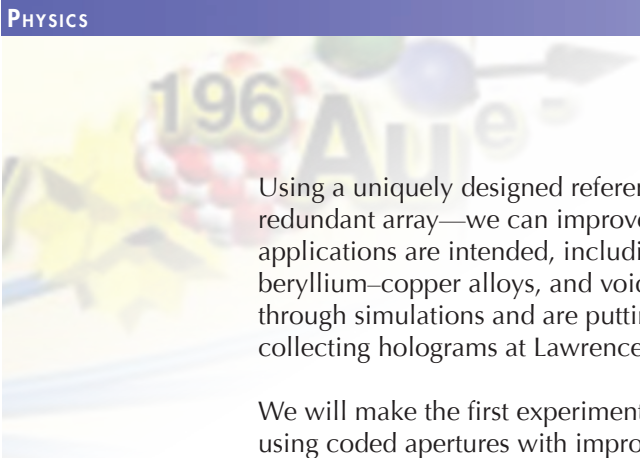
Hollar, J., X. Rouby, and S. Ovyn, 2008. *Forward physics triggers*. LLNL-TR-402528.

Fourier Transform Holography with Coded Apertures

Stefan Hau-Riege   07-LW-086

Abstract

In Fourier transform holography, resolution is limited by the reference object size, and a small object scatters weakly. We propose to develop a new imaging technique that will boost holographic signals by two orders of magnitude to achieve an approximate 2-nm resolution.

Using a uniquely designed reference object with point-like autocorrelation—a uniformly redundant array—we can improve signal and resolution. Material science and biological applications are intended, including imaging laser-target aerogel foams, copper inclusions in beryllium–copper alloys, and voids in plutonium. We have already demonstrated the technique through simulations and are putting it into practice by fabricating such reference objects and collecting holograms at Lawrence Berkeley's Advanced Light Source.

We will make the first experimental demonstration of our new holographic imaging technique using coded apertures with improved signal and resolution, which was conceived and simulated at Lawrence Livermore. We intend to fabricate a high-resolution lithographic uniformly redundant array and use it to image samples of interest to LLNL. As an additional parallel development, we propose to use known reference virus structures to obtain images at sub-nanometer resolution. We expect to produce high-resolution, three-dimensional holograms and publish our results in a peer-reviewed journal.

Mission Relevance

Our advanced imaging technique will enable analysis of the mechanical properties of materials of interest to the Stockpile Stewardship Program. When ultimately applied to bio-imaging, this technique will also benefit the homeland security mission by providing an extremely powerful tool for determining pathogen structure. It will place LLNL at the forefront of imaging science, and advance collaborations at two major x-ray facilities: Berkeley's Advanced Light Source and the Linac Coherent Light Source at Stanford.

FY08 Accomplishments and Results

After pioneering Fourier–Hadamard transform x-ray holography in FY07, we concentrated on three-dimensional imaging in FY08. Specifically, we (1) fabricated samples of ultralow-density tantalum oxide and germanium oxide aerogels for imaging with uniformly redundant array structures; (2) successfully acquired three-dimensional diffraction data at the Advanced Light Source, and determined the structure of our fabricated samples; (3) attempted, for the fabrication of macromolecular complexes, alignment of ketone-bearing tobacco mosaic virus protein shells via oxime formation with self-assembled mono-layers of alkoxyamine-bearing alkane thiols; and (4) observed limited immobilization, thereby determining that alignment of the virus protein shells was not achieved. With this project, we demonstrated uniformly redundant array imaging with short x-ray pulses beyond the continuous wave damage threshold at the FLASH free-electron laser facility at Deutsches Elektronen-Synchrotron in Germany. In conclusion, we have developed and demonstrated a new diffraction imaging technique (massively parallel x-ray holography) with a substantially improved signal-to-noise ratio that will become an integral part of imaging efforts on coherent light sources. In addition to programmatic applications, our work has sparked a renewed interest in holographic imaging, and our technique is being used on third- and fourth-generation light sources all over the world.

Publications

Marchesini, S., et al., 2008. "Massively parallel x-ray holography." *Nat. Photon.* **2**, 560. UCRL-JRNL-234707.

Fast-Ignition Proof-of-Principle Experiments

Erik Storm   08-SI-001

Abstract

The objective of this project is to investigate the feasibility of a new approach to fusion ignition. As opposed to baseline laser-fusion ignition schemes, "fast ignition" uses an approach that directly compresses the fusion fuel to high densities and then ignites it with a separate laser beam, which sends a fast pulse of hot electrons into the compressed fuel capsule. This is a scientifically and technologically challenging approach that, if successful, will offer the potential for large advances in efficiency over the potential baseline approach to ignition. We will design and undertake integrated fast-ignition experiments on high-power lasers 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 and new regimes of excited-state nuclear physics. We will study and validate key aspects of fast-ignition physics related to fuel assembly and electron transport through subscale experiments on the Titan and Omega lasers, and develop an integrated target design that could be experimentally benchmarked on the National Ignition Facility (NIF).

This project will define the requirements for high-gain fast ignition for future fusion-class laser systems. In particular, we will optimize an 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 facilities such as NIF and will be important in recruiting and retaining exceptional scientists for the Laboratory.

FY08 Accomplishments and Results

We (1) conducted two campaigns on Titan, obtaining data that will determine the optimal laser intensity and contrast for electron conversion efficiency in subsequent experiments on the NIF Advanced Radiographic Capability (ARC) laser; (2) carried out two campaigns on Omega to measure gold cone ablation and mixing; (3) designed electron-coupling experiments on the Omega Extended Performance (EP) laser to be conducted in FY09; (4) designed transport-validation experiments to be conducted on the Titan and Omega EP lasers in FY09; (5) designed and tested a prototype high-energy K-alpha imager on Titan; (6) developed two indirect-drive

cryogenic target designs based on continuous-ramp and discrete-shock radiation drive; and (7) determined fast-ignition ignitor pulse requirements and developed a system design that would enable the ARC to meet fast-ignition pointing and intensity requirements.

Proposed Work for FY09

In FY09 we propose to (1) complete the point design for the integrated warm coupling experiment, (2) continue point design testing and risk mitigation experiments on Omega, (3) perform laser–electron coupling experiments in cone geometry on the Titan laser and extend the experiments in planar and cone geometries to the Omega EP laser, (4) perform particle-in-cell and Large Scale Plasma (LSP) code simulations to model Titan and Omega EP data and extrapolate to ARC parameters, (5) test and qualify NIF hard-x-ray K-alpha imaging diagnostics on Omega in integrated direct-drive implosions, (6) examine intra-split-beam phase control on ARC and bench-test the alignment and pointing enhancements, and (7) design and execute a NIF hydrodynamics campaign to test implosion performance using ARC x-ray backlighting.

Publications

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Resolving Inconsistencies in Astrophysical Absorption Spectroscopy

James Dunn   08-ERD-003

Abstract

We propose an experimental and theoretical study to resolve topical inconsistencies and controversy in the interpretation of astrophysical x-ray spectra. Our efforts towards generating a complete and accurate atomic-structure database will help resolve the atomic physics uncertainty and provide a better understanding of ionized matter surrounding black holes and active galactic nuclei. We will build a high-resolution grating spectrometer and field it on the high-repetition-rate lasers of the LLNL Jupiter Laser Facility to measure high-quality spectra of K-shell oxygen and L-shell iron lines in laser-heated plasma both in emission and absorption. These new data will be compared with predictions from atomic physics codes to help resolve astrophysical observations and theoretical atomic energy levels.

Astrophysical spectra are often Doppler-shifted and broadened, and uncertainties exist in the incomplete atomic energy-level database, which makes interpretation difficult. A high-resolution absorption spectroscopy platform of ionized plasmas containing K-shell oxygen and L-shell iron is essential to address the needs of the astrophysical community. This technology would allow access to multiple excited levels in low-ionization-charge states of interest. Absorption spectroscopy is the only way to measure inner-shell excited states that de-excite by radiationless (Auger) decay. An accurate database derived from this technique would allow the identification of atomic structure measurements of features commonly observed from astrophysical objects.

Mission Relevance

This work supports and utilizes the Laboratory's capability and expertise in high-energy-density science to develop spectroscopic atomic-structure databases to interpret x-ray spectra relevant to astrophysics, which supports Laboratory missions related to stockpile stewardship, energy security, and advances in fundamental science. In addition, the work will create a new absorption platform on low-temperature and lower-atomic-number materials for making precision opacity measurements relevant to the weapons program.

FY08 Accomplishments and Results

In FY08, we (1) built a high-resolution grating spectrometer and fielded it on LLNL's Comet high-power laser; (2) recorded high-resolution K-shell oxygen emission spectra with high signal-to-noise ratios from a low-density aerogel target, for the first study of the project spectral region; (3) transferred the instrument to the JANUS laser to develop the intense x-ray laser backlighter required for absorption measurements; and (4) developed a target of mixed-layer, mid-atomic-number materials that exhibited a strong, short burst of spectrally smooth emission in the 1.5-to-2.5-nm waveband, in line with our goals. These time-resolved spectra lasted several hundred picoseconds and followed the laser pulse shape. This project established a new laboratory-based absorption spectroscopy platform for studying the atomic structure of K-shell oxygen and L-shell iron to interpret complicated spectra measured from astrophysical plasmas. The next step is to apply the techniques developed in this work to studies on opacity.

