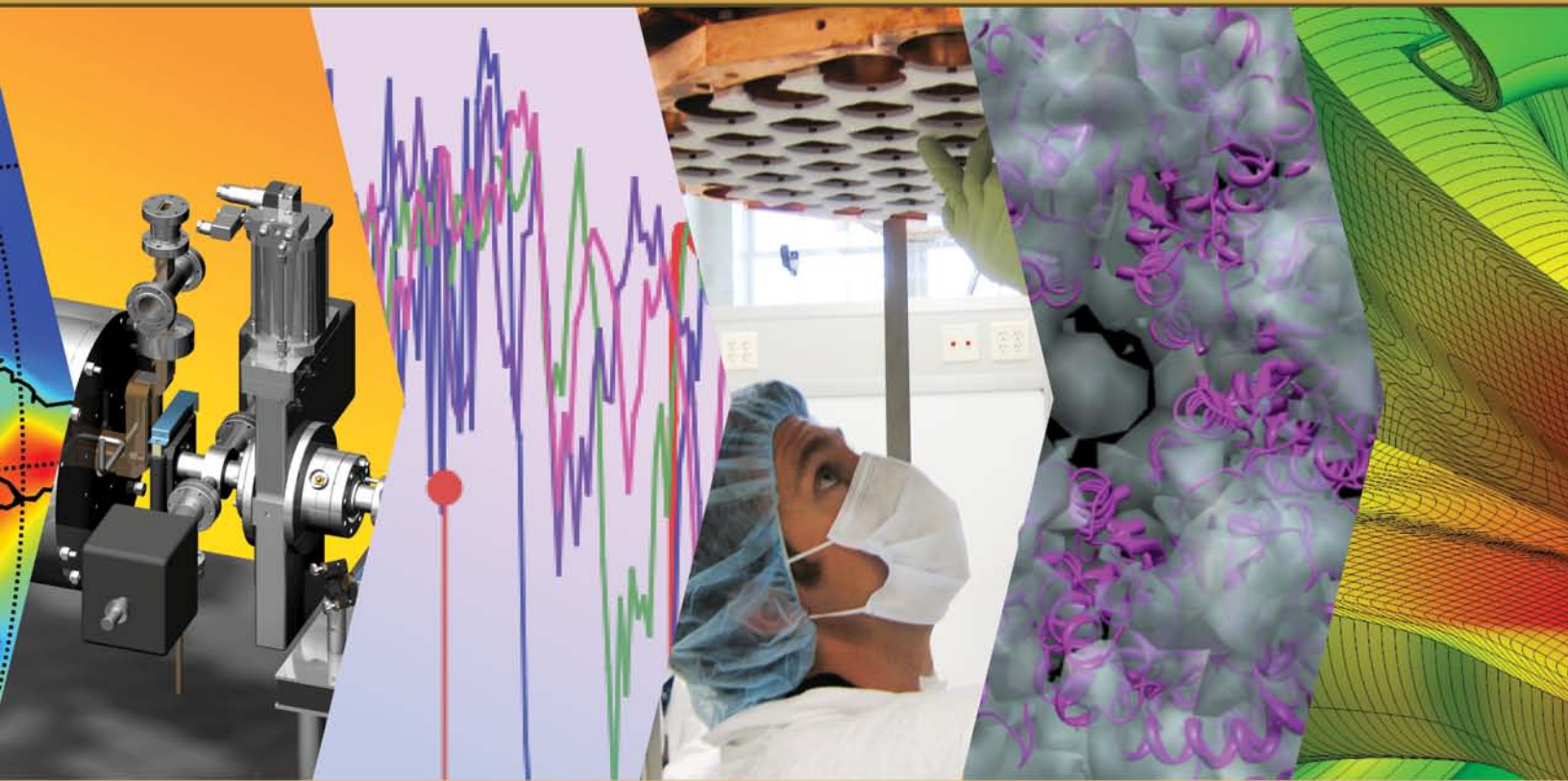


FY2010

LABORATORY DIRECTED RESEARCH AND DEVELOPMENT



ANNUAL REPORT

Lawrence Livermore National Laboratory



About the Cover:

Laboratory Directed Research and Development 2010 projects depicted on the back and front covers (left to right): "New Algorithms to Scale Domain Decomposition Up to BlueGene Architectures," David Hysom (08-ERD-014); "Strain-Rate Effects on Plasticity and Defects," James Hawreliak (08-ERD-033); "High-Temperature Thermal X-Radiation Sources at Short-Pulse Lasers," Marilyn Schneider (08-ERD-024); "Collection of Refractory Debris from the National Ignition Facility for Stewardship-Relevant Measurements," Dawn Shaughnessy (09-ERD-026); "The Advance of Uncertainty Quantification Science," Richard Klein (10-SI-013); "Precision Mono-Energetic Gamma-Ray Science for NNSA Missions," Christopher Barty (09-SI-004); "Advanced Computational and Experimental Analysis of Plasma Equations of State and Transport," Brian Wilson (08-ERD-027); "Advanced Rare-Event Detectors for Nuclear Science and Security," Adam Bernstein (10-SI-015); "Coupling Advanced Cryo-Electron Microscopy with High-Performance Computing to Resolve Biomolecular Function," Felice Lightstone (09-ERD-009); and "Modern Finite Elements for Lagrangian Hydrodynamics," Tzanio Kolev (09-ERD-034).

UCRL-TR-113717-10

Available to DOE and DOE contractors from the
Office of Scientific and Technical Information
P.O. Box 62
Oak Ridge, TN 37831

Prices available from (423) 576-8401
<http://www.osti.gov/bridge/>

Available to the public from the
National Technical Information Service
U.S. Department of Commerce
5285 Port Royal Rd.
Springfield, VA 22161
<http://www.ntis.gov/>

or

Lawrence Livermore National Laboratory
Technical Information Department Digital Library
<https://library-ext.llnl.gov/>

Disclaimer

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

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Acknowledgments

The Laboratory Directed Research and Development Program extends its sincere appreciation to the principal investigators of fiscal year 2010 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: Barbara Jackson, administrator; Nancy Campos, database manager; Steve McNamara, computer specialist; and Kristen Croteau, resource manager. We extend particular thanks to Judith Kammeraad, who successfully directed the LDRD Program in 2010, as well as for the two previous years.

Scientific Editors: Kenneth Jackson, Paul Chrzanowski, Rob Sharpe

Publication Editors: Jeffrey Sketchley, Paul Kotta

Proofreader: Karen Kline

Publication Designer: Lucy Dobson

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 \$88.7 million for fiscal year 2010 sponsored 146 projects. These projects were selected through an extensive review process to ensure the highest scientific quality and mission relevance. Each year, the number of deserving proposals far exceeds the funding available, making the selection a tough one indeed.

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

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



George Miller, Director

Contents

About Lawrence Livermore National Laboratory.....	2
About the FY 2010 Laboratory Directed Research and Development Annual Report.....	3
Program Overview—Innovation for Our Nation	4
Structure of the LDRD Program	5
The LDRD 2010 Portfolio	6
Highlights of 2010 LDRD Accomplishments.....	8
LDRD Metrics.....	17
Awards and Recognition.....	19

Advanced Sensors and Instrumentation

Broadband Heterodyne Infrared Spectrometer: A Path to Quantum Noise-Limited Performance— Joseph Tringe (08-ERD-016)	30
Tracing the Shadows of Planetary Systems—Bruce Macintosh (08-ERD-043)	31
Point-of-Care Diagnostic for Foot-and-Mouth Disease Virus—Jane Bearinger (08-ERD-044).....	32
Cadmium–Zinc–Telluride Sandwich Detectors for Gamma Radiation—Adam Conway (08-ERD-051)	33
Hybridization, Regeneration, and Selective Release of DNA Microarrays— Elizabeth Wheeler (08-ERD-064)	34
Optimized Volumetric Scanning for X-Ray Area Sources—Angela Foudray (09-ERD-045)	35
Superimposed Plasmonic and Photonic Detection Platform—Sarah Baker (09-LW-003).....	36
Antibiotic Heteroresistance in Methicillin-Resistant <i>Staphylococcus Aureus</i> : Microchemostat Studies at the Single-Cell Level—Raymond Lenhoff (09-LW-112)	38
Real-Time Space Situational Awareness—Scot Olivier (10-SI-007)	39
Compact, Efficient Lasers for Inertial Fusion–Fission Energy—Robert Deri (10-SI-010)	40
Embedded Sensors for Monitoring Complex Systems—Jack Kotovsky (10-ERD-043)	42

Passive, Standoff Detector of High-Density Masses with a Gravity Gradiometer Based on Atom Interferometry—Stephen Libby (10-FS-003).....	43
--	----

Biological Sciences

A New Selectable Marker System for Genetic Studies of Select-Agent Pathogens— Brent Segelke (08-ERD-002)	46
The Elegant Molecular Syringe: Characterizing the Injectisome of the <i>Yersinia pestis</i> Type III Secretion System—Brett Chromy (08-ERD-020)	46
Viability-Based Detection Methods for Pathogens in Complex Environmental Samples— Staci Kane (08-ERD-025)	47
Important Modes to Drive Protein Molecular-Dynamics Simulations to the Next Conformational Level— Babak Sadigh (08-ERD-037)	48
New Molecular Probes and Catalysts for Bioenergy Research—Michael Thelen (08-ERD-071)	49
Coupling Advanced Cryo-Electron Microscopy with High-Performance Computing to Resolve Biomolecular Function—Felice Lightstone (09-ERD-009).....	50
Flexible and Rapid Therapeutic Countermeasures for Global Biosecurity— Jane Bearinger (09-ERD-054)	51
Biological Testing of Systems Biology: Validation of Flux-Balance Analysis Predictions— Benjamin Stewart (09-ERI-002)	53
The Role of Dendritic Cells in Tularemia Pathogenesis—Sahar El-Etr (09-LW-036).....	54
Effect of Aging on Chondrocyte Function—Gabriela Loots (09-LW-072)	55
Versatile Delivery and Immune-Stimulatory Platform for Just-in-Time Vaccine Development— Craig Blanchette (09-LW-077).....	56
Genomics of Cell-to-Cell Communication: Identification of DNA Sensors in Humans— Gabriela Loots (10-ERD-020).....	57
Understanding the Role of Virus Evolution in Interspecies Transmission Events— Monica Borucki (10-LW-020).....	58
Establishing Cancer Stem Cell Longevity and Metastatic Potential—Bruce Buchholz (10-LW-033)	59
Radiation Biodosimetry Using Loop-Mediated Isothermal Amplification—Paul Wilson (10-LW-041).....	60

Chemistry

The Viral Discovery Platform—Christopher Bailey (08-SI-002)	64
Rapid Radiochemical Separations for Investigating Chemistry of the Heaviest Elements— Dawn Shaughnessy (08-ERD-030)	65
Probing the Organization of the Cell Membrane—Peter Weber (08-LW-015)	67
Nuclear Forensics: An Integrated Approach for Rapid Response—Ian Hutcheon (10-SI-016).....	68
Microbes and Minerals: Imaging Carbon Stabilization—Jennifer Pett-Ridge (10-ERD-021)	70

Earth and Space Sciences

Coordinated Analysis of Geographic Indicators for Nuclear-Forensic Route Attribution— M. Lee Davisson (08-ERD-065).....	74
Improving Atmospheric Flow Prediction at Intermediate Scales—Jeffrey Mirocha (09-ERD-038)	75
Mapping Patterns of Past Drought in California: Late-Holocene Lake Sediments as Model Diagnostics— Susan Zimmerman (09-ERI-003)	76
Stardust Science: Nanoscale Analytical Studies of Materials—John Bradley (09-ERI-004).....	77
Natural Perchlorate in Groundwater: Source, Formation Mechanisms, and Fate— Darren Hillegonds (09-LW-104).....	79
An Adaptive, Coupled Regional Climate and Hydrologic Modeling System for Accurate Wind-Power and Water-Resource Simulation—Carol Woodward (10-ERD-011).....	80
Enhancing Climate Model Diagnosis and Intercomparison—Karl Taylor (10-ERD-060)	81