Publications

Dunn, J., et al., 2008. *Calibration of a high-resolution soft x-ray spectrometer.* Intl. Conf. X-ray Lasers, Belfast, U.K., Aug. 17–22, 2008. LLNL-ABS-404849.

Dunn, J., et al., 2008. *High-resolution soft x-ray spectroscopy of low Z K-shell emission from laser-produced plasmas.* 17th Topical Conf. High-Temperature Plasma Diagnostics, Albuquerque, NM, May 11–15, 2008. LLNL-ABS-403445.

Dunn, J., et al., in press. "High-resolution soft x-ray spectroscopy of low-Z K-shell emission from laser-produced plasmas." *Rev. Sci. Instrum.* LLNL-JRNL-404496.

High-Energy-Density Experiments on Short-Pulse X-Ray Light Sources

Klaus Widmann   08-ERD-004

Abstract

Extreme states of matter are central to many critically important scientific questions, from understanding planetary interiors to demonstrating the inertial-confinement fusion energy concept. This project will establish the capability and expertise for LLNL to perform high-energy-density science experiments using fourth-generation short-pulse x-ray light sources. In particular, we will develop the basic capability of measuring the energy balance and, therefore, the fraction of free-electron laser energy that is absorbed by the target as a function of laser intensity. Moreover, we will use interferometric techniques to monitor the hydrodynamic expansion of the heated target. By breaking new scientific ground, this project will pave the way to high-energy-density experiments at the next generation of light sources now under development.

We expect to (1) measure vacuum or extreme ultraviolet focal spots in situ with 1-µm spatial resolution, (2) measure the energy density in targets heated with free-electron lasers and the subsequent hydrodynamic expansion of the high-energy-density state, and (3) characterize absorption as a function of irradiance, which should shed light on the absorption process of high-intensity ultrafast x-ray pulses. This will clarify and quantify, for the first time, the difference between x-ray heating and short-pulse laser heating. In combination with the simultaneous measurement of expansion, we expect to determine the electron temperature of this high-energy-density state, opening the door to equation-of-state measurements.

Mission Relevance

Understanding the high-energy-density regime is at the scientific foundation of the Stockpile Stewardship Program. By enabling the capability for free-electron laser, high-energy-density experiments, this project supports the Laboratory's national security mission.

FY08 Accomplishments and Results

For FY08, we (1) successfully demonstrated our capability to focus the x-ray beam at the FLASH free-electron laser facility in Germany to a diameter of only a few micrometers, and thus were able to obtain x-ray intensities of 10^{16} W/m^2; (2) performed initial experiments of the laser focal spot size using post-shot metrology of poly(methyl methacrylate) plastic samples; (3) determined that the surface quality of our molybdenum–silicon multilayer off-axis parabola cannot exceed 0.2-nm root-mean-square and that elaborate metrology of the gradient coating has been the key to a micrometer-sized focal spot; (4) demonstrated that silicon x-ray diodes are well suited for the energy balance measurements and that the x-ray intensity in our focal spot was high enough to induce saturation absorption in a metal in the extreme ultraviolet regime; and (4) initiated design of an interferometer suitable to be fielded at FLASH and the Linac Coherent Light Source at Stanford.

Nonequilibrium Electron Dynamics in Warm Dense Matter

Andrew Ng   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–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 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.

FY08 Accomplishments and Results

In FY08, we successfully performed the first single-shot measurements with a chirped probe. We found that gold foil heated with 800-nm pulses undergoes a transition from single-photon absorption to two-photon absorption with increasing energy densities. This discovery led to a shift in our focus to the 800-nm pump for studying electron dynamics under selective excitation. For the theoretical effort, we developed a computationally efficient procedure to calculate the dielectric function without compromising numerical convergence. To strengthen our computational capability for these efforts, we collaborated with Lawrence Berkeley National Laboratory through a user program in the Molecular Foundry facility.

Proposed Work for FY09

For FY09, our key experimental efforts will be chirped-pulse reflectivity–transmissivity measurements at the Europa laser facility, combined with picosecond x-ray absorption spectroscopy, both with 800-nm laser excitation. These will yield the first single-shot data on the temporal evolution of free-electron density and electron density of states. Our primary theory work will be adapting interpolation and random k-point sampling of electron density to calculations of physical parameters for warm dense gold, as well as using the constant entropy method to examine the role of nonequilibrium electron distribution. The results will allow us to elucidate nonadiabatic effects in electron–phonon coupling.

Publications

Ogitsu, T., et al., 2008. *Finite temperature simulations of the conductivity of aluminum and gold.* LLNL-POST-408472.
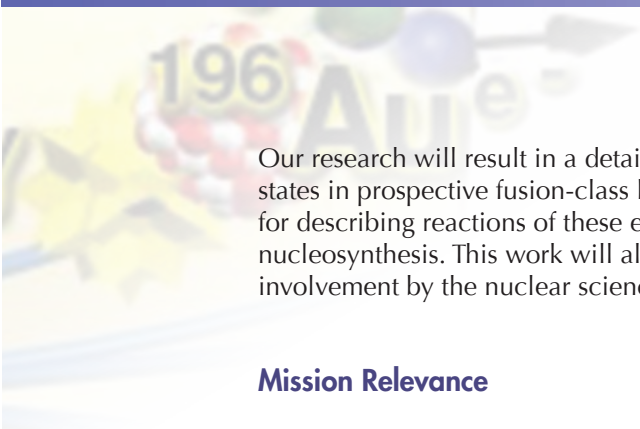
Ping, Y., et al., 2007. "Dielectric function of warm dense gold." *Phys. Plasmas* **15**, 056303. UCRL-CONF-237013.

Studying Reactions of Excited Nuclear States

Lee A. Bernstein   08-ERD-008

Abstract

Fusion-class lasers offer an unprecedented opportunity to observe reactions of nuclei in highly excited nuclear states because of the exceptionally short time over which the "burn" occurs and the enormous compression of the target capsule. These reactions can provide information that is critical to understanding how heavy elements are made in astrophysical environments. We will study these reactions by determining the relative number of products that result from tracer nuclides reactions in target capsules. This project will experimentally determine the excited-state lifetimes required for interpretation of fusion-class laser shot data and create the theoretical tools needed to determine their importance in astrophysics.

Our research will result in a detailed understanding of the lifetimes of quasi-continuous excited states in prospective fusion-class laser tracer products. It will prepare the modeling framework for describing reactions of these excited states and explore their importance in astrophysical nucleosynthesis. 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 of excited states will improve interpretation of radiochemical data, which are a key nuclear weapons diagnostic used in both stockpile stewardship and homeland security (nonproliferation) applications. The research also supports the Laboratory's mission in breakthrough science by improving the interpretation of radiochemical data relevant to the formation of elements in astrophysical environments.

FY08 Accomplishments and Results

In FY08, we (1) performed an experiment using the Livermore-developed silicon telescope array for reactions studies and the Livermore–Berkeley array for collaborative experiments to determine the feasibility of measuring quasi-continuum lifetimes of highly excited nuclear states that will be produced in future fusion-class laser experiments; (2) analyzed the data and created a plan for a follow-on "production" experiment, and observed and measured reactions of highly excited nuclear states that had been populated by (n, gamma) reactions in a high-energy-density plasma comparable to stellar interiors; and (3) prepared a paper detailing our findings for submittal to *Physical Review Letters*.

Proposed Work for FY09

In FY09 we propose to (1) plan an experiment at the Omega laser facility to observe, for the first time, inverse internal conversion—one of the most important of the processes relevant to stellar s-process nucleosynthesis—and measure its cross section; (2) continue participation in the development of a new type of radiochemical-based nuclear diagnostics that will be critical to performing this new class of science at advanced fusion-class lasers; and (3) present results of experiments highlighting the effects of a population of excited nuclear states, induced by nuclear–plasma interaction, on nuclear reactions relevant to stellar s-process nucleosynthesis.

Exploration of Laser–Plasma Interactions for High-Performance Laser-Fusion Targets

David J. 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 occur 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 (PIC) 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.

FY08 Accomplishments and Results

We (1) performed 2D and 3D PIC simulations with the Z3 code of Raman scatter in a laser speckle, which showed Langmuir-wave front bowing in ignition conditions; (2) conducted theory and Vlasov simulations of trapping-induced frequency shifts in Raman scatter and compared the results; (3) developed a simple threshold for Langmuir-wave electron trapping nonlinearity to overcome collisions and speckle-side loss; and (4) kinetically calculated the dispersion and threshold for Langmuir decay instability.

Proposed Work for FY09

For FY09, we will (1) complete our threshold calculations for trapping and Langmuir decay instability in a plasma wave, (2) compare these thresholds to kinetic simulations and apply them to National Ignition Facility simulations, (3) conduct 2D and 3D Raman simulations and diagnose them for enhanced scattering and hot electron spectra, and (4) continue studies of electron and ion trapping in ion waves and Brillouin scattering.

Publications

Bénisti, D., D. J. Strozzi, and L. Gremillet, 2008. "Breakdown of electrostatic predictions for the nonlinear dispersion relation of a stimulated Raman scattering driven plasma wave." *Phys. Plasmas* **15**, 030701. UCRL-JRNL-230843.

Berger, R. L., et al., 2008. *Kinetic simulation of driven nonlinear ion acoustic waves*. 38th Ann. Anomalous Absorption Conf., Williamsburg, VA, June 1–6, 2008. LLNL-POST-404395.

Cohen, B. I., et al., in press. "Stimulated Brillouin backscattering and ion acoustic wave secondary instability." *Phys. Plasmas*. LLNL-JRNL-407238.

Langdon, A. B., et al., 2008. *Two- and three-dimensional simulations of stimulated Raman scatter in NIF ignition conditions*. 38th Ann. Anomalous Absorption Conf., Williamsburg, VA, June 1–6, 2008. LLNL-ABS-402957.

Palastro, J. P., et al., 2008. "Kinetic dispersion of the Langmuir decay instability and its relevance for ignition plasmas." *Bull. Am. Phys. Soc.* **53**, 14. LLNL-ABS-406548.

Strozzi, D. J., D. Bénisti, and L. Gremillet, 2008. "Kinetic modeling of Raman scattering with adiabatic electron response." *Bull. Am. Phys. Soc.* **52**, 195. UCRL-PRES-235988.

Strozzi, D. J., et al., 2008. *Assessing risk of plasma-wave trapping nonlinearities in stimulated Raman scattering*. 38th Ann. Anomalous Absorption Conf., Williamsburg, VA, June 1–6, 2008. LLNL-CONF-404028.

Williams, E. A., et al., 2008. *Langmuir wave de-trapping and SRS inflation thresholds*. 38th Ann. Anomalous Absorption Conf., Williamsburg, VA, June 1–6, 2008. LLNL-PRES-404366.

Towards a Universal Description of Nuclei with Monte Carlo Methods

William E. Ormand   **08-ERD-018**

Abstract

We propose to investigate the application of Monte Carlo methods to solving the nuclear many-body problem, a long-standing issue in nuclear physics. This issue may hold the key to developing a universal picture of nuclei, a key goal of nuclear physics. Building on our recent breakthrough on the "sign problem" with a previous LDRD project, we will apply the auxiliary-field Monte Carlo (AFMC) method to develop a universal picture describing the structure of nuclei spanning the periodic table. The power of the AFMC method is that it provides exact results for systems with extraordinarily large dimensions and enables, for the first time, basic calculations needed to address the nuclear many-body problem. We will first apply our unique AFMC capability to large-scale problems with existing interactions, then combine AFMC with mean-field methods to develop the first truly microscopic and universal picture of nuclei. This work, if successful, 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 that 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. This will provide the Laboratory 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.

FY08 Accomplishments and Results

For FY08, we (1) performed benchmark calculations for three nuclei and achieved excellent agreement with exact shell-model calculations for ground-state energy, thermal energy, and density of states; (2) performed calculations for iron-54 and iron-60 and prepared our results for *Physical Review Letters*; (3) developed computer programs for the Hubbard Model (condensed matter physics), which began yielding promising results; and (4) initiated coupling of the AFMC and Hartree–Fock methods.

Proposed Work for FY09

In FY09, we will (1) complete our examination of solutions to the sign problem for the Hubbard model, (2) apply the "zero temperature" formalism of the AFMC method to extract ground-state properties for upper fp-shell nuclei ranging from iron to selenium, (3) develop the requisite mean-field codes for the basis states and single-particle wave functions to compute two-body matrix elements for the configuration-interaction calculations of mid-mass nuclei with the AFMC technique, and (4) establish a procedure to determine effective interaction for a universal description 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 D. 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, our analytical theory, and numerical simulations based on Livermore BOUT and UEDGE codes, we will develop optimum 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, and 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 tokamak consortium ITER (International Thermonuclear Experimental Reactor) and completion of its 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.

FY08 Accomplishments and Results

We (1) assessed techniques and developed initial theory for driving non-axisymmetric magnetic perturbations via plasma currents to reduce heat bursts from the plasma core, (2) upgraded the UEDGE and BOUT codes for snowflake divertors with tilted plates, (3) identified the key parameter that predicts simulated heat-flux reduction by tilting divertor plates, (4) found a range of enhanced heat flux reduction for the snowflake divertor in the planned Fusion Development Facility, (5) worked with collaborators at Princeton to develop a possible snowflake divertor for their planned National High-Power Advanced Torus Experiment facility, and (5) collaborated with General Atomics and Princeton to show that snowflake configurations can be created on the existing DIII-D and National Spherical Torus Experiment tokamaks without new hardware, including planning corresponding experiments on both tokamaks.

Proposed Work for FY09

For FY09, we propose to (1) complete an analytical assessment of the feasibility of inducing magnetic stochasticity using plasma-driven currents in the tokamak; (2) perform UEDGE analysis of a snowflake divertor in the radiative mode and determine specific, relevant design specifications for the planned new fusion facilities at Princeton and General Atomics; (3) perform BOUT simulations of the induced convection for various types of surface perturbations for divertor plates; (4) devise specific experiments, in collaboration with Princeton and General Atomics, for benchmarking the BOUT results; (5) identify best materials for the induced convection and currents approach to reducing heat loads; and (6) publish results in peer-reviewed journals and submit appropriate patent applications.

Publications

Joseph, I., R. H. Cohen, and D. D. Ryutov, 2008. *Control of edge localized modes through toroidally asymmetric current perturbations in the tokamak scrape-off layer.* Resonant Magnetic Perturbations Modeling Workshop, San Diego, CA, Aug. 25–26, 2008. LLNL-PRES-406589.

Joseph, I., R. H. Cohen, and D. D. Ryutov, 2008. *Driving toroidally asymmetric current through the tokamak scrape-off layer to suppress edge localized modes.* LLNL-JRNL-408174.

Ryutov, D. D., et al., 2008. *A snowflake divertor: A possible way of improving the power handling in future fusion facilities.* 22nd International Atomic Energy Agency Fusion Energy Conf., Geneva, Switzerland, Oct. 13–18, 2008. LLNL-CONF-407193.

Ryutov, D. D., et al., 2008. "Magnetic field structure of a snowflake divertor." *Plasma Phys.* **15**, 092501. LLNL-JRNL-404468.
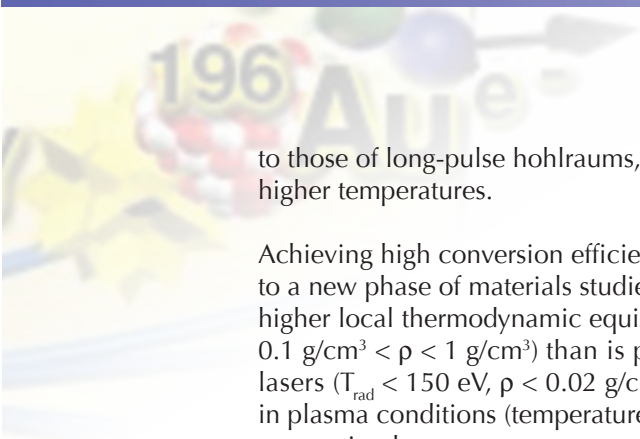
Umansky, M. V., et al., 2008. *Edge transport modeling for FDF comparing standard and snowflake divertors.* LLNL-PRES-404335.

High-Temperature, Thermal X-Radiation Sources at Short-Pulse Lasers

Marilyn B. Schneider   **08-ERD-024**

Abstract

Probing radiatively heated matter at high temperatures and in local thermodynamic equilibrium is important for benchmarking radiation transport, opacity, equation of state, and atomic physics codes. This project will develop a platform to use short-pulse lasers to create hot (thermal) radiation sources to radiatively heat samples. We will first optimize the conversion of laser energy into thermal ("soft") x-rays by varying pulse length, intensity, target material, and laser-target geometry. We will use this knowledge to optimize conditions for a confined-geometry (hohlraum) target. Our goal is to reach conversion efficiencies (>80%) equivalent

to those of long-pulse hohlraums, which would enable short-pulse lasers to reach much higher temperatures.

Achieving high conversion efficiencies in short-pulse hohlraums would open the door to a new phase of materials studies. If successful, we will be able to drive materials to higher local thermodynamic equilibrium temperatures and densities ($T_{rad} > 200$ eV, 0.1 g/cm$^3 < \rho < 1$ g/cm^3) than is possible by radiatively heating materials with long-pulse lasers ($T_{rad} < 150$ eV, $\rho < 0.02$ g/cm^3). We also plan to measure the emission of an iron sample in plasma conditions (temperature and density) similar to those at the bottom of the sun's convection layer.

Mission Relevance

This project will enable laboratory-based experiments on materials important to the Stockpile Stewardship Program. Our research 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.

FY08 Accomplishments and Results

In FY08, we (1) made baseline measurements to understand the conversion of laser light to soft x-rays, concentrating on copper foils because the K-alpha spectrometers and imagers (which measure hot electrons inside the target) are specifically built for a narrow x-ray range; (2) built a broadband soft x-ray spectrometer; (3) used the Janus laser, an x-ray streak camera, and the Elecron Beam Ion Trap facility to calibrate the spectrometer; and (4) measured the conversion of laser light to soft x-rays at the Titan laser as a function of pulse length, spot size, laser energy, and energy partition to hot electrons.

Proposed Work for FY09

The work in FY09 will optimize the conversion efficiency of laser light into soft x-rays. To do this effectively, we must understand the mechanisms of the bulk heating of targets only a few micrometers thick, then develop theoretical models that explain the experimental results. Specifically, we will (1) measure the time history of the heating of the back side of copper targets, (2) correlate the measured soft x-ray spectra with the measured hot electron temperature and with the energy partitioned into hot electrons, (3) optimize the laser conditions for the x-ray radiation source at Titan, (4) field the x-radiation source on Titan, and (5) develop a theoretical model of the heating mechanisms.