Energy Supply and Use

Fossil-Fuel Emission Verification Capability—Thomas Guilderson (07-ERD-064)	84
Direct Simulation of Dynamic Fracturing during Carbon Storage and Prediction of Potential Storage Failures—Scott Johnson (08-ERD-039)	85
A Hydrogen–Oxygen–Argon Internal Combustion Engine System: The Mechanical Equivalent of a Fuel Cell—Salvador Aceves (08-ERD-042)	86
Toward More Intrinsically Secure Nuclear Fuel Cycles—Keith Bradley (08-ERD-056)	88

Dynamic Chamber Processes for LIFE: Simulations and Experiments on Beam Propagation and Chamber Clearing—Jeffery Latkowski (10-SI-009)	88
Design of Novel Catalysts to Capture Carbon Dioxide—Roger Aines (10-ERD-035).....	90
Prediction of Underground Coal Gasification Cavity Growth, Coal Conversion, and Geophysical Signatures—David Camp (10-ERD-055)	92

Engineering and Manufacturing Processes

High-Resolution Projection Microstereolithography for Advanced Target Fabrication—Christopher Spadaccini (08-ERD-053)	96
Enabling Transparent Ceramic Optics and Advanced Armor with Nanostructured Materials Tailored in Three Dimensions—Klint Rose (09-ERD-029).....	97
Maskless, Low-Cost, High-Performance Polymer Waveguides—Eric Duoss (09-ERD-057).....	98
Novel Separation of Actinides—Raymond Mariella (10-FS-001).....	99

Materials Science and Technology

Nanomaterials for Fusion Application Targets—Alex Hamza (08-SI-004)	102
Dynamics of Material Motion and Transformation following Localized Laser-Energy Deposition in Transparent Dielectrics—Stavros Demos (08-ERD-001).....	104
Fundamental Mechanisms Driving the Amorphous-to-Crystalline Phase Transformation—Nigel Browning (08-ERD-032)	105
Strain-Rate Effects on Plasticity and Defects—James Hawreliak (08-ERD-033)	107
New Physical Mechanisms for Next-Generation Fusion-Laser Dynamic Sensors and Diagnostics—Michael Armstrong (08-ERD-034)	108
Do Brittle Metals Change Character under Extreme Shock Conditions?—Damian Swift (08-ERD-038)	110
Chemical and Structural Modification and Figure Control during Glass Polishing—Tayyab Suratwala (08-ERD-055).....	111
Physics of Local Reinitiation and Morphological Evolution of Mitigated Sites for Ultraviolet Optics—Manyalibo Matthews (08-ERD-057)	113

Radiation-Tolerant Materials—Michael Fluss (09-SI-003)	115
Nanosecond Characterization of Dynamic Void Evolution in Porous Materials— Anthony Van Buuren (09-ERD-002)	118
Understanding the Surface Properties That Lead to Optical Degradation in High-Fluence, High-Average-Power Optical Materials—Jeffrey Bude (09-ERD-003).....	119
Multi-Resolution Adaptive Monte Carlo for Microstructure Simulations—Vasily Bulatov (09-ERD-005)	121
Collection of Refractory Debris from the National Ignition Facility for Stewardship-Relevant Measurements—Dawn Shaughnessy (09-ERD-026)	122
Magnetorheological Finishing for Large-Aperture High-Fluence Optical Applications— Joseph Menapace (09-ERD-049)	124
Characterization of Tritium Uptake and Release by Inertial-Confinement Fusion Reactor Materials— James Fair (09-ERD-050).....	125
Methods for Mitigation of Damage to Multilayer Mirrors—Christopher Stolz (09-ERD-051)	126
Biomolecule-Directed Synthesis of Highly Ordered, Nanostructured Porous Zinc Oxide— Thomas Han (09-LW-024).....	127
Direct Observation of Phase Transformations and Twinning under Extreme Conditions: In Situ Measurements at the Crystal Scale—Joel Bernier (10-ERD-053)	128
Material–Coolant Interactions in Fusion Reactors—Joseph Farmer (10-ERD-056)	129
Thermodynamic and Kinetic Modeling of Advanced Nuclear Fuels—Patrice Erne Turchi (10-ERD-059)	131
Development of High-Performance Lead-Free Solders for Microelectronics and Semiconductor Applications—John Elmer (10-LW-002).....	132
In Situ Spectroscopy and Microscopy for the Study of Advanced Materials for Energy Storage— Jonathan R. Lee (10-LW-045)	133

Mathematics and Computing Sciences

Storage-Intensive Supercomputing—Maya Gokhale (07-ERD-063).....	138
New Algorithms to Scale Domain Decomposition Up to BlueGene Architectures— David Hysom (08-ERD-014)	139

Robust Ensemble Classifier Methods for Detection Problems with Unequal and Evolving Error Costs— Barry Chen (08-ERD-022)	140
Enhanced Event Extraction from Text Via Error-Driven Aggregation Methodologies— Tracy Lemmond (08-ERD-023)	141
Scalable Methods for Discrete-Ordinate Transport Algorithms on Massively Parallel Architectures— Robert Falgout (08-ERD-026)	143
Efficient Numerical Algorithms for Vlasov Simulation of Laser-Plasma Interactions— Jeffrey Hittinger (08-ERD-031)	144
Understanding Viral Quasi-Species Evolution through Computation and Experiment— Carol Zhou (08-ERD-036)	145
Supercomputing-Enabled Transformational Analytics Capability (SETAC)— Celeste Matarazzo (09-SI-013)	146
Quantitative Analysis of Vector Field Topology—Peer-Timo Bremer (09-ERD-014)	148
Rapid Exploitation and Analysis of Documents—David Buttler (09-ERD-017)	150
Adding Validation and Novel Multiphysics Capabilities to the First-Principles Molecular Dynamics Qbox Code—Erik Draeger (09-ERD-019)	150
Role Discovery in Dynamic Semantic Graphs—Tina Eliassi-Rad (09-ERD-021)	151
Modern Finite Elements for Lagrangian Hydrodynamics—Tzanio Kolev (09-ERD-034)	153
Lagrange Multiplier Embedded-Mesh Method—Michael Puso (09-ERD-044)	155
Towards Understanding Higher-Adaptive Systems—Brenda Ng (09-LW-030)	156
The Advance of Uncertainty Quantification Science—Richard Klein (10-SI-013)	158
ExaCT: Exascale Computing Technologies—Bronis de Supinski (10-SI-014)	160
Parallel Discrete-Event Simulation of Cyber Attack and Defense Scenarios and Automated Rollback Code Generation—David Jefferson (10-ERD-025)	162
CgWind: A Parallel, High-Order Accurate Simulation Tool for Wind Turbines and Wind Farms— William Henshaw (10-ERD-027)	164
Binary Analysis—Daniel Quinlan (10-ERD-039)	165
Uncertainty Visualization—Peter Lindstrom (10-ERD-040)	166

M3Net: Taxonomy Construction and Topic Mapping for Multimedia Message Manager Traffic— Douglas Poland (10-ERD-041)	167
Eigensolvers for Large-Scale Graph Problems—Van Henson (10-ERD-054)	168

Nuclear Science and Engineering

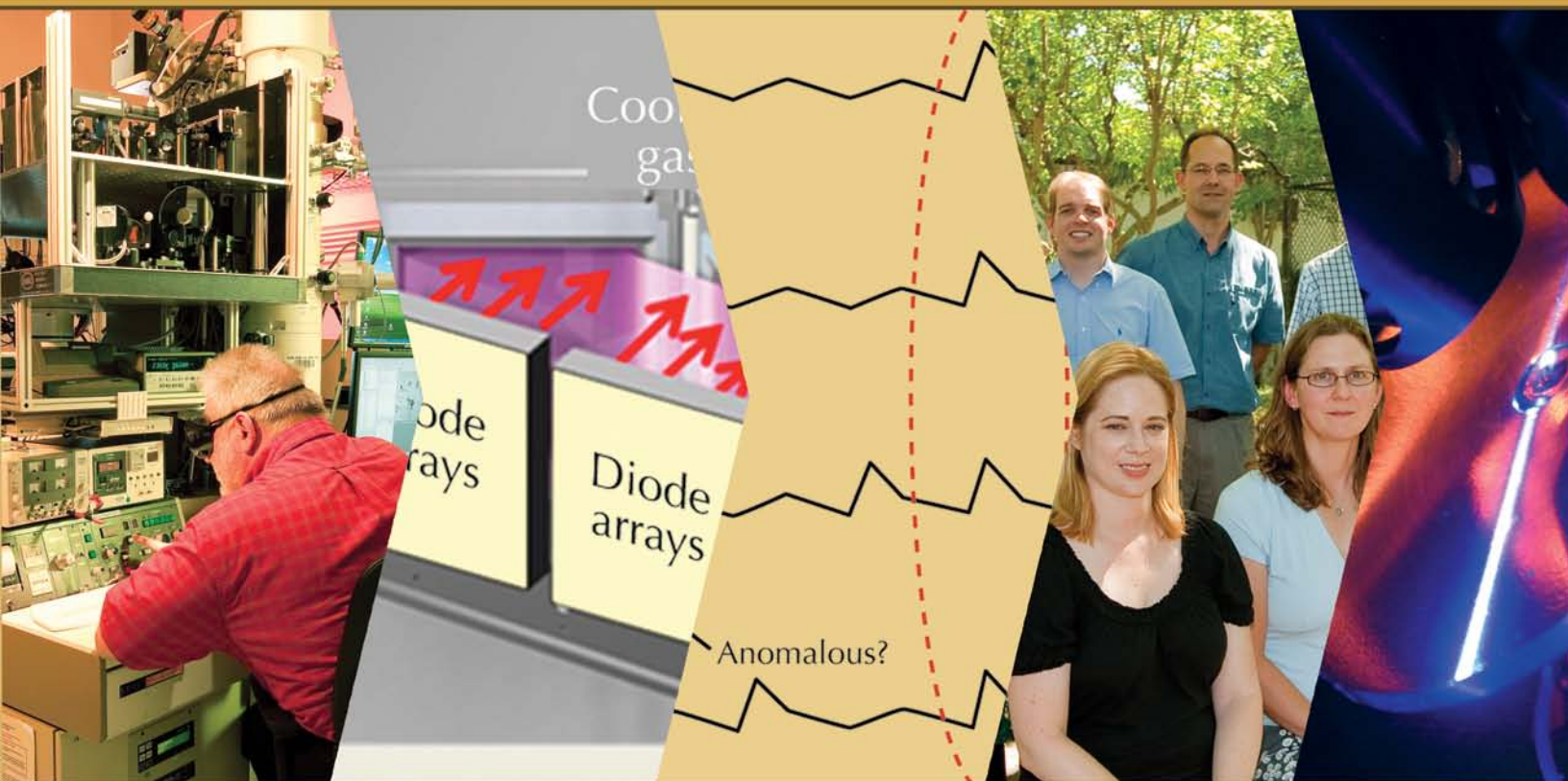
Detection, Classification, and Estimation of Radioactive Contraband from Uncertain, Low-Count Measurements—James Candy (07-ERD-019)	172
How Carbon and Oxygen Can Be Made in Stars: An Ab Initio Approach to Nuclear Reactions— Petr Navratil (09-ERD-020)	174
Shock Temperatures from Neutron Resonance Spectroscopy—James McNaney (09-ERD-037)	175