Publications

Baldis, H. A., et al., 2008. *Laser plasma interactions in high energy density plasmas.* 38th Anomalous Absorption Conf., Williamsburg, VA, June 2–6, 2008. LLNL-PRES-404341.

Cone, K. V., et al., 2008. *Heating mechanisms of thin targets using short pulse lasers.* 38th Anomalous Absorption Conf., Williamsburg, VA, June 2–6, 2008. LLNL-POST-404338.

Advanced Computation and Experimental Analysis of Plasma Equations of State and Transport

Brian G. 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 experimental validation will address the effects of pressure ionization through measurements of photoabsorption in shock-heated samples. These first-ever measurements of how partially degenerate atomic systems are modified at very high densities and finite temperatures will provide a stringent test of our new computational methods.

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.

FY08 Accomplishments and Results

In FY08 we (1) developed an improved method to initialize ion configurations to facilitate the simulations, concentrating on zero-temperature amorphous system simulations; (2) continued extending and combining the existing Korringa–Kohn–Rostoker codes of our collaborators at the University of Illinois and the University of Munich to apply to finite-temperature and amorphous systems; and (3) began an accurate computation of the electronic structure of a disordered cluster of atoms.

Proposed Work for FY09

For FY09, we will (1) implement a generalization of geometrically based Voronoi tessellation to enable multiple scattering simulations of spatially amorphous systems—this will allow an optimized average spherical approximation basis set to be employed by the Mecca code, which in turn will allow zero-temperature amorphous system simulations; (2) 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 the Mecca code; and (3) develop a multicenter but nonspherically symmetric potential extension of a plasma equation of state, using orbital-free density functional methods as a first approximation.

Impurity and Alloying Effects on Material Strength from First Principles

Robert E. 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, oxygen impurity strengthening, and alloy core-structure modification. The project will be largely computational, but also will include further development and application of novel diamond-anvil cell experiments to validate results of our computational 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, oxygen impurity strengthening, and alloy core modification. Diamond-anvil cell experiments conducted as part of the project will provide validation for the oxygen impurity strengthening; other results will be validated with existing experimental data. The principal significance of these achievements will be demonstration of 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.

FY08 Accomplishments and Results

In FY08 we (1) calculated alloy minority constituent properties in a body-centered-cubic metal from first principles, (2) conducted diamond-anvil cell measurements at the Advanced Photon Source of the yield strength of pure vanadium through the phase transition of body-centered cubic to rhombohedral, (3) initiated a theoretical investigation of how alloying affects that phase transformation, and (4) conducted hundreds of first-principles density-functional theory calculations to determine how minority constituents affect defect mobilities in vanadium.

Proposed Work for FY09

In FY09 we will focus on the strength of body-centered-cubic metal alloys. Specifically, we will (1) calculate the gamma surface (energy as a function of shear displacement) of tantalum–tungsten alloys using first-principles techniques, (2) infer the dependence of the Peierls barrier on alloy concentration at high pressure using gamma surface values in a Peierls–Nabarro model, (3) measure the strength of tantalum–tungsten alloys at high pressure using the pressure-gradient technique and a diamond anvil cell, (4) conduct calculations of the shear modulus of vanadium alloys with our university collaborator, and (5) begin experiments on vanadium alloy strength in the 0.5-to-1.0-Mbar range using a diamond anvil cell, if calculations of the shear modulus of the alloy are promising.

Publications

Rudd, R. E., and J. E. Klepeis, in press. "Multiphase improved Steinberg–Guinan model for vanadium." *J. Appl. Phys.* LLNL-JRNL-406789.
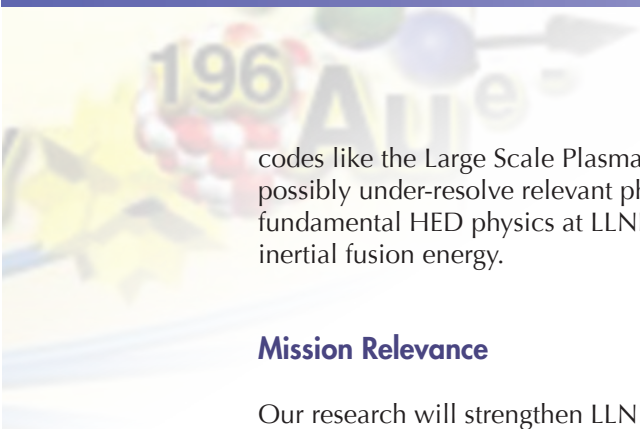
Characterization of Short-Pulse Laser Interaction with Solid Matter

Andreas J. Kemp   08-ERD-040

Abstract

The possible uses of short-pulse lasers in driving plasma devices with complex geometries are only now beginning to be realized. Today's large implicit codes can perform more-detailed kinetic simulations of the relevant reactions at a higher precision, but are impractical for problems such as the cone-size targets that are used in fast ignition and other high-energy-density (HED) experiments. In this project, we will use both analytics and existing collisional kinetic simulations to characterize the laser-generated electron distributions that are important for large-scale implicit simulations.

Our objective is to study basic mechanisms of short-pulse laser–solid interaction for HED physics and fast ignition, and to provide an improved scientific basis for laser–plasma interactions in general and electron-distribution functions for large implicit codes such as the Large Scale Plasma code in particular. As we address fundamental physics issues of HED physics experiments involving large spatial scales, high densities, and long time durations using an explicit collisional kinetic approach, we will be able to process results in large implicit

codes like the Large Scale Plasma code that currently lack laser–plasma interaction and possibly under-resolve relevant physics aspects on small spatial scales. Our results will benefit fundamental HED physics at LLNL—radiography, equation of state, opacity, fast ignition, and inertial fusion energy.

Mission Relevance

Our research will strengthen LLNL's work in short-pulse laser–matter interaction and HED physics, especially radiography, equation of state, and opacity physics in support of stockpile stewardship, and fast ignition for inertial fusion energy in support of the Laboratory's energy security mission.

FY08 Accomplishments and Results

In FY08, we (1) studied short-pulse laser coupling to fast-ignition–relevant plasmas, which typically feature density gradients with scale lengths of several micrometers, using kinetic Particle-in-Cell simulations; (2) studied energetic electron jets along solid target surfaces irradiated beyond a critical angle—we determined there is a small fraction of electrons that co-propagate with the laser pulse along the target surface; and (3) analyzed surface heating in short-pulse laser–plasma interaction using two-dimensional collisional simulations. Overall, we have made significant progress in our theoretical study of short-pulse laser–plasma interaction relevant for fast ignition efforts at LLNL, and addressed several important physics issues, which have been detailed in *Physical Review Letters*.

Publications

Akli, K., et al., 2008. "Laser heating of solid matter by light-pressure-driven shocks at ultrarelativistic intensities." *Phys. Rev. Lett.* **100**, 165002. UCRL-JRNL-230851.

Kemp, A. J., Y. Sentoku, and M. Tabak, 2008. "Hot-electron energy coupling in ultraintense laser–matter interaction." *Phys. Rev. Lett.* **101**, 075004. LLNL-JRNL-403005.

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, have put this understanding—and a corresponding experimental validation of it—within reach. Partnering with university collaborators and with Los Alamos and

Berkeley National Labs, we will perform lattice QCD calculations of the equation of state (EOS) 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 EOS of nuclear matter, (2) the nucleon–nucleon phase shifts, and (3) three-nucleon systems using quark degrees of freedom, ultimately leading to the extraction of unknown three-nucleon force parameters. Computing the EOS of nuclear matter would be a significant advance in high-temperature lattice QCD and will be crucial for understanding the petabytes of heavy ion data that will be generated at facilities such as Relativistic Heavy Ion Collider at Brookhaven and the Large Hadron Collider at the CERN European Organization for Nuclear Research. The results of our calculations will help benchmark low-energy QCD with experiments and calculate properties of the nuclear force that are not currently accessible experimentally, but which are essential to calculating few-body nuclear reactions with precision.

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.

FY08 Accomplishments and Results

In FY08, we calculated the EOS for a lattice with the space–time lattice constants of $N_t = 8$ and $ml = 0.1$ ms for two fermion actions referred to as "p4" and "asqtad;" (2) performed transition temperature calculations for $ml = 0.2$ ms for both actions, and also for the "domain wall fermion" action with dimensions of 96 in the fifth dimension; (3) hosted a workshop on lattice strong dynamics, which launched a new collaboration to perform calculations relevant to high-energy-physics experiments at the Large Hadron Collider; and (4) performed initial calculations for the two-body nuclear phase shifts in the nucleon–nucleon system.

Proposed Work for FY09

In FY09 we will (1) begin EOS calculations at finite density with staggered fermion actions, (2) perform EOS calculations with the improved chirally symmetric domain-wall fermion action, (3) complete an analysis of nucleon–nucleon scattering length and begin work on the theory required to perform calculations of the three-nucleon interaction, and (4) perform preliminary strong dynamics calculations for physics beyond the Standard Model.

Publications

Beane, S. R., et al., 2008. "Multipion systems in lattice QCD and the three-pion interaction." *Phys. Rev. Lett.* **100**, 082004. LLNL-JRNL-353413.

Detmold, W., et al., 2008. "Multi-pion states in lattice QCD and the charged-pion condensate." *Phys. Rev. D* **78**, 014507. LLNL-JRNL-402365.

Luu, T., 2008. *Three fermions in a box.* Lattice 2008, 26th Intl. Symp. Lattice Field Theory, Williamsburg, VA, July 14–19, 2008. LLNL-PROC-407504.

Luu, T., R. Soltz, and P. Vranas, 2007. "Simulating the birth of the universe on a petaflop." *Comput. Sci. Eng.* **9**(6), 55. LLNL-JRNL-404088.

Vranas, P., et al., 2008. "Massively parallel quantum chromodynamics." *IBM J. Res. Dev.* **52**(1/2), 189. LLNL-JRNL-404093.

Analysis in Three Dimensions Plus Time of Plasma Microturbulence Simulations

William M. Nevins   **08-ERD-048**

Abstract

Plasma microturbulence is the dominant mechanism of heat loss in tokamaks, and will determine the fusion gain achieved in future confined-plasma fusion reactors. A fundamental issue in plasma microturbulence is energy flow—turbulent energy is produced by instabilities at a low radial wave number. The conventionally accepted theory is that this energy scatters to a 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. In this project, we will use 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 extend the current state-of-the-art 2D-plus-time code, GKV, to achieve 3D-plus-time analysis of these data sets by decomposing the data into subsets of several correlation lengths and times per dimension. These subsets can then be processed in parallel to produce accurate estimates of correlation functions and spectral densities. We will also develop the tools needed to extract more information than currently possible from 3D numerical simulations of plasma microturbulence.

We will develop a 3D-plus-time data analysis capability and use it to explore the 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 the fusion gain is critical to the success of magnetic fusion because it will determine how much fusion power can be produced.

FY08 Accomplishments and Results

In FY08, we (1) chose the interactive data language for our interpreter and graphics package; (2) completed a 2D-plus-time analysis code employing the algorithm proposed for 3D-

plus-time data analysis and used it to analyze data from the GYRO, GEM, GS2, and GENE plasma turbulence simulation codes; and (3) selected and hired a postdoctoral researcher knowledgeable in the analysis of data from plasma microturbulence simulations, who joined the project in December.

Proposed Work for FY09

In FY09 we will transform our prototype 3D-plus-time analysis software into a package suitable for use by third parties and use this package to analyze energy flow in 3D-plus-time datasets.

Cryogenic Bolometers for Double-Beta Decay Experiments

Eric B. Norman   08-ERD-049

Abstract

The Cryogenic Underground Observatory for Rare Events (CUORE), at the Gran Sasso National Laboratory in Italy, will be a large detector designed to search for the neutrinoless double-beta decay of tellurium-130. 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 (TeO_2) crystal bolometer production, and background reduction that will improve the performance of CUORE, and thus improve its sensitivity to neutrinoless double-beta decay.

We intend to 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 tellurium-130 to both the ground state and excited states of xenon-130, as well as the two-neutrino electron capture/beta-plus decay of tellurium-120 and the charge-nonconserving decay of the electron into a neutrino and a gamma ray. We will develop procedures for producing TeO_2 crystals to meet CUORE's stringent requirements on radio-purity, uniformity, and surface finish. Furthermore, we expect to identify materials with lower radioactive contamination than those used previously in components for CUORE. 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 detection of 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.

FY08 Accomplishments and Results

We (1) conducted a search at CUORICINO for the neutrinoless double-beta decay of tellurium-130 and published the results in *Physical Review C*; (2) began the analysis of CUORICINO data for the double-electron capture and beta plus–electron capture decays of telluriume-120; (3) acquired 500 TeO_2 crystals for our CUORE experiments; (4) used two large LLNL plastic scintillators at the Gran Sasso National Laboratory to study the effects of cosmic ray muons on the CUORICINO background, showing that muons will contribute a negligible amount to the background at CUORE; and (5) worked on the low-background gamma-ray counting of materials used in the production of TeO_2 crystals for CUORE.

Proposed Work for FY09

In FY09, we plan to (1) search for the double-beta decay of tellurium-130 to excited states of xenon-130, (2) measure the half-life of tellurium-130, and (3) take advantage of new opportunities afforded by CUORE-0—a small-scale CUORE detector—to refine background elimination techniques and obtain better sensitivity in searches for double-beta decay and other rare decay modes.

Publications

Arnaboldi, C., et al., 2008. "Results from the CUORICINO zero-neutrino double beta decay experiment." *Phys. Rev. C* **78**, 035502. LLNL-JRNL-408037.

Dolinski, M., 2008. *Neutron interactions in the CUORE neutrinoless double beta decay experiment.* LLNL-TH-408040.

Partition-of-Unity, Finite-Element Method for Large-Scale Quantum Molecular Dynamics on Massively Parallel Computational Platforms

John E. 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 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— partition-of-unity, finite-element analysis. Our method 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.

FY08 Accomplishments and Results

In FY08, we (1) formulated and implemented a prototype partition-of-unity method for solving the Schrodinger and Poisson equations; (2) implemented the partition-of-unity concept in LLNL's finite-element electronic structure code; (3) validated our code against existing codes, achieving total energy convergence to micro-Hartrees; and (4) carried out fully self-consistent calculations on d- and f-electron metals to demonstrate efficiency. These calculations on real, physical systems have shown even greater efficiency gains than previously suggested by calculations on model problems. For example, calculations for lithium hydride showed a reduction in total basis set size by a factor of 16, indicating a total speedup by a factor of 50 relative to current state-of-the-art plane-wave-based codes.

Proposed Work for FY09

In FY09, we will (1) formulate QM forces for Livermore's partition-of-unity finite-element (PUFE) code, (2) implement the forces in our prototype and PUFE codes, (3) parallelize the PUFE code, and (4) apply our code to the study of the elastic moduli of systems with dilute impurities (oxygen in vanadium at high pressure).

Publications

Pask, J. E., 2008. *Partition-of-unity finite-element approach for large, accurate ab initio electronic structure calculations*. IMA Mathematical and Algorithmic Challenges in Electronic Structure Theory, Minneapolis, MN, Sept. 29–Oct. 3, 2008. LLNL-PRES-403799-DRAFT.

Pask, J. E., 2008. *Partition-of-unity finite-element approach for large, accurate ab initio electronic structure calculations*. SIAM Conf. Mathematical Aspects of Materials Science, Philadelphia, PA, May 11–14, 2008. LLNL-ABS-401977.

Sukumar, N., and J. E. Pask, in press. "Classical and enriched finite element formulations for Bloch-periodic boundary conditions." *Int. J. Numer. Meth. Eng.* LLNL-JRNL-403676-DRAFT.

Sukumar, N., and J. E. Pask, 2008. *Partition of unity finite element method to solve the Kohn–Sham equations of density functional theory*. 8th World Congress on Computational Mechanics and 5th European Congress on Computational Methods in Applied Sciences and Engineering, Venice, Italy, June 30–July 4, 2008. LLNL-ABS-400460.

Measurement and Prediction of Laser-Induced Damage in the Presence of Multiple Simultaneous Wavelengths

Mike C. Nostrand   08-ERD-054

Abstract

Accurate predictions of laser-induced optical damage are critical for laser experimentation in which optical damage limits performance and in which 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-length variations. We will first collect damage and conditioning data to enable empirical fits as a function of parameters for inertial-confinement fusion lasers, then develop a predictive computational capability for describing the damage expected from the beamline of this class of laser. 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 produce 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 silicon 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.

FY08 Accomplishments and Results

In FY08, we (1) created and successfully implemented a multiple simultaneous wavelength capability including construction of a 4ω converter; (2) performed studies that have resulted in significant optimization of sample-preparation techniques; (3) performed tests on pulse-length dependent conditioning, but found a much greater effect of pulse-shape on surface damage and have transferred efforts to understanding this effect; (4) collected silicon dioxide and KDP surface-damage data; (5) determined that silicon dioxide fits show good agreement for growth, but found a deficit in understanding for KDP growth; (6) determined that the absorption distribution model is useful for understanding KDP–laser interactions, but adaptation will be necessary for applicability to silicon dioxide; and (7) developed and tested predictive tools that will guide the discovery of more efficient techniques.

Proposed Work for FY09

We will (1) continue to upgrade and refine our predictive capabilities from the increased amount of online data available and expand the work to include KDP, (2) continue modeling of flaws and incorporate those models into our online predictive capabilities, (3) continue pulse-shape work on 3ω and expand it to additional wavelengths, (4) develop and refine rules for optics flaws, and (5) further develop our laser-management software to include more and better operation rules, more efficient load-leveling of optic recycling and maintenance, more efficient visualization and analysis of laser beams, and predictive capabilities that extend further into the future.

Publications

Carr, A., et al., 2008. *Defect classification using machine learning.* SPIE Boulder Damage 2008, Boulder, CO, Sept. 22–24, 2008. LLNL-PROC-408339.

Carr, C. W., et al., 2008. *Using shaped pulses to probe energy deposition during laser-induced damage of SiO$_2$ surfaces.* SPIE Boulder Damage 2008, Boulder, CO, Sept. 22–24, 2008. LLNL-PROC-408345.