Physics

Fast-Ignition Proof-of-Principle Experiments—Pravesh Patel (08-SI-001)	178
Nonequilibrium Electron Dynamics in Warm Dense Matter—Yuan Ping (08-ERD-005)	181
Studying Reactions of Excited Nuclear States—Lee Bernstein (08-ERD-008)	182
Exploration of Laser-Plasma Interactions for High-Performance Laser-Fusion Targets— David Strozzi (08-ERD-017)	184
Innovative Divertors for Future Fusion Devices—Dmitri Ryutov (08-ERD-019)	185
High-Temperature Thermal X-Radiation Sources at Short-Pulse Lasers— Marilyn Schneider (08-ERD-024)	187
Advanced Computational and Experimental Analysis of Plasma Equations of State and Transport— Brian Wilson (08-ERD-027)	188
Impurity and Alloying Effects on Material Strength from First Principles—Robert Rudd (08-ERD-035)	189
Analysis of Plasma Microturbulence Simulations in Three Dimensions Plus Time— William Nevins (08-ERD-048)	190
Cryogenic Bolometers for Double-Beta Decay Experiments—Nicholas Scielzo (08-ERD-049)	191
Partition-of-Unity Finite-Element Method for Large-Scale Quantum Molecular Dynamics on Massively Parallel Computational Platforms—John Pask (08-ERD-052)	193

Measurement and Prediction of Laser-Induced Damage in the Presence of Multiple Simultaneous Wavelengths—Mike Nostrand (08-ERD-054)	194
Mesoscale Studies of Hydrodynamic Instability Growth in the Presence of Electric and Magnetic Fields—Peter Amendt (08-ERD-062)	195
Nuclear Astrophysics at the National Ignition Facility: Feasibility of Studying Reactions of the Stars on Earth—Richard Boyd (08-ERD-066)	196
Study of Kelvin–Helmholtz Instability in High-Energy-Density Hydrodynamic Processes—Hye-Sook Park (08-ERD-069)	198
X-Ray Scattering on Compressed Matter—Siegfried Glenzer (08-ERI-002)	199
Proton Fast Ignition—Pravesh Patel (08-ERI-004)	201
Plasma Waveguide for Electron Acceleration—Laurent Divol (08-LW-070)	202
Precision Mono-Energetic Gamma-Ray Science for NNSA Missions—Christopher Barty (09-SI-004)	203
Physics and Chemistry of the Interiors of Large Planets: A New Generation of Condensed Matter—Gilbert Collins (09-SI-005)	207
From Super-Earths to Nucleosynthesis: Probing Extreme High-Energy-Density States of Matter with X Rays—Bruce Remington (09-SI-010)	209
The Microphysics of Burning, Hot Dense Radiative Plasmas—Frank Graziani (09-SI-011)	210
Improved Spectral Line-Shape Models for Opacity Calculations—Carlos Iglesias (09-ERD-004)	212
First-Principles Planetary Science—Kyle Caspersen (09-ERD-012)	213
Imaging X-Ray Line-Shape Diagnostic for Burning Plasmas—Peter Beiersdorfer (09-ERD-016)	213
Ultrafast Nanoscale Dynamic Imaging Using X-Ray Free-Electron Lasers—Stefan Hau-Riege (09-ERD-023)	215
Scrape-Off-Layer Flow Studies in Tokamaks—Thomas Rognlien (09-ERD-025)	217
Understanding the Initiation of High-Voltage Vacuum Insulator Flashover—Timothy Houck (09-ERD-028)	218
Critical Enabling Issues for Burning-Plasma Diagnostics—Steven Allen (09-ERD-030)	219

Experimental Determination of Dense Plasma Effects on Bound States in Extreme States of Matter— Ronnie Shepherd (09-ERD-032).....	220
Uses of Ignition at the National Ignition Facility—L. John Perkins (09-ERD-036).....	221
Arc Initiation of High Explosives—James McCarrick (09-ERD-042).....	223
An Atomic Inner-Shell X-Ray Laser Pumped by the Linac Coherent Light Source— Nina Rohringer (09-LW-044)	224
Direct Search for Decay of the Thorium-229 Nuclear Isomer—Jason Burke (09-LW-061).....	226
Investigation of Short-Pulse Laser-Pumped Gamma-Ray Lasers—Ronnie Shepherd (09-LW-080).....	227
Science and Technology of Unconventional Fiber Waveguides for Emerging Laser Missions— Jay Dawson (10-SI-006)	228
Advanced Rare-Event Detectors for Nuclear Science and Security—Adam Bernstein (10-SI-015).....	229
Mix at the Atomic Scale—Paul Miller (10-ERD-004)	230
High-Gradient Inverse Free-Electron Laser Accelerator—Scott Anderson (10-ERD-026)	231
Modeling and Measuring Quark–Gluon Plasma Shock Waves—Ron Soltz (10-ERD-029)	233
Unlocking the Universe with High-Performance Computing—Pavlos Vranas (10-ERD-033)	234
Discovery and Synthesis of Materials for High-Energy-Density Science—Stanimir Bonev (10-ERD-038)	236
An Intense Laser-Based Positron Source—Scott Wilks (10-ERD-044).....	237
Multiscale Polymer Flows and Drag Reduction—Todd Weisgraber (10-ERD-057)	238
Fundamental Research in Advanced Quantum Simulation Algorithms—Jonathan DuBois (10-ERD-058)	239
Feasibility of a Hybrid Rubidium Resonance and Exciplex Pump Laser—Raymond Beach (10-FS-002).....	240
Feasibility of Diode-Laser Array as Surrogate Source for Laser Lethality Studies— W. Howard Lowdermilk (10-FS-004)	241
Suppressing Counterflow Turbulence with a Shear-Thickening Agent—Peter Beiersdorfer (10-FS-005)	242



Overview

About Lawrence Livermore National Laboratory

A premier applied-science laboratory, Lawrence Livermore National 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, military operations, and missile defense, for example—that evolve in response to emerging

threats. For broader national needs, LLNL executes programs in energy security, climate change and long-term energy needs, environmental assessment and management, bioscience and technology to improve human health, and for 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 Department of Energy (DOE)/National Nuclear Security Administration (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.

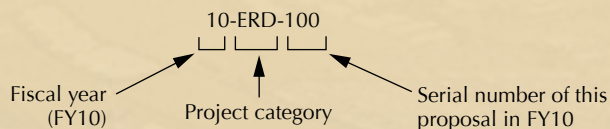
About the FY 2010 Laboratory Directed Research and Development Annual Report

The Laboratory Directed Research and Development (LDRD) annual report for fiscal year 2010 (FY10) 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 some highlights of accomplishments and awards for the year.

Project Summaries: A summary of each project, submitted by the principal investigator. Project summaries include the scope, motivation, goals, relevance to DOE/NNSA and LLNL mission areas, the technical progress achieved in FY10, and a list of publications that resulted from the research.

Summaries are organized in sections by research category (in alphabetical order), and within each research category projects appear for the various project categories: Strategic Initiative (SI), Exploratory Research (ER), Laboratory-Wide Competition (LW), and Feasibility Study (FS). Each project is assigned a unique tracking code—an identifier that consists of three elements. The first is the fiscal year the project began, the second represents the project category, and the third identifies the serial number of the proposal for that fiscal year. For example:



Program Overview— Innovation for Our Nation

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 in 2010, Laboratory Director George Miller and the Chief Research and Development Officer Tomás Díaz de la Rubia were responsible for the LDRD Program. Execution of the program was delegated to the director of the Institutional Science and Technology Office, Judith Kammeraad. The LDRD Program at LLNL is in compliance with DOE Order 413.2B and other relevant DOE orders and guidelines.

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

Strategic Context for the LDRD Portfolio

The FY10 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 2009, the Laboratory director called for the development of a new strategic roadmap that sets institutional strategic goals and identifies science and technology needs in selected mission focus areas, in fundamental research, and in critical science, technology, and engineering capabilities. *The Roadmap to the Future* was developed by multidisciplinary teams under the guidance of the Chief Research and Development Officer. This document set the strategic context for the LDRD competition for five years, starting in 2009. As a living document, it will be updated annually to respond to our ever-changing mission needs. Further strategic context is provided by the 2006 U.S. Department of Energy Strategic Plan² and by the NNSA mission.³ The DOE strategic plan articulates strategic themes for achieving the DOE mission of discovering solutions to power and secure America's future. In FY10, the Laboratory's LDRD Program strongly supported 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.

² 2006 U.S. Department of Energy Strategic Plan. <<http://science.energy.gov/~media/fes/pdf/International%20Activities/2006-DOE-Strategic-Plan.pdf>> (retrieved March 31, 2011).

³ *Our Mission: National Nuclear Security Administration* <<http://nnsa.energy.gov/ourmission>> (retrieved March 31, 2011).

4. **Environmental Responsibility**—Protecting the environment by providing a responsible resolution to the environmental legacy of nuclear weapons production.

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

Mission Focus Areas

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

Science, Technology, and Engineering Pillars

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

The DOE and NNSA oversee the Laboratory's LDRD Program to ensure that it accomplishes its objectives. This oversight includes field and headquarters reviews of both the technical content and management processes. The value of LDRD to DOE as well as to the country is evidenced in the DOE 2008 report to 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 Laboratory-Wide (LW) competition. During the year, the LDRD Program also funds a few projects in a fourth category, Feasibility Study/Project Definition (FS).

Strategic Initiative

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

Exploratory Research

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

⁴ Department of Energy (DOE) FY 2008 Report to Congress—Laboratory Directed Research and Development (LDRD) at the DOE National Laboratories. <<http://www.mbe.doe.gov/cf1-2/ldrld.htm>> (retrieved March 24, 2011).

Laboratory-Wide Competition

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

Feasibility Study/Project Definition

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

Project Competency Areas

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

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

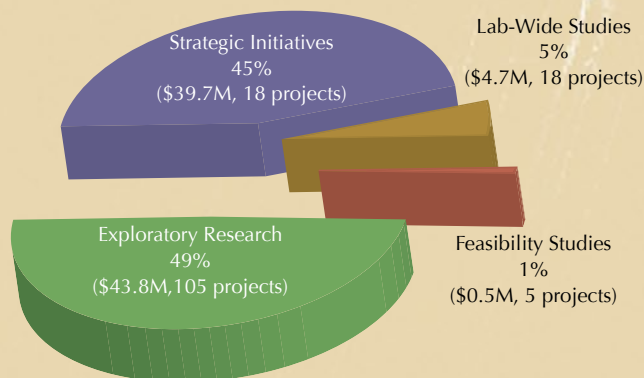
The LDRD 2010 Portfolio

Portfolio Overview

The FY10 LDRD portfolio was carefully structured to continue the LDRD Program's vigorous support for the strategic vision and long-term goals of DOE, NNSA, and LLNL. The projects described in this annual report underwent a stringent peer-reviewed

selection process and received ongoing management oversight.

In FY10 the LDRD Program funded 146 projects with a total budget of \$88.7M. The distribution of funding among the LDRD project categories is shown in the following pie chart.



Distribution of funding among the LDRD project categories. Total funding for FY10 was \$88.7M.

Strategic Initiative

In FY10, the LDRD Program funded 18 SI projects. Although the SI category represented only about 12% of the total number of LDRD projects for FY10, it accounted for nearly 45% of the budget. SI projects ranged in funding from \$1.3M to \$5.4M.

Exploratory Research

The LDRD Program funded 105 ER projects for FY10. The largest project category, ERs accounted for 72% of the number of LDRD projects and just over 49% of the budget for the fiscal year. Projects in this year's ER category ranged in budget from \$70K to \$2.1M.

Laboratory-Wide Competition

In FY10, 18 LW projects were funded, which represent about 12% of the LDRD projects for the year and slightly over 5% of the budget. The LW projects for FY10 ranged in funding from \$70K to \$338K.

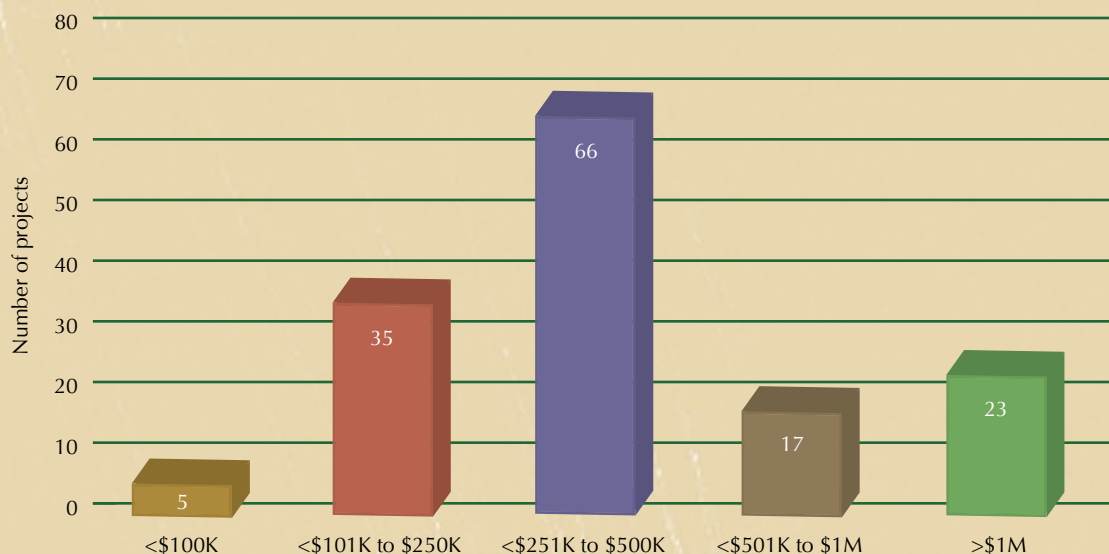
Feasibility Study

The LDRD Program funded just 5 FS projects in FY10, which represent just over 3% of the LDRD projects for the year and under 1% of the budget. The FS projects for FY10 ranged in funding from \$50K to \$125K.

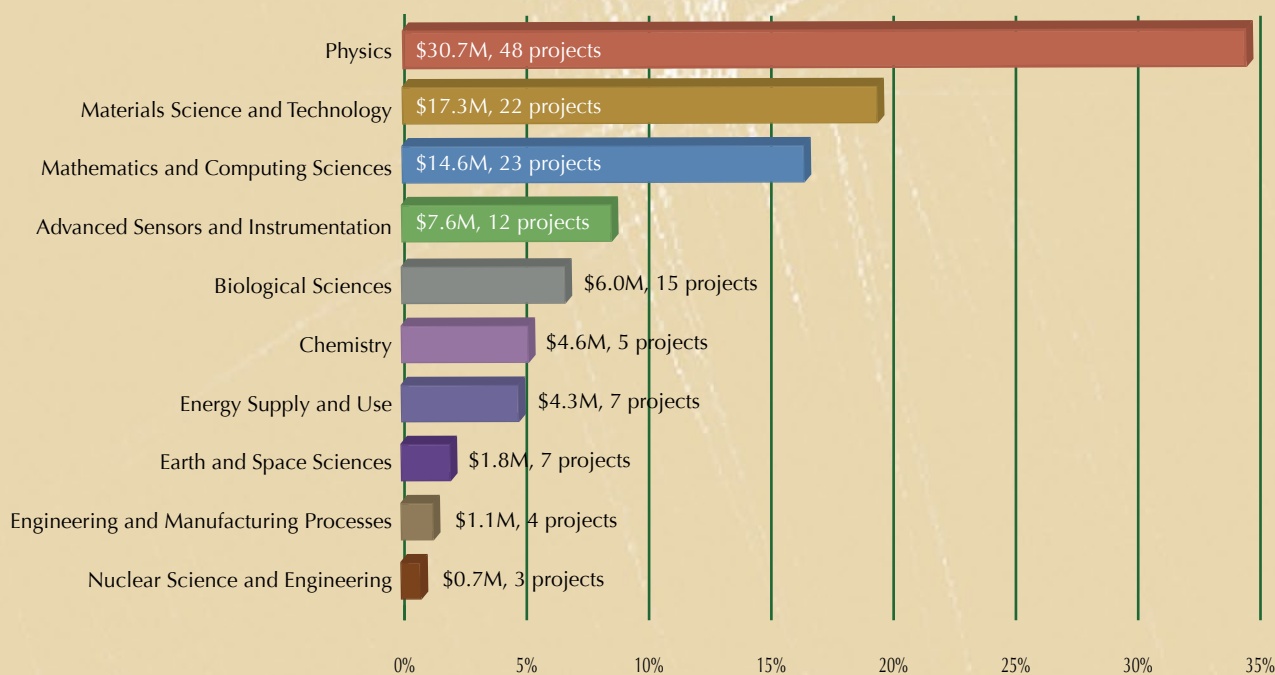
The following bar chart shows the funding distribution by dollar amount for the 146 FY10 projects—69% of the projects were in the \$101K to \$500K range, with a little over 3% falling below \$100K. Projects in the \$501K to \$1M funding range accounted for just under 12% of the total, and

another 16% of the projects received more than \$1M. The average funding level for the 146 projects was about \$607K.

The percentage of LDRD funding and number of projects in each research category for FY10 are shown in the bottom bar chart.



Number of projects and levels of funding. The average funding level for an LDRD project in FY10 was \$607K.



Percentage of LDRD funding and number of projects in each research category in FY10.

Highlights of 2010 LDRD Accomplishments

In FY10, the LDRD Program at LLNL continued to be extremely successful in achieving its goals of scientific discovery, providing new concepts for core missions, and creating an exciting research environment that attracts outstanding young talent to the Laboratory. Below is a selection of highlights that exemplify LDRD's noteworthy research results and timely support for the Laboratory's five-year strategic *Roadmap to the Future*, as well as for critical national needs.

Scalable Methods for Discrete-Ordinate Transport Algorithms on Massively Parallel Architectures— Robert Falgout, Principal Investigator (08-ERD-026)

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

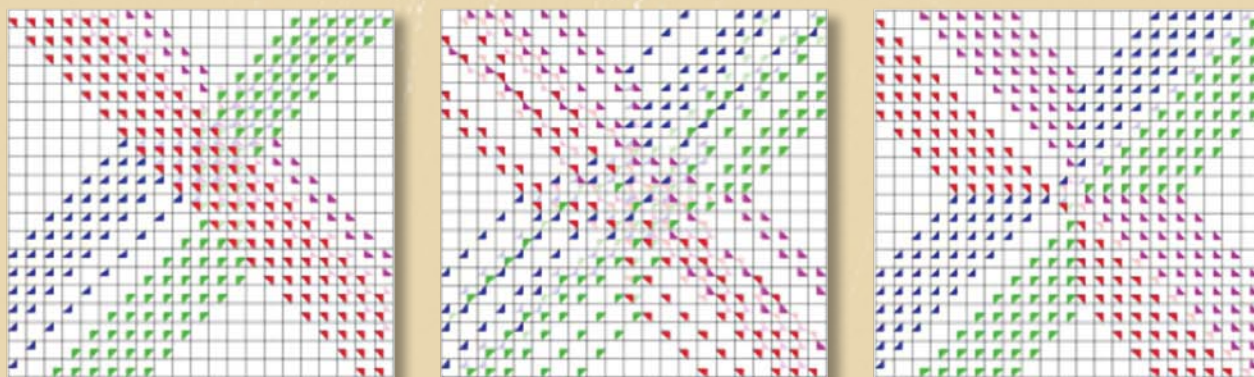
One of the Laboratory's primary missions is stockpile stewardship—maintaining the safety and reliability of the nation's nuclear weapons. In the absence of actual weapons testing, the Laboratory conducts “virtual testing” on some of the world's most powerful computational platforms, such as the massively parallel BlueGene/L, with over 130,000 processors. At the heart of this simulation capability is some of the world's most sophisticated computer code—physics codes that simulate the behavior of stockpile materials under extreme conditions. Obviously, computer codes for an application of

such critical national importance must meet the most demanding of accuracy and performance standards.

A fundamental aspect of these physics codes is the mono-energetic Boltzmann radiation and neutron transport equations. These equations describe the transport, absorption, scattering, and emission of x rays and neutrons as they pass through a stockpile-related material, altering the material's properties as they do so. The algorithms that solve these equations must be not only robust but also scalable. Scalability—the ability to harness the full processing power of large-scale systems—is increasingly important as ever more powerful, more massively parallel computers come on line for stockpile stewardship.

This LDRD team developed new, robust algorithms—discrete-ordinate transport algorithms—to solve the linear and nonlinear systems in radiative transfer and neutron transport equations. Building upon highly successful multigrid solvers used in key LLNL physics codes, they extended the solver capabilities with deterministic parallel, multilevel solutions, significantly enhancing the simulation power of critical codes and making them effective over a wider range of regimes. They also developed sweep algorithms for their multigrid methods as part of the team's strategy for achieving algorithms that are scalable to state-of-the-art, massively parallel systems.

To develop the sweep algorithms, the team began by creating a performance model, used it to demonstrate an algorithm that achieved the minimum stages possible, and demonstrated the algorithm's ability to scale to large numbers of processors. Issues addressed along the way include “collision,” in



These interference patterns visualize the computational issue of collision, in which multiple angles converge on the same processor at the same time. (Colors indicate the mesh corner from which the angles originate.) The differences in patterns when choosing angles by rank (left), randomly (center), and by longest remaining travel distance (right) indicate the importance of angle choice in developing sweep algorithms. These algorithms assured that team's advanced transport algorithms would be scalable to the new, massively parallel computers coming on line for stockpile stewardship.

which multiple angles involved in transport calculations converge on the same individual processor at the exact same time.

They next developed a generic sweeping algorithm for comparing techniques for scaling beyond 100,000 processors and multiple algorithms for sweeping on mesh-refined grids. Finally, they developed parallel sweep algorithms and related performance models for the long-characteristics discretization of the Boltzmann equations, demonstrating equivalent performance with large datasets to existing techniques but without leaving processors idle at any stage. The properties required for algorithm scalability to hundreds of thousands of processors were also established.

The successful project also developed a multigrid method for discrete-ordinate transport that was shown to be robust across a wide range of spatial resolutions, scattering ratios, and other parameters, as well as a multigrid method for the full space-angle-energy Boltzmann equation, among other deliverables.

The team's new sweep algorithms are already in the process of being adopted by stockpile stewardship researchers, who have also expressed interest in further developing an algebraic version of the team's multigrid solver. Says principal investigator Robert Falgout about the project's impact in front-line research: "The solution of radiation and neutron transport equations is a key component in scientific simulations important to LLNL and the nation. This LDRD project developed the techniques necessary to solve these equations efficiently on the ultraparallel computer architectures that are now beginning to appear."

Nuclear Forensics: An Integrated Approach for Rapid Response—Ian Hutcheon, Principal Investigator (10-SI-016)

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

The very real danger of nuclear terrorism has created a pressing need for faster, more-accurate capabilities to pinpoint the source of nuclear

materials either retrieved from post-detonation debris or intercepted prior to use. Nuclear forensic analysis, coupled with reliable data on material characteristics, can help identify the perpetrators and, equally importantly, rule out those not involved.

Current nuclear forensic capabilities, however, derive largely from the nuclear weapons testing and surveillance programs of the Cold War and from stockpile stewardship. Although accurate, these techniques rely on time-consuming, labor-intensive methods. In the critical hours after nuclear material is discovered, both the speed and accuracy of forensic analysis are of the essence. Furthermore, gaps exist in our understanding of how forensics-relevant compounds behave during detonation.

This project is pursuing a revolutionary, forward-thinking scientific strategy to develop a "single day" nuclear forensic and attribution system. The system will enable officials to answer three critical questions in a nuclear terror crisis: What was the device? Who were the perpetrators? Are there more devices?

The scientist who is leading the team, Ian Hutcheon, says their goal "is to develop new approaches to answer these questions up to ten times faster than is currently possible and with the highest possible fidelity." To this end, the project encompasses four overarching, interrelated fields—mass spectrometry, actinide science, actinide material synthesis, and fallout characterization—the results of which will synergize into a game-changing capability.