Norton, M. A., et al., 2008. *Laser damage growth in fused silica with simultaneous 351 nm and 1053 nm irradiation.* SPIE Boulder Damage 2008, Boulder, CO, Sept. 22–24, 2008. LLNL-PROC-408343.
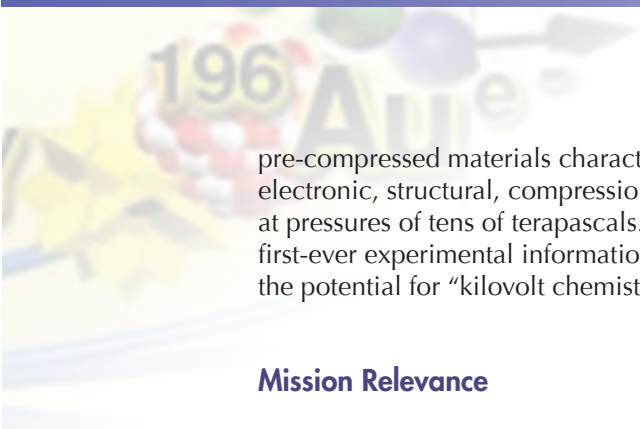
Physics and Chemistry of Planetary Interiors: A New Generation of Condensed-Matter Experiments

Gilbert W. Collins   08-ERD-058

Abstract

We will develop and validate the capability to perform extreme condensed-matter experiments on fusion-class laser systems, then systematically characterize condensed matter in the gigabar pressure range, with up to tenfold higher compression. We will focus on establishing a new generation of experiments that will access the currently unexplored regime of ultrahigh compression, with applications that range from understanding the origin and evolution of planets to testing and significantly extending first-principle, quantum mechanical theories of condensed matter.

This project will extend the capability of high-pressure condensed-matter experiments from the megabar to the gigabar regime. Ramp loading experiments at the National Ignition Facility will characterize solids in the 1- to 10-TPa range to examine constitutive properties, atomic-packing structure, melting, and other phenomena. We will provide experimental constraints on models of planetary interiors, evolution, and origin through single- and multiple-shock compression of

pre-compressed materials characteristic of planetary fluids. This will allow us to determine the electronic, structural, compressional, melting, and chemical bonding of hydrogen and helium at pressures of tens of terapascals. Finally, strong shock compression will be used to obtain the first-ever experimental information on chemistry at extreme (petapascal) conditions, including the potential for "kilovolt chemistry."

Mission Relevance

Understanding matter at extreme conditions is fundamental to LLNL's national security mission. By extending the regime of accurate high-pressure, condensed-matter data, we will provide rigorous constraints for materials relevant to stockpile stewardship in a regime for which no data currently exist.

FY08 Accomplishments and Results

Last year we (1) initiated a worldwide effort to explore ultradense material states on fusion-class lasers, which produced several experimental designs and discoveries; (2) developed compression techniques to study solid state properties of materials at terapascal pressures, hydrogen and helium at many grams per cubic centimeters, and extreme chemistry where the characteristic bonding energy is a kilovolt; and (3) tested these techniques on the Jupiter and Omega laser facilities, which resulted in the metallization of helium, melting of diamond, and discovery of new polymeric fluid phases. Overall, this new field has generated significant enthusiasm in the scientific community and recognition for the Laboratory. We have developed and used new techniques to explore ultradense states of matter, resulting in the metallization of helium, the observation that diamond melts to a liquid metal with a higher density than the solid, and the discovery of new polymeric fluid phases at several terapascal pressures and electronvolt temperatures.

Publications

Bradley, D. K., et al., 2008. "Stress-density response of diamond under shockless compression to 800 GPa." LLNL-JRNL-401827.

Eggert, J., et al., 2008. "Melting of diamond." LLNL-JRNL-234391.

Hicks, D., et al., 2008. "High precision measurements of the diamond Hugoniot in and above the melt region." *Phys. Rev. B.* **78**(17), 174102. LLNL-JRNL-406173.

Smith, R., et al., 2008. "Ultra-fast dynamic compression technique to study kinetics of phase transformations in bismuth." *Phys. Rev. Lett.* **101**, 065701. LLNL-JRNL-401818.

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

Peter A. 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 the origin of these fields is believed to have direct implications for 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 and ion fluids—that is, a plasma. This project will explore such plasma effects on important hydrodynamic instabilities such as Rayleigh–Taylor and Richtmyer–Meshkov.

The main deliverable 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 enough. 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 impact not only ignition on fusion-class lasers but also many high-energy-density studies with relevance to the Laboratory's national security mission.
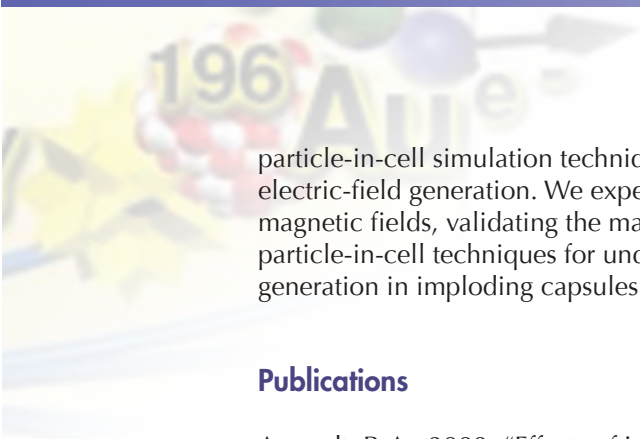
Mission Relevance

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 impacting investigations of high-energy-density imploding systems.

FY08 Accomplishments and Results

In FY08, we (1) developed a prediction that ionization gradients in inertial-confinement-fusion capsules can lead to higher levels of Rayleigh–Taylor instability growth, particularly for low-atomic-number ablators; (2) determined that potential astrophysical applications of this predicted phenomenon include supernovae and protostellar HII regions; (3) discovered that self-consistent electric fields in an accelerating plasma can produce charge separations and a significant redistribution of electrons; and (4) determined that such a profile adjustment can affect our interpretation of measured x-ray self-emission and charged particle slowing in inferring implosion core behavior.

Proposed Work for FY09

In FY09 we will concentrate on (1) continued development of analytic tools for gauging electric and magnetic fields on instability growth, (2) exercising new three-dimensional radiation-hydrodynamics capabilities with magnetic field generation, and (3) studying the viability of

particle-in-cell simulation techniques to understand the mechanisms underlying the observed electric-field generation. We expect continued progress on applying the analytic techniques to magnetic fields, validating the magnetic-field generation package, and developing the 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 instability." *Phys. Rev. Lett.* **101**(11), 115004. LLNL-JRNL-403824.

Nuclear Astrophysics at the National Ignition Facility: Feasibility of Studying Reactions of the Stars on Earth

Richard Boyd   08-ERD-066

Abstract

Our objective is to begin planning nuclear astrophysics experiments to be conducted at the National Ignition Facility (NIF) to determine how nuclides were synthesized and, more broadly, to study the evolution of stars. Because these experiments can only be performed at NIF at its full energy, our work will focus on studies that must precede the experiments. Target simulations will be performed using the HYDRA code for several reactions, some of which are believed to be viable candidates, and others for which viability needs to be established. 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. The latter information will determine the feasibility of each experiment. Yields will be optimized by varying such parameters as the pellet design, laser energy, and laser profile. The diagnostics required for future shots will also be determined, and their ability to determine the information required of the NIF shots will be analyzed. 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 use of NIF to conduct nuclear astrophysics experiments, in support of the Laboratory's national security mission, and will lead to advances in understanding nuclear reactions that are relevant to stockpile stewardship. In addition, our research will contribute to the Laboratory's mission in basic science.

FY08 Accomplishments and Results

In FY08 we (1) performed simulations of various compound laser-induced reactions including those of ^{3}He(^{4}He,γ)^{7}Be and ^{14}N(p,γ)^{15}O and determined both gave insufficient yields to be studied at NIF with the standard ignition parameters—when their constituents were included in ignition shots, the yields increased dramatically, but only because of reactions induced by the added deuterium and tritium; (2) determined that simulations of ^{10}B(p,α)^{7}Be also produced an estimated yield that was too small; (3) determined that the ^{6}Li(p,α)^{3}He reaction produced a sufficient simulated yield that it could be used as a target in subsequent simulations designed to optimize NIF parameters for nuclear astrophysical shots; and (4) made significant progress, in collaboration with the Colorado School of Mines group, toward designing a radiochemical diagnostic that involves pumping out all shot debris and selectively freezing it on cryopanels for observation of radionuclide decays. This group also contributed to the radiochemical diagnostic being developed by NIF personnel.
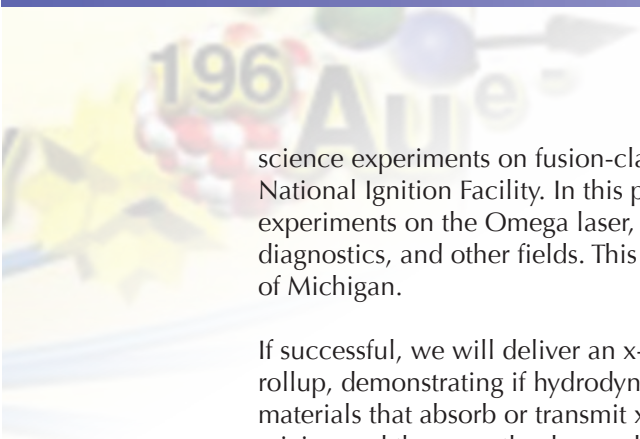
Proposed Work for FY09

FY09 will be devoted to continuing our feasibility studies for nuclear astrophysics experiments on NIF. Work will initially focus on simulations of the ^{6}Li(p,α)^{3}He reaction, because that seems to produce sufficient yield to be used to optimize NIF parameters such as laser pulse and target size. A feasibility study of using NIF to measure the ^{59}Fe(n,γ)^{60}Fe reaction will be conducted. This reaction is of special significance to gamma-ray astronomy. Its study would involve several stages: making a ^{59}Fe material, inserting that into a NIF target, then analyzing the results at the LLNL Center for Accelerator Mass Spectroscopy. The Colorado group will continue efforts to develop radiochemical diagnostics for NIF. A new effort will be initiated by collaborators at Ohio University to develop a neutron time-of-flight system. Finally, a new initiative to test Big Bang nucleosynthesis will begin—this involves theoretical work both to extend the reaction network and to include a proper description of nonthermal particles in Big Bang nucleosynthesis calculations. It will also involve feasibility studies of reactions, mostly involving ^{7}Be targets, that need to be studied experimentally for a meaningful description of Big Bang nucleosynthesis. Test of NIF codes via comparison to Big Bang nucleosynthesis yields will be performed, and a possible NIF experiment as a test of Big Bang nucleosynthesis reactions will also be studied for feasibility.