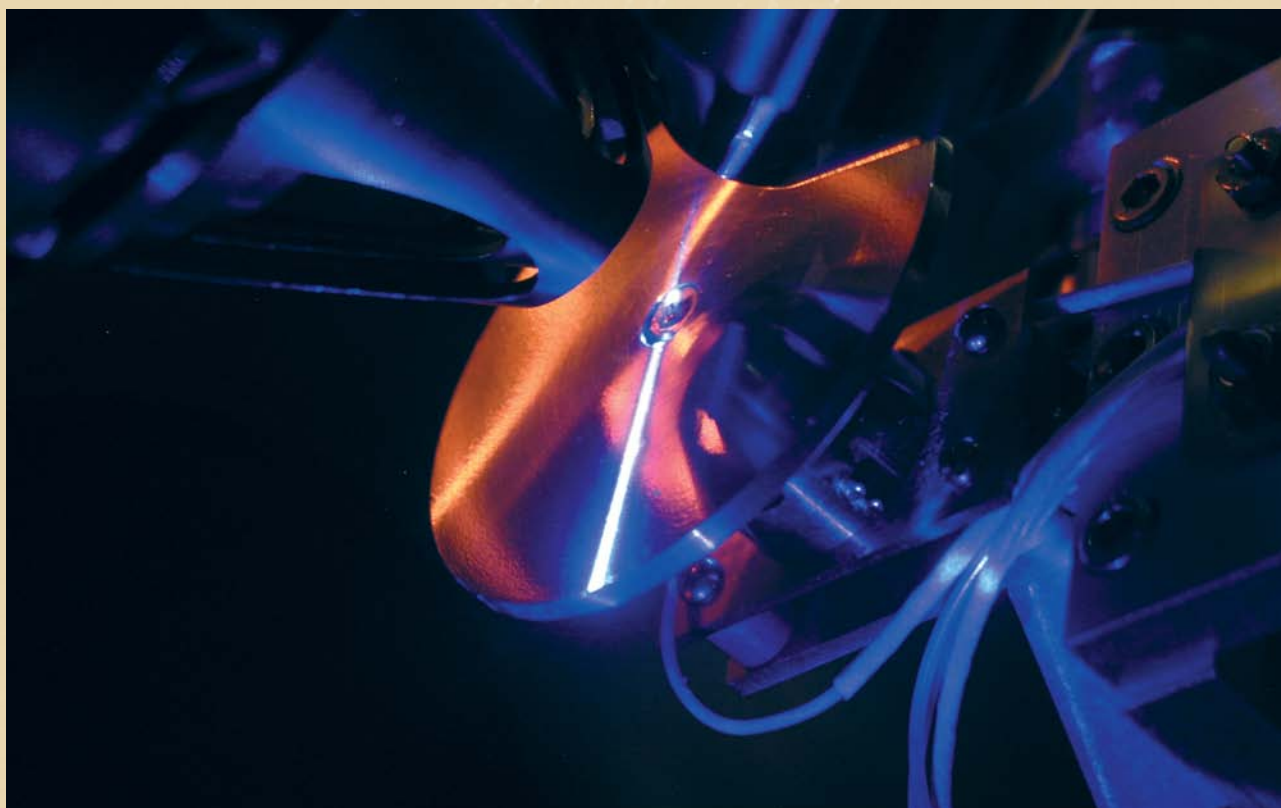
The team's mass spectrometry effort centers on resonance ionization mass spectrometry (RIMS, shown in the figure) for the rapid and accurate determination of radioisotope ratios—critical data for identifying where, how, and by whom a nuclear material was made. The RIMS technique can produce such data within hours, without the time-consuming chemical separation of samples. The team's original goal was to develop RIMS capable of determining uranium and plutonium isotope ratios with a precision of 0.5% within 4 hours, but in work conducted at Argonne National Laboratory's RIMS facility, they exceeded both of these goals, achieving a precision better than 0.5% and a sample-processing time of less than 1 hour with multiple uranium isotopes and uranium oxides.

The team also made progress in the other two prongs of the mass spectrometry effort. Using simulation software, they investigated the ion optics of a cavity ion source, which will help obtain accurate isotope ratios from much smaller samples than are required now. They also developed a new detector for the accelerator mass spectrometry analysis of neutron-activated chromium, iron, and nickel—the activation products of transition metals being an important forensic signature of a nuclear device's structural components. This work leverages the world-leading capabilities of LLNL's Center for Accelerator Mass Spectrometry.

Understanding how actinide compounds behave in the extreme conditions of a nuclear detonation lies at the heart of accurate nuclear forensics. The goal of the team's actinide synthesis effort is to provide previously unavailable data through the in situ investigation of how uranium oxides are transformed during a detonation. The compounds are being prepared with different techniques to identify signatures for determining how a nuclear

material was produced and where its raw materials were obtained. These samples were also used to develop new scanning electron microscopy methods to examine grain shape and other properties as potential signatures. In addition, using x-ray absorption spectroscopy at the Advanced Light Source at Lawrence Berkeley National Laboratory and state-of-the-art quantum modeling, the team achieved the first-ever parameter-free, first-principles calculation of the electronic structure of uranium oxide.

As for this project's role in enabling LLNL to recruit and retain top-tier scientific talent, Hutcheon states: "By linking cutting edge science with a compelling national problem, the LDRD project has proved to be an effective means to attract vital new talent to LLNL. The project currently employs five postdoctoral researchers and has supported the conversion of two postdoctoral researchers to flex-term positions." The project also furthers both recruitment and collaborations by "actively engaging with researchers at leading U.S. universities to address pressing questions in nuclear forensic analysis."



In resonance ionization mass spectroscopy (RIMS) at a collaborator's facility, laser light tuned to uranium resonances is used to determine a uranium sample's isotope ratios—important signatures of where and how the material was made. This work furthers one of the project's goals—to develop a new RIMS capability for determining a nuclear material's origin far more quickly than is possible now.

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

Mission Focus Area	Biosecurity
Science, Technology, and Engineering Pillars	Measurements and Experimental Science

The key to minimizing the impact of a bioterror attack is to detect and identify the pathogen as rapidly as possible, so that first responders can take appropriate measures, including administering the correct vaccine to the uninfected and appropriately treating those already infected. Rapid identification of the pathogen used in such a scenario requires a field-deployable technology that can produce actionable results in real time. Current technologies, however, are time consuming and not easily used in the field, requiring cell culturing, polymerase chain reaction, or other means to amplify the suspected agent. Some current techniques also require pre-labeling of the pathogen with molecules that aid in detection.

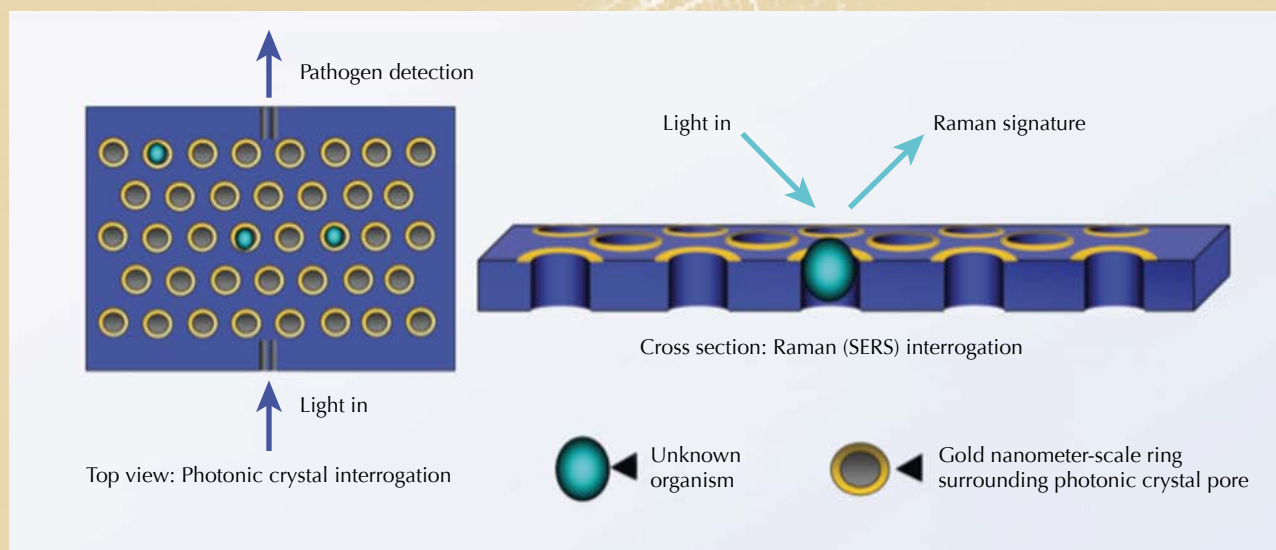
This LDRD project aims to overcome these and other limitations by integrating two cutting-edge technologies never before combined into a single pathogen-detection system: photonic crystals with functionalized pores and surface-enhanced Raman spectroscopy (SERS) utilizing the plasmonic

resonance of the pores. The photonic crystal will detect the presence of a pathogen, after which the SERS-plasmon system will determine exactly what type of pathogen it is. The resultant device will be field-deployable, require no pre-amplification or labeling of the sample, and produce results in real time.

Photonic crystals have already been shown capable of acting as highly sensitive biosensors: when a pathogen is trapped in a pore, its presence can be detected as changes in the refractive index using light passed through the crystal (as shown in the left-hand side of the figure). The team on this LDRD project is creating the first-ever photonic biosensor with flow-through pores, for far more efficient detection than is possible with the previous photonic-crystal biosensors, which have been made with dead-end pores.

Furthermore, the team will functionalize the array of flow-through pores with gold nanometer-scale rings around each pore opening. The rings will increase the probability of a pathogen of interest being caught by capture molecules anchored to the pore surface. By being fixed at the surface, the pathogen is easier to subsequently identify with the second half of this detection platform: SERS.

The SERS will exploit localized surface plasmon resonances that the gold nanometer-scale rings generate when subjected to light at their excitation



A schematic illustration of integrated photonic-plasmonic detection and identification. In the first step, the presence of a pathogen in a gold-enhanced pore in the crystal platform is detected as changes in the properties of light passing through the crystal. Next, surface-enhanced Raman spectroscopy (SERS) is used to identify the pathogen based on its Raman-shift signature.

frequency. This approach has the highest sensitivity-to-refractive change of any nanometer-scale particle system and has already demonstrated the ability to detect even a single pathogen particle. The results of this Raman interrogation are matched against a database of known pathogen signatures to identify the specific pathogen trapped in the pores. The extreme precision required in fabricating the components of the photonic-plasmonic platform will be achieved at Livermore's state-of-the-art electron-beam lithography and focused ion beam facilities.

In addition to demonstrating the detection of particles (as pathogen simulants) in crystal pores by measuring optical band edge shift, the team has also successfully demonstrated the signal-amplifying plasmon resonance of gold coating and the use of this resonance to detect molecular mono-layers with SERS tuned to these frequencies. They have also optimized processes for measuring the crystals' optical spectra. With regard to overall integration of the components, the team has optimized crystal fabrication in ways that facilitate integration with fluidics components, conducted computer simulation on integrating the crystals with SERS structures, and determined the basic geometric and materials requirements for integrating those two components along with sample fluid flows. The team is thus on track to fabricate a prototype device and functionalize it for organism simulant capture. Work done in FY10 was featured on the cover of the *Applied Physical Letters*.

"While our multifunctional sensor platform is still in the early stages of development," says principal investigator Sarah Baker, "the technology has the potential to miniaturize optical sensors so that they can be integrated directly into computer chips and with other lab-on-a-chip components, allowing portable and fast detection of particles of interest."

As a postdoctoral researcher awarded this opportunity, she can testify first-hand about the power of LDRD as a recruiting tool: "Having the opportunity to lead a project for the first time and to dictate the project content is very appealing to postdoc candidates . . . and is therefore a very effective recruiting tool," she says. "Leading a fundamental science

project is also an excellent opportunity to network with other Livermore scientists in order to locate equipment and expertise here, ultimately showcasing the breadth of the Laboratory's capabilities."

Supercomputing-Enabled Transformational Analytics Capability (SETAC)—Celeste Matarazzo, Principal Investigator (09-SI-013)

Mission Focus Area	Cyber Security, Space Security, and Intelligence
Science, Technology, and Engineering Pillars	High-Performance Computing and Simulation

Across the country and around the world, there is an increased reliance on Internet applications for commerce, defense, research, education, and health care. In particular, government operations have come to depend on the Web and are, therefore, vulnerable to a variety of attacks. Forms of attack vary but most are attempts to read, alter, or destroy data or to compromise a computer's operating system to take control of the machine. It is estimated that more than 60,000 machines per day are co-opted into loose networks of computers, called botnets, some of which are operated by foreign professionals. As a result, cyber security has become a top national priority requiring the best computer experts in government, academia, and business. Some of these experts are working on an LDRD project whose goal is to develop a fundamentally new approach for cyber defense.

The Supercomputing-Enabled Transformational Analytics Capability (SETAC) will provide real-time behavioral analytics for cyber-security data. The proposed system capabilities will include

- Identification and classification of high-volume streaming computer network traffic
- High-performance sensor nodes to increase processing capabilities and provide distributed detection across a computational network
- A computing test bed to develop advanced global collection and analysis approaches
- New computer algorithms (step-by-step procedures) to analyze data across a distributed system

- System- and component-level metrics for performance assessment

According to principal investigator Celeste Matarazzo, “as a research project in cyber security situational awareness, SETAC addresses challenges not only of today’s Internet but of the Internet as it will be in three to five years.”

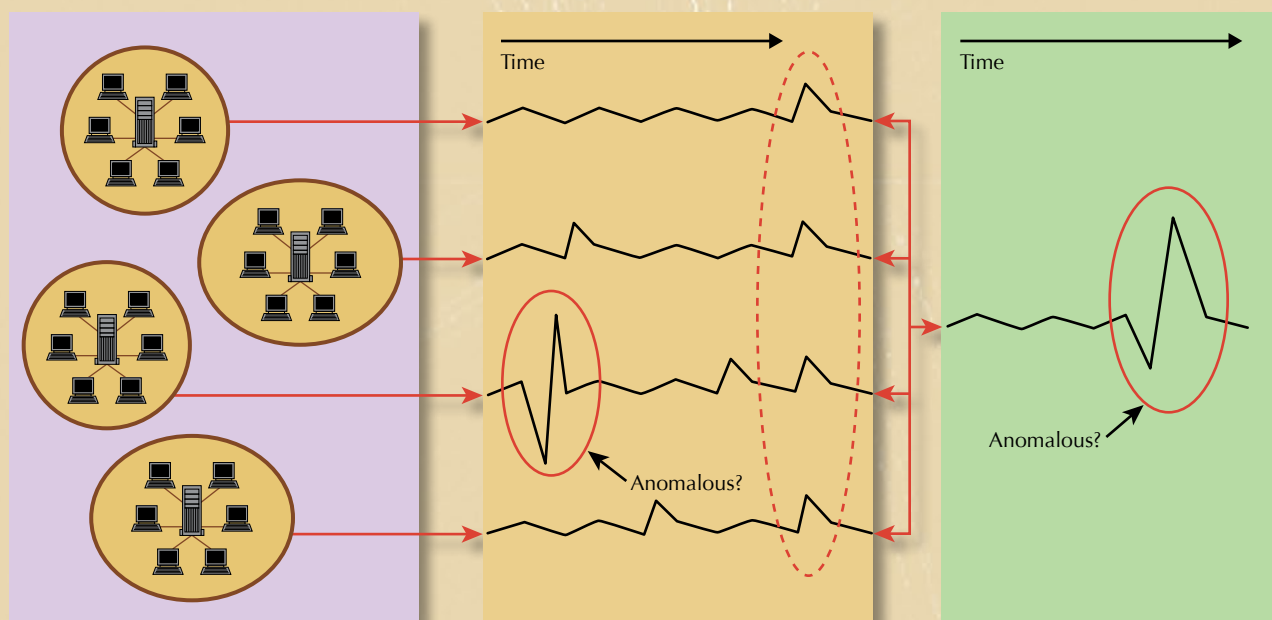
The project’s goal is to dramatically increase the ability to detect, characterize, and combat malicious attacks on large computer networks. The LDRD effort focuses on establishing situational awareness—that is, a state of continual awareness—of network behavior to better detect malicious intrusions in real time, while being respectful of individuals’ privacy. In this way, human analysts will have the opportunity to respond to threats immediately.

The LDRD research team includes computer scientists, statisticians, mathematicians, and engineers. Academic partners include the University of California at Riverside and Davis and Carnegie Mellon University. The team is also collaborating with experts at Sandia National Laboratories, Pacific Northwest National Laboratory, and Cisco, Inc. Matarazzo explains that “SETAC has generated broad

interest throughout the academic and research communities, and has resulted in the hiring of numerous undergraduate and graduate students and postdoctoral researchers that are motivated by the difficult and exciting challenges faced in cyber security and want to make an impact to improve the security of the nation.”

To date, effective situational awareness of computer networks has been challenging because of the problem’s scale and complexity. Hundreds of millions of Internet connection records are made each day at Livermore alone, for example. Furthermore, the cyber threat is extremely dynamic because adversaries can continually change the Internet Protocol (IP) addresses from which they conduct their operations, making detection difficult. Another challenge is malicious software (malware) that can change its behavior over time.

As part of the situational awareness effort, SETAC researchers are using complex algorithms distributed throughout the network together with novel hardware architectures derived from supercomputers. The researchers plan to deploy the algorithms (also called software sensor agents) to collect, analyze,



The Supercomputing-Enabled Transformational Analytics Capability is designed to detect both local and global patterns of behavior. For example, sensors continuously observe the behavior of the four computers shown at left. A spike in activity of one computer indicates a possible anomalous local behavior (center). A simultaneous spike in activity of all four computers indicates a possible anomalous global behavior (right). The information collected is then shared with other sensors, and a security analyst is alerted for further investigation.

and share data across the unclassified Lawrence Livermore computer network. These distributed software sensor agents will also access data provided by commercial tools such as antivirus software and “learn” to quickly recognize suspicious behavior and take any necessary protective actions.

Sensor agents developed for the project will look for anomalous scenarios such as multiple machines simultaneously performing the same action or an unauthorized action, a large amount of data suddenly being sent outside the Laboratory, a computer accessing a supercomputer that it has never previously accessed, or a computer communicating with an outside server that frequently changes its IP address. Should a sensor detect an anomalous scenario, it shares this information with other sensors to determine if similar behavior is occurring elsewhere on the network—if so, a security analyst would be alerted.

The three primary characteristics of SETAC—distributed decision making, an emphasis on behavior modeling using machine learning approaches, and real-time analysis and detection—are novel features of cyber defense. SETAC’s situational awareness emphasis is preferable to today’s typical cyber defense, which relies on commercial software at the organization’s network perimeter and analysis after an attack has occurred and damage has been done. “Current cyber defense has limitations,” says Matarazzo. “For example, once an internal machine is breached, the entire network is at risk, because of the difficulty in preventing the spread of malware from within the organization.”

In FY10 LDRD investigators deployed hundreds of software sensor agents throughout the Laboratory’s computer network, extended their behavior-based machine-learning algorithms, developed a probabilistic activity model of computer hosts in the system framework for anomaly detection, and evaluated the usefulness of host data for cyber security indicators. Remaining efforts will focus on a systems test at the DETERlab test bed, a public facility for medium-scale experiments in computer security, as well as investigating active learning methods in which response can be measured by the SETAC sensor and analytic capabilities to actively assess levels of network damage. Most importantly, the SETAC project funded by LDRD is developing new

approaches that contribute to national efforts such as the Comprehensive National Cyber Security Initiative, one of the largest single national security research and development investments in the U.S. today.

Design of Novel Catalysts to Capture Carbon Dioxide—Roger Aines, Principal Investigator (10-ERD-035)

Mission Focus Area	Energy and Climate
Science, Technology, and Engineering Pillars	High-Performance Computing and Simulation

The need to reduce atmospheric levels of carbon dioxide (CO₂) is spurring efforts to develop the means to actively absorb large amounts of CO₂ from industrial waste gas and even from the air itself. Current technologies, however, are far too large and expensive to encourage widespread industrial adoption on a scale to counter climate change. This is because of the slow speed of the chemical reaction by which CO₂ is absorbed into solution as carbonic acid. In fact, if this conversion of CO₂ were not the rate-limiting step, CO₂ absorption could be accomplished a thousand times more quickly than is currently possible, it is estimated.

Catalysts or enzymes that accelerate this chemical process would enable smaller, less expensive CO₂ removal facilities. For instance, at coal-fired utility plants, the right catalyst would dramatically increase the throughput of existing systems and permit new, high-efficiency, small-footprint systems that cost much less to operate because of greatly reduced energy consumption.

In natural organisms, CO₂ is converted into carbonic acid by the natural enzyme carbonic anhydrase, one of the fastest-acting enzymes known. “The human body,” explains this project’s principal investigator, Roger Aines, “separates CO₂ from blood at one-fifth the energy cost using this enzyme.” Because the natural enzyme, however, is not nearly robust enough for the high-temperature conditions of industrial CO₂ removal, Aines and his team must improve on nature: “Our project,” he continues, “seeks to replicate the function of that enzyme in a rugged, industrializable small molecule that will similarly reduce the energy cost of capturing CO₂ from power generation.”

This LDRD project is leveraging Livermore's capabilities in computer simulations, systems analysis, and biology, along with the chemical-synthesizing and testing capabilities of a proven industrial partner, to develop such carbon-capturing catalysts. The team's overall innovation plan is as follows:

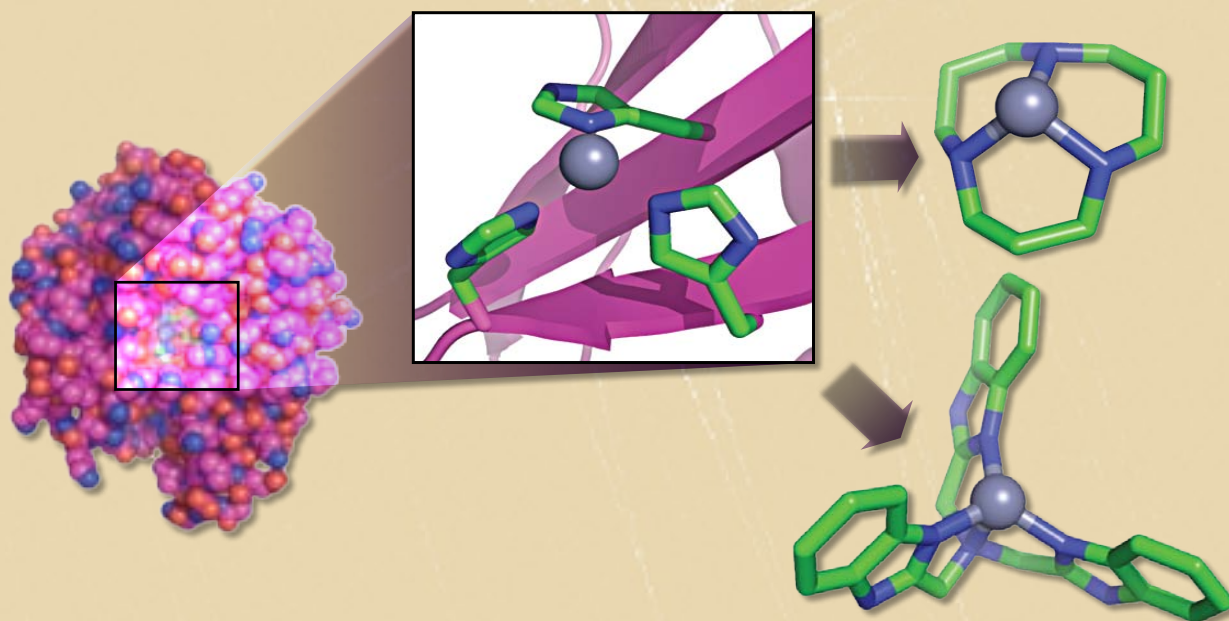
- Identify the features of natural carbonic anhydrase that are essential to convert CO_2
- Design synthetic catalysts and predict their performance with quantum mechanical simulations
- Synthesize the most promising candidates
- Test the synthesized catalysts in an industrial facility

In particular, the second step—simulation—is enabling the researchers to analyze many molecular options and configurations much more quickly and inexpensively than if each candidate catalyst had to be synthesized and tested to determine its actual properties. In fact, in the project's first year, the team has already synthesized and tested new catalysts that had been identified through computational analysis as the most promising candidates. Furthermore, new computational approaches developed in the course of this work are up to five times faster than previous

techniques and will speed up the team's computational screening of catalysts even further.