Supernova Experiments Preparation for the National Ignition Facility

John Freddy Hansen   08-ERD-069

Abstract

An unanswered question in high-energy-density hydrodynamics is whether or not Kelvin–Helmholtz (KH) instability can be studied in a controlled fashion. A controlled KH instability experiment would be a valuable step towards demonstrating the ability to field a number of

science experiments on fusion-class lasers, including eventual supernova experiments on the National Ignition Facility. In this project, we will conduct KH instability and related supernova experiments on the Omega laser, leveraging LLNL's expertise in target design, simulation, diagnostics, and other fields. This project will be conducted in collaboration with the University of Michigan.

If successful, we will deliver an x-ray radiograph of a material's controlled KH instability rollup, demonstrating if hydrodynamics experiments can resolve multiple interspersed layers of materials that absorb or transmit x-rays, 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 KH instability is central to many hydrodynamic processes important to the Laboratory's stockpile stewardship efforts. 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 code.

FY08 Accomplishments and Results

We determined positively that KH instability can be studied in a controlled fashion under high-energy-density conditions. In collaboration with the University of Michigan, we conducted four shots at the Omega laser, producing spectacular KH instability x-ray radiographs showing well-resolved, multiple interspersed layers containing a wealth of physics information beyond expectations. Specifically, we discovered the transition to turbulence between 45 and 75 ns, a feature that may be a layer of material stripped away from the denser part of a KH instability rollup by turbulent mass stripping. We also observed, possibly for the first time, a transonic bubble—a region where the flow is locally supersonic in an otherwise subsonic environment—in a KH instability.

Proposed Work for FY09

In FY09 we will conduct further Omega experiments exploring the transition to turbulence and the unexpected and novel transonic bubble. For the former, we hope to complete a time series of x-ray radiographs showing a KH instability initially rolling up during the laminar period, then dispersing after transition to turbulence. For the latter, we hope to observe transonic bubbles by varying experimental parameters and observing a change to the bubble radius in a fashion consistent with transonic bubble theory.

Publications

Hurricane, O., et al., 2008. *A high-energy-density shock-driven Kelvin–Kelmholtz shear layer experiment.* 50th Ann. Mtg. American Physical Society Division of Plasma Physics, Dallas, TX, Nov. 17–20, 2008. LLNL-ABS-405184.

Micro-Targets for High-Energy-Density Physics: Three-Dimensional Simulations of Ultra-Intense Laser-Absorption Experiments

Scott C. Wilks   08-ERI-001

Abstract

Our objective is to design the highest temperature, solid-density laser targets to advance capabilities for equation-of-state and related experiments. We will optimize coupling of the laser energy to the target by varying not only the laser intensity and spot size, as is usually done, but also the target dimensions to allow for uniform heating of the solid. We will use a three-dimensional (3D) particle-in-cell (PIC) code to simulate, for the first time, an entire laser solid target in both space and time, relying solely on basic physics—Maxwell's equations, the Lorentz force, and a collisional and ionization model for particles on a submicron grid. We plan to obtain the most detailed and accurate account of laser-generated electron coupling to a target to date.

We expect this work to result in a well-defined, robust target design that can be used as a source for a variety of high-energy-density physics studies where a solid-density, hot (~1-keV) source is required. This would allow a new class of experiments to be performed that would add to the data base of equation of state for materials of interest. Our results also would extend to the basic physics of how hot electrons couple their energy to a solid. In addition, we hope to answer other important physics questions such as electron distribution (spatial and energy) from laser–matter interaction in 3D and how K-alpha production can be maximized.

Mission Relevance

High-energy-density physics lies at the heart of virtually all physics research at Lawrence Livermore, from inertial-confinement fusion to weapons-related research in support of both energy and national security. The ability to achieve ignition and to maintain a safe and reliable stockpile both require data on materials under extreme conditions for use in computer simulations. For this project, we are proposing to use computer simulation to design a new target that isochorically heats material to near-kilovolt temperatures to provide just such data.

FY08 Accomplishments and Results

In FY08, we (1) investigated enhancements to the energy conservation model, along with recent 3D radiation–hydrodynamics code results; (2) simulated an entire experiment with a 3D PIC code using ATLAS and compared the results with existing data; (3) gained insight into absorption and deposition of energy using our 3D PIC simulation; (4) used a 3D radiation-hydrodynamics code to study the effects of the inclusion of radiation for the highest energy cases; and (5) experimentally verified an important finding made through our simulations—that proton and ion acceleration efficiency increases dramatically in small targets, thus limiting the maximum achievable temperatures in small targets.

Proposed Work for FY09

In FY09, we will (1) design an algorithm for an electron source employing the PIC and HYDRA codes; (2) prepare a code script joining the two computer codes, using PIC as an "inline source" for HYDRA during the short-pulse laser phase; and (3) apply the coupled code to a reduced-mass target experiment and publish the results.

Publications

Chen, H., et al., 2007. *Angular distribution of fast electrons and protons in short-pulse laser–target interaction.* 49th Ann. Mtg. Am. Phys. Soc. Division of Plasma Physics, Orlando, FL, Nov. 12–16, 2007. UCRL-ABS-232921.

Kemp, A., 2007. *Laser heating of solid matter by light pressure-driven shocks at ultra-relativistic intensities.* 49th Ann. Mtg. Am. Phys. Soc. Division of Plasma Physics, Orlando, FL, Nov. 12–16, 2007. UCRL-PRES-236323.

Wilks, S. C., et al., 2007. *Isochoric heating of reduced-mass targets by ultra-intense lasers.* 49th Ann. Mtg. Am. Phys. Soc. Division of Plasma Physics, Orlando, FL, Nov. 12–16, 2007. UCRL-PRES-236325.

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 spectral broadening of the Compton scattered spectrum. Our approach combines the recently demonstrated x-ray scattering technique and K-alpha radiation produced with an 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 technique 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 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 importance to the Laboratory.

FY08 Accomplishments and Results

In FY08, we performed experiments at the Titan laser facility, and determined that the spectrally resolved scattering of ultrafast K-alpha x rays provided experimental validation of modeling of compression and heating of shocked matter. The elastic scattering component characterized the evolution and coalescence of two shocks launched by a nanosecond laser pulse into lithium hydride with unprecedented temporal resolution of 10 ps. At shock coalescence, we observed rapid heating and collective plasmon oscillations that indicate transition to the dense metallic plasma state. The plasmon frequency determines the material compression, which is found to be a factor of three consistent with independent experiments at Omega, thereby reaching conditions in the laboratory important for the study of the physics of planetary formation.

Proposed Work for FY09

In FY09, we will (1) combine the x-ray scattering experiments at LLNL's Titan laser with additional diagnostics of shock velocities to test equation-of-state modeling, (2) perform x-ray scattering with long-pulse-laser–produced x-ray backlighters from compressed beryllium on the Omega laser using coalescing shock waves to access high pressures and compression, (3) conduct cryogenic hydrogen target experiments, and (4) post-process the scattering spectra calculations to help define diagnostics requirements for the design of a K-alpha scattering experiment at the Advanced Radiographic Capability facility.

Publications

Garcia Saiz, E., et al., 2008. "Probing warm dense lithium by inelastic x-ray scattering." *Nat. Phys.* **10.1038**, 1103. LLNL-ABS-406742.

Kritcher, A., et al., 2008. "Ultrafast x-ray Thomson scattering of shock-compressed matter." *Science* **322**(5898), 69. LLNL-JRNL-404372.

Lee, H. J., et al., in press. "X-ray Thomson scattering measurements of density and temperature in shock-compressed beryllium." *Phys. Rev. Lett.* LLNL-JRNL-406683

Proton Fast Ignition

Pravesh K. Patel   08-ERI-004

Abstract

We will explore proton fast ignition, from its conceptual phase to proof-of-principle subscale demonstration experiments. We will perform systematic experiments on the 350-J Titan laser and the 5.2-kJ Omega Extended Performance laser 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. We will leverage extensive collaborations, which will also foster significant university use of LLNL laser facilities.

Through experiments and modeling, we will establish the feasibility of full-scale proton fast ignition. The outstanding physics issues we will resolve 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 hydro, 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 the Omega Extended Performance laser—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.

FY08 Accomplishments and Results

In FY08, we (1) performed experiments on the Titan laser to measure proton conversion efficiency as a function of pulse length, and to investigate optimization of the proton beam through the use of hydrated targets—focusing data was obtained using a new mesh technique to accurately measure the diameter and flux of the focused proton beam; (2) performed extensive Large Scale Plasma (LSP) simulations to model the experimental data, and prepared the results for publication; and (3) submitted a proposal and obtained time on the OMEGA Extended Performance laser to extend our proton-scaling measurements to laser intensities and pulse lengths relevant to fast ignition.