The project's functional, small-molecule approach is designed to arrive at catalysts that are robust and easy to manufacture. First they identify individual small molecules, each of which mimics a specific function of natural carbonic anhydrase—a large, complex molecule that would be too expensive to replicate. Next, the researchers determine the optimum structure into which these individual components can be combined—a structure that preserves the individual functionalities while also providing the requisite structural hardness. The team has already designed catalytic molecules that are based on natural proteins but achieve their active site with a much smaller number of atoms. Work next year will emphasize designs that mimic the hydrogen bonding of natural carbonic anhydrase.

On his LDRD project's support of Lab recruitment, Aines says, "half of the staff of this project have been at the Lab for less than two years, including three postdocs and four recent hires. The ability to apply the Lab's resources, including high-performance computers, to environmental problems is very attractive to young scientists seeking to solve the climate problem."



In creating robust synthetic catalysts capable of enabling faster, less expensive carbon dioxide absorption for industrial applications, this LDRD project is analyzing the natural enzyme carbonic anhydrase (left) to identify the structural features (center) responsible for converting carbon dioxide to carbonic acid. Next, the team uses this information to design more-robust small molecules (right) that mimic the natural enzyme's functions.

Compact, Efficient Lasers for LIFE—Robert Deri, Principal Investigator (10-SI-010)

Mission Focus Area	Laser Inertial Fusion Energy
Science, Technology, and Engineering Pillars	High-Energy-Density Science

A potential path to commercially feasible fusion energy is laser inertial fusion energy (LIFE), which uses laser energy to ignite fusion fuel through inertial confinement. The LIFE approach can potentially help meet the world's growing demand for energy with fusion technology—an energy source that, unlike conventional fission nuclear energy, generates only negligible nuclear waste, avoids the concerns of proliferation, and poses little risk to surrounding communities. As the concept is developed, LIFE can leverage the extensive experience at LLNL gained in developing the National Ignition Facility (NIF). Making LIFE economically feasible will require further technological advances beyond NIF to reduce costs and plant footprint, for instance, but recent developments in laser and materials science and technology could be utilized to dramatically reduce both cost and size while at the same time attaining efficient and reliable plant operation.

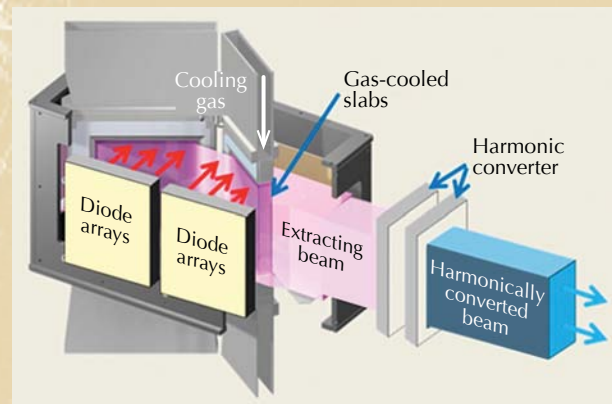
This LDRD team is building the foundation in advanced laser technology that will make LIFE commercially viable. They are assessing multiple technologies for use in LIFE, including:

- Laser diode pumps, which can improve efficiency
- Advanced laser gain media with long storage lifetimes, which can reduce diode requirements and costs
- Far-field spatial filters, to reduce a form of laser beam distortion known as “pinhole closure”
- Optics with improved durability, where lessons learned from NIF such as finishing and coating techniques will be applied
- Power conditioning and control, such as locating the field-effect transistors that control diode power inside the diode package to leverage the diode cooling system

Determining the optimal combination of these and many other technical options is the critical first step in achieving feasible LIFE power plants. Once this is done, the next step is to create plant designs incorporating these options by optimizing and combining the selected technologies in a cost-effective architecture. In keeping with this basic strategy, the team's principal deliverables will be a LIFE cost-per-performance analysis model—with which a wide range of architectural variants will be analyzed—and a baseline and a backup site design, for future detailed analysis and refinement.

Laser diode pumps, for instance, are key components in LIFE. These diodes can improve efficiency, but their costs will also dominate the total cost of a LIFE power plant. However, the team, working with manufacturers, has determined that up to 80% of diode costs are for assembly and packaging. To achieve both cost performance and efficiency targets, the team plans to leverage both successes achieved at NIF—such as simplified diode package assemblies—and new engineered materials and structures that have become available since NIF was designed and built.

This year, the team developed simulation tools to assess the effect of advanced laser gain media—such as reducing thermo-mechanical stress through a phenomenon known as birefringence—and used the



Conceptual illustration of the cost-performance model to be developed to analyze the tradeoffs of various configurations of laser ignition fusion energy (LIFE) for commercial-scale power generation. The computational model will comprise three sub-units: diode pumping, extraction, and harmonic beam conversion.

tools to develop a 16-cubic-meter “beamline in a box” architecture using neodymium-doped glass and a compact, efficient pump cavity design. They also verified that the new beam-line design achieves an infrared pulse output greater than 16 kilojoules and an electrical-to-optical conversion efficiency exceeding 10%. The team also used their new simulation tools to investigate other gain media and used the results to create new designs for diode pumps, a Pockels cell, and other subsystems. These designs will be further developed in FY11.

The project team is working closely with industrial partners capable of producing the components for the baseline design, as well as consulting with manufacturing engineers to estimate fabrication and assembly costs, identify design areas where vendor competition can be enhanced, and reduce costs through lessons learned and innovations in manufacturing. In short, cost-effectiveness is being designed in from the ground up.

By resolving the key issues in laser inertial fusion energy, the project “will directly contribute to enhanced U.S. energy and environmental security,” says principal investigator Robert Deri, “by providing a source of abundant, clean power without nuclear waste disposal, safety, carbon sequestration, or proliferation issues.” Deri also affirms LDRD’s powerful impact on recruiting and retention at the Laboratory: “This project provides a venue for developing the next generation of high-energy lasers, enabling LLNL to provide the exciting opportunities in state-of-the-art laser design needed to retain top researchers in this field.”

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 FY10, LDRD costs at LLNL were \$88.7M, which is 5.72% of total Laboratory costs. The number of patents resulting from LDRD-funded

research since 2006 and the percentage of total patents that were derived from LDRD research and development are 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 typically made several years before the technology is actually patented. Furthermore, although an LDRD-sponsored project makes essential contributions to such technologies, subsequent programmatic sponsorship also contributes to a technology’s further development.

It is notable that the number of patents decreased significantly from 2006 to 2009. This is most likely because from 2005 through 2007, patents were not an institutional priority. In December 2007, a functional management assessment of the patenting and licensing processes at LLNL was conducted by the new contractor. The findings and recommendations pointed to an immediate need to transform the manner in which intellectual properties were selected for and actually patented. Starting in 2008, patents again became a priority, and the Industrial Partnerships Office at LLNL took significant steps to encourage and submit new patent applications. The number of patent applications per year at LLNL is now increasing, as shown by the 17% increase in 2010 from 2009 applications. In 2010, LDRD projects generated 50% of Livermore’s total patents, even though the LDRD program constitutes a little under 6% of the Laboratory’s budget.

Patents	2006	2007	2008	2009	2010
All LLNL patents	63	62	57	46	54
LDRD patents	29	32	23	20	27
LDRD patents as percentage of total	46%	52%	40%	43%	50%

Patents resulting from LDRD-funded research as a percentage of all LLNL patents for the last five years.

As with patents, records of invention submitted by LDRD researchers account for a significant percentage of the total for the Laboratory. Overall, LDRD records of invention for 2006 to 2010 account for over 42% of the 734 total. In 2010, there were

160 records submitted at Livermore, with 66 (41%) of those attributable to LDRD-supported projects. The general trend in the number of records of invention, which showed a notable decrease in FY08, has recovered more rapidly than the trend for patents. This is due to the fact that records of invention arise readily from active research and are the precursors to patent applications, but the number of those that become patent applications and eventually patents is strongly limited by the high cost of that process—it is also a process that typically takes several years.

Records of invention	2006	2007	2008	2009	2010
All LLNL records	157	162	110	145	160
LDRD records	74	69	44	56	66
LDRD records as percentage of total	47%	43%	40%	39%	41%

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

Finally, LDRD also plays a role in producing Laboratory copyrighted material. From 2006 to 2010, LDRD-supported projects accounted for over 25% of the 336 Livermore copyrights. In 2010, there were 63 LLNL copyrights, with 20 (32%) that could be attributed to LDRD research.

Publications in Scientific Journals

LDRD publications in scientific journals demonstrate that research and development under LDRD furthers the progress of the broad scientific and technical community by contributing new scientific results, innovative technologies, and fundamental breakthroughs. In a typical year, Laboratory scientists and engineers collectively publish around 1,000 papers in a wide range of peer-reviewed journals. In 2010 there were 910 such articles, of which at least 186 (20%) resulted from LDRD projects. The downward trend in total Laboratory publications in recent years is in part related to a decrease in the size of the scientific and engineering workforce at LLNL. During FY08 this population at Lawrence

Livermore decreased by 15% (from 3,412 to 2,891), and the number of postdoctoral researchers declined by 19% (from 147 to 119). Since that year, the total population of scientists and engineers at LLNL has remained relatively constant at the lower number (~2900), and the postdoctoral population began to recover in 2010. Because most of LLNL's postdoctoral researchers are sponsored by LDRD and represent a substantial component of the Laboratory's publishing scientists and engineers, the number of postdoctoral researchers is an important contributing factor for the lower number of total LLNL publications from 2007 through 2010. However, over the last several years, the percentage of LDRD-supported articles has remained relatively consistent, with a five-year average of nearly 19% of total Laboratory publications. The following table shows the number of journal articles per calendar year resulting from LDRD-funded research since 2006 and the percentage of total articles that were derived from LDRD research and development.

Journal Articles	2006	2007	2008	2009	2010
All LLNL articles	1237	1162	1097	1001	910
LDRD articles	223	237	212	161	186
LDRD articles as percentage of total	18%	20%	19%	16%	20%

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

Collaborations

External collaborations are absolutely essential to the conduct of research and development in LDRD. By collaborating formally and informally with other national laboratories, academia, and industry, LDRD investigators are able to access world-leading facilities and knowledge—both in the U.S. and abroad—and serve as active and prominent members of the broad scientific and technical community. External collaborations are also vital for assembling the best teams for pursuing many research and development opportunities, by 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 FY10 portfolio included 70 formal LDRD-funded collaborations involving 49 LDRD projects (34% of the total projects funded). Collaborating institutions included the University of California (23% of total collaborations), other academic institutions (51%), DOE sites (9%), and other collaborators (e.g., other government agencies and industry, 17%). These statistics do not include the numerous informal collaborations that PIs pursue in the course of their LDRD projects.

Postdoctoral Researchers

Because LDRD funds exciting, potentially high-payoff projects at the forefront of science, the program is essential for recruiting top talent in new and emerging fields of science and technology. In FY10, the LDRD Program supported nearly 80% of the Laboratory postdoctoral researchers—there was an average of 123 postdoctoral researchers at the Laboratory in FY10, of which 98 were supported in some way by LDRD projects. The Laboratory continues significant recruitment efforts to increase the total number of postdoctoral researchers.