Proposed Work for FY09

In FY09 we will (1) perform proton-focusing experiments on Titan, (2) investigate scaling with pulse length and pre-plasma, (3) investigate variations on the standard hemispherical target design, (4) perform two-dimensional PIC and three-dimensional LSP simulations to benchmark conversion efficiency and focusing data from Titan, and (5) conduct shots on the Omega Extended Performance laser to extend these results to higher-intensity and longer-duration pulses, more closely replicating realistic fast-ignition laser conditions.

Publications

Chen, H., 2008. *High performance compact magnetic spectrometers for energetic ion and electron measurement in ultra intense short-pulse laser solid interactions.* 17th High Temperature Plasmas Diagnostics Conf., Albuquerque, NM, May 11–15, 2008. LLNL-ABS-401465.

MacPhee, A. G., in press. "Diagnostics for fast ignition science." *Rev. Sci. Instrum.* LLNL-CONF-403625.

MacPhee, A. G., 2008. *Plasma diagnostics for electron fast ignition ICF.* 17th High Temperature Plasmas Diagnostics Conf., Albuquerque, NM, May 11–15, 2008. LLNL-ABS-401698.
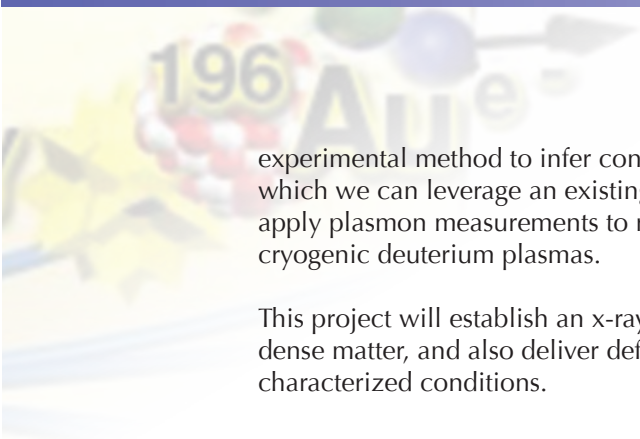
Offermann, D. T., 2008. *Observations of improvement in conversion efficiency to laser accelerated protons using Er-hydride coated targets.* American Physical Society April Mtg. and High Energy Density Physics and High Energy Density Laboratory Astrophysics Conf., St. Louis, MO, Apr. 11–15 2008. LLNL-ABS-401089.

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, performance of materials compressed by laser-driven foils, equation-of-state data such as obtained with the Purgatorio code, and primary weapon performance. Existing experimental data for comparisons with code predictions cannot be used to test theoretical calculations of conductivity in relevant regimes because they cannot access all relevant temperature–density regimes and lack independent and reliable diagnostics of these parameters. 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 aluminum plasmas. The proposed

experimental method to infer conductivities from plasmon spectra will be tested in a regime in which we can leverage an existing experimental and theoretical database. 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 also deliver definitive 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 definitive 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.

FY08 Accomplishments and Results

In FY08, we have (1) met all our proposed milestones and completed development of x-ray sources and scattering experiments at the Omega, Titan, Vulcan, and free electron laser in Hamburg; (2) demonstrated, from these experiments, plasmons and transitions to dense metallic plasmas in shocked matter; (3) succeeded in the first temperature measurements with detailed balance that are enabling direct calculation of Landau damping, which will be applied to plasmon measurements to determine collisions from broadening of the plasmon peak; and (4) identified a postdoctoral researcher to aid in our research.

Proposed Work for FY09

In FY09, we will perform two new experiments at the x-ray free electron laser with a new high-efficiency, high-resolution soft x-ray spectrometer. The goal is to measure plasmon from cryogenic hydrogen beam plasmas heated by an ultrashort-pulse laser beam. Dynamics will be measured by varying the pump-probe delay time. We will also continue to perform conductivity measurements on beryllium using the Omega laser. In addition, we will perform experiments at the Omega Extended Performance facility using K-alpha techniques. The plasmon broadening will be interpreted with calculations using various approximations for the dynamic collision frequency, and current conductivity models will be tested.

Publications

Garcia Saiz, E., et al., 2008. "Probing warm dense lithium by inelastic x-ray scattering." *Nat. Phys.* **10.1038**, 1103. 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., in press. "X-ray Thomson scattering measurements of density and temperature in shock-compressed beryllium." *Phys. Rev. Lett.* LLNL-JRNL-406683.

Zero-Order Phased Fiber Arrays

Michael J. 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 endeavors toward this goal employ methods that do not preserve the spectral properties of the constituent fibers and are thus not applicable to short-pulse lasers. 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 relative lengths to within a few wavelengths of each other, thus making a zero-order phased array. Our strategy for accomplishing this would open the door to joule-class pulsed-fiber sources and perhaps to novel applications such as resonant amplifiers for mode-locked pulse trains.

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 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 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.

FY08 Accomplishments and Results

In FY08 we developed temporal and spectral schemes for monitoring and controlling the lengths of a pair of fibers by developing radiofrequency-based techniques for measuring the length of independent amplifiers to within 1 ps. We then used piezoelectric–based actuators to stretch the fibers until their lengths were matched to within 40 μm. The latter was confirmed by verifying that the combined amplifier pair matched the 25-nm spectrum of the mode-locked oscillator that supplied them both. In addition, we put these techniques to use to successfully tune and measure the lengths of four amplifiers to within 1 ps.

Proposed Work for FY09

In FY09, we propose to demonstrate phasing of two 1-W broadband lasers to show that our broadband technique is applicable to modest-power lasers. In addition, we will demonstrate co-phasing and re-compression of two 10-nJ stretched-pulse amplifiers to show that broadband

phasing is viable for short-pulse lasers and can be used to scale pulse energies for future DOE endeavors to generate x and gamma rays.

Relativistic Electron–Positron Jets

Scott C. 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 laser. This project will leverage LLNL's laser diagnostics and is supported by a theory suggesting that choosing a special 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 testbed 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. This high-profile research will also help to recruit leading scientists in this cutting-edge field.

FY08 Accomplishments and Results

The proposed research exceeded our expectations in the first year. In FY08, we characterized the first dense relativistic electron–positron plasma jet ever created in a laboratory. We measured the directionality, number density, and energy spectrum of the jets. This accomplishment provides LLNL with a new testbed for exotic jets that were previously impossible to study in a laboratory setting. In addition, we performed calculations on positron focusing, which enabled us to determine the realistic number and energy of positrons obtained.

Proposed Work for FY09

We will (1) analyze electron and positron data from both TITAN and Omega Extended Performance laser shots; (2) compare the experimental results with theoretical predictions;

(3) field high-energy bremsstrahlung and annihilation radiation detectors for first time on TITAN to measure high-energy x-rays, deduce the expected number of pairs, and compare our predictions with the measured positron creation rate as determined by the spectrometer; (4) conduct simulations of dense jets interacting with low-density foams to study shock formation related to proposed gamma-ray burst mechanisms; and (5) scale TITAN and Omega Extended Performance laser results to a pair experiment on the National Ignition Facility's Advanced Radiographic Capability.

Publications

Chen, H., et al., in press. "Relativistic positron creation using ultra intense short pulse lasers." *Phys. Rev. Lett.* LLNL-JRNL-406720.

Plasma Waveguide for Electron Acceleration

Dustin H. 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.

FY08 Accomplishments and Results

We have met our FY08 proposed objectives by (1) demonstrating a 20-cm long external magnetic field, (2) expanding our plasma target to be compatible with a 20-cm long experiment, and (3) producing a multiple-centimeter-long low-density channel.

Proposed Work for FY09

Our objective in FY09 is to demonstrate a 5-cm-long density channel suitable to guide a 200-TW laser at conditions to produce a multiple-gigaelectronvolt electron beam (where electron density is equal to 10^{18} cm^{-3}). Specifically, we will use the HYDRA code along with initial experimental results to extend the B-field, the gas target, and the intensity of the laser beam at the necessary conditions to produce a 5-cm-long channel for laser wakefield acceleration.

Publications

Froula, D. H., et al., 2008. *Laser wakefield acceleration at Lawrence Livermore National Laboratory*. 13th Advanced Accelerator Concepts Workshop, Santa Cruz, CA, July 27–Aug. 2, 2008. LLNL-ABS-404985.

Froula, D. H., et al., 2009. "Magnetically controlled plasma waveguide for laser wakefield acceleration." *Plasma Phys. Control. Fusion* **51**, 024009. LLNL-JRNL-403962.

Leurent, V., et al., 2008. *Measurement of x-ray betatron radiation from a laser wakefield accelerator.* 13th Advanced Accelerator Concepts Workshop, Santa Cruz, CA, July 27–Aug. 2, 2008. LLNL-PROC-406432.

Leurent, V., et al., 2008. *Ultra-short x-ray radiation coming from a laser wakefield accelerator.* 13th Advanced Accelerator Concepts Workshop, Santa Cruz, CA, July 27–Aug. 2, 2008. LLNL-ABS-404984.

Pollock, B. B., et al., 2008. *Magnetically controlled optical plasma waveguide for electron acceleration.* 13th Advanced Accelerator Concepts Workshop, Santa Cruz, CA, July 27–Aug. 2, 2008. LLNL-ABS-404976.

Pollock, B. B., et al., 2008. "Multicentimeter long high density magnetic plasmas for optical guiding." *Rev. Sci. Instrum.* **79**(10), 10F550. LLNL-CONF-403602.