Awards and Recognition

A primary goal of LDRD is to foster excellence in science and technology that will, 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 recent honors attest to the exceptional capabilities, talents, and performances of these researchers, while simultaneously highlighting the success and vitality of the LDRD Program at Livermore.

14th International Detonation Symposium Best Poster Award/DOE SERch National Science Competition

Summer student Han Wang won an LLNL best poster award at the 14th International Detonation Symposium and was invited to the upcoming DOE SERch national science competition in support of an LDRD project investigating the arc initiation of high explosives (09-ERD-042).

14th Pacific–Asia Conference on Knowledge Discovery and Data Mining Best Paper Award

At the 14th Pacific–Asia Conference on Knowledge Discovery and Data Mining, external collaborator Christos Faloutsos was part of a team that won a best paper award for “OddBall: Spotting Anomalies In Weighted Graphs.” The work was part of an LDRD project on supercomputing-enabled transformational analytics capability (09-SI-013).

Alameda County Women's Hall of Fame

Lisa Poyneer is the latest of several LDRD researchers to be inducted into Alameda County Women's Hall of Fame in 2010 for her scientific achievements in the development of the Gemini Planet Imager. Using algorithms she developed, the Gemini Planet Imager promises a performance level that is up to 100 times greater than current instruments of its kind. Poyneer is currently a member of an LDRD team tracing the shadows of planetary systems (08-ERD-043).



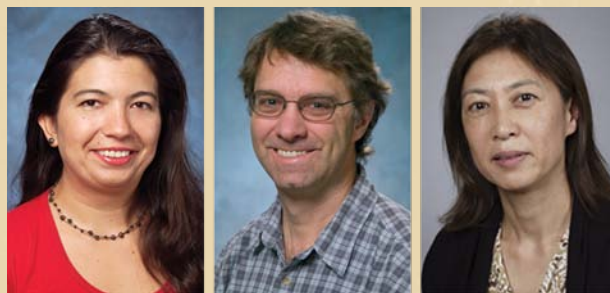
Lisa Poyneer

American Physical Society Fellows

Three of the four fellows of the American Physical Society named from LLNL in 2010 were LDRD-supported researchers. Election is limited to no more than one half of one percent of the association's membership for a given year.

- Olgica Bakajin, a former LLNL chief scientist, was cited in the biological physics category for her contributions to the development of new instrumentation for studies of protein folding and for fundamental understanding of transport and selectivity at the nanometer scale. Bakajin's work also could lead to a better understanding of membrane channels. She now serves as chief technology officer of Porifera, which licensed an LLNL carbon nanotube technology that she helped develop. She was the principal investigator for a project to discover folding rules for proteins (05-ERD-078), and a co-investigator for several other projects including research into the structure and transport of water and hydrated ions in nanometer-scale channels (07-LW-056) and molecular transport in one-dimensional lipid bilayers (05-LW-040).
- Jon Eggert, a physicist in the Physical and Life Sciences Directorate, was cited for significant achievements in linking dynamic and static compression of condensed matter in the shock compression of condensed matter category. Eggert has served as a co-investigator for several projects examining the physics and chemistry of the interiors of large planets (09-SI-005, 04-ERD-065, and 00-ERD-044), as well as a project investigating new regimes of material strength at ultrahigh strain rates and pressures (06-ERD-027).
- Hye-Sook Park, a physicist at the National Ignition Facility, was cited for development of seminal experimental techniques to create and probe plasmas with extreme density and

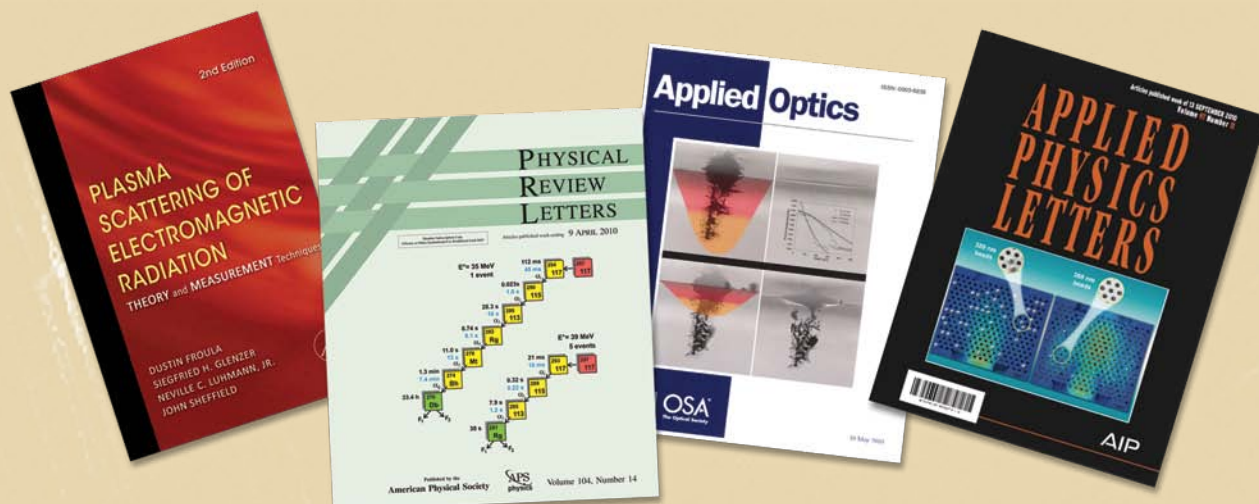
temperature in the plasma physics category. Park was the principal investigator for the study of Kelvin–Helmholtz instability in high-energy-density hydrodynamic processes (08-ERD-069), as well as a project to develop an advanced radiography capability at future large fusion-class lasers (05-ERD-006). She has also participated in additional research efforts in high-power lasers and high-energy-density states of matter (09-SI-010 and 07-ERD-004).



Olgica Bakajin, Jon Eggert, Hye-Sook Park

Books and Journal Covers

In 2010, several LDRD-supported projects were featured on the covers of peer-reviewed journals, and one in a new textbook on electromagnetic radiation. Research on x-ray scattering in warm dense matter (08-ERI-002) has been featured in the book, *Plasma Scattering of Electromagnetic Radiation*. The journal *Physical Review Letters* showcased two new element-117 decay chains, which were part of an LDRD project on rapid radiochemical separations for investigating chemistry of the heaviest elements (08-ERD-030). The cover of the May 10, 2010 issue of *Applied Optics* featured a project on the physics of local reinitiation and morphological evolution of mitigated sites for ultraviolet optics (08-ERD-057). The *Applied Physics Letters* cover of the September 13, 2010 issue highlighted an LDRD project on a superimposed plasmonic and photonic detection platform (09-LW-003).



A new textbook co-authored by LDRD researchers Siegfried Glenzer and Dustin Froula, who have led projects on laser propagation and laser-matter interactions is shown at left. Two new element-117 decay chains discovered during bombardment of berkelium-249 with calcium-48 at the Joint Institute for Nuclear Research in Dubna, Russia are shown on the cover of Physical Review Letters. A comparison of thermal and microstructural differences caused by mid- and far-infrared lasers used for repairing laser-induced microfractures on silica surfaces appeared on the cover of Applied Optics. A flow-through silicon-based photonic crystal that can detect fewer than five virus particles in real time and could offer significant advances for public health monitoring and biosecurity was featured on the cover of Applied Physics Letters.

DOE Outstanding Mentor Award

DOE established the Outstanding Mentor Award in 2002 to foster a complex-wide culture that values mentorship and establish practices that go above and beyond the normal responsibilities to students in the mentoring relationship. The awards are unique in that the recipients are nominated by students from

the previous summer. As in previous years, many named as 2010 recipients are LDRD researchers, including principal investigator Adam Bernstein and co-investigator Kareem Kazkaz, who are developing advanced rare-event detectors for nuclear science and security (10-SI-015). Klint Rose is investigating methods to enable transparent ceramic optics and



DOE outstanding mentors for 2010: Dawn Shaughnessy, Amy Gaffney, Jeff Westcott, Kareem Kazkaz and Christine Orme. (Standing) Trevor Willey, Director George Miller, Phil Burger, Klint Rose, Zafer Demir, Steve Langer, Robert Rieben, Gary Laguna, Roger Henderson and Roger Qiu. (Absent when photo was taken: Adam Bernstein and Tina Eliassi-Rad.)

advanced armor with nanometer-structured materials tailored in three dimensions (09-ERD-029); Tina Eliassi-Rad has studied role discovery in dynamic semantic graphs (09-ERD-021); Dawn Shaughnessy is developing rapid radiochemical separations for investigating chemistry of the heaviest elements (08-ERD-030); Christine Orme has performed research into understanding shape control in the synthesis of nanometer-scale particles (06-LW-090) and engineering titanium for improved biological response (00-ERI-006); Trevor Willey is a co-investigator for projects on nanosecond characterization of dynamic void evolution in porous materials (09-ERD-002) and formerly examined the structure and properties of nanometer porous materials (05-ERD-003); and Roger Qiu is part of a team exploring methods for mitigation of damage to multilayer mirrors (09-ERD-051) and formerly developed use of a micro-fluidic liquid cell for molecular imaging in aqueous phases using atomic force microscopy (04-FS-034).

DOE Undergraduate Intern Honors

For the first time in LLNL history, a summer intern paper was selected for an American Association for the Advancement of Science poster and DOE publication by the DOE Summer Undergraduate Laboratory Intern Program. Kyle Brady was honored for his work on the passive, standoff detector of high-density masses with a gravity gradiometer based on atom interferometry (10-FS-003).

Excellence in Fusion Engineering Award

Pravesh Patel was honored by Fusion Power Associates in December 2010 for his work in relativistic laser-plasma interaction and leadership in developing the fast-ignition concept for inertial confinement fusion. Patel is currently the principal investigator for a project on proton fast ignition (08-SI-001) and previously headed research on the opacity of the solar interior (05-ERD-045). In addition, he has served as a team member for several



Pravesh Patel

other laser-plasma and high-energy-density physics projects (04-ERD-028, 03-LW-001, and 02-ERD-006). The Excellence in Fusion Engineering Award was established in 1987 to recognize persons in the relatively early part of their careers who have shown both technical accomplishments and potential to become exceptionally influential leaders in the fusion field.

Federal Laboratory Consortium's Far West Region Competition

Lawrence Livermore was awarded an Outstanding Technology Development Award for work in developing a microarray that can detect more than 2,000 viruses and 900 bacteria in 24 hours. LDRD support came from the viral discovery platform project (08-SI-002), for which winners Shea Gardner, Tom Slezak, Kevin McLoughlin, and Crystal Jiang all served as co-investigators.

Fusion Power Associates Distinguished Career Award

Dmitri Ryutov was one of two recipients of the FPA 2010 Distinguished Career Award that recognizes "individuals who have made distinguished career-spanning contributions to fusion development." His seminal contributions over his career span most, if not all, of the major plasma physics applications, including fusion energy, astrophysics, and high-energy-density physics. He is an innovator in tokamak design and other magnetic-confinement concepts. Ryutov is the principal investigator for the study of innovative divertors for future fusion devices (08-ERD-019), and is a member of the research team for astrophysical collisionless shock generation by laser-driven laboratory experiments (11-ERD-054). He has previously worked as a co-investigator for projects on the creation of a neutron star atmosphere (04-ERD-028) and x-ray optics and applications for fourth-generation light sources (00-ERD-025).



Dmitri Ryutov

Gordon Battelle Prize

In the category of Scientific Discovery, Oak Ridge National Laboratory and Lawrence Livermore National Laboratory shared the Gordon Battelle Prize for discovery of a new chemical element $Z = 117$. LDRD researcher Dawn Shaughnessy's work on rapid radiochemical separations for investigating chemistry of the heaviest elements (08-ERD-030) played a key role in this search for new heavy elements. Voted one of the five most significant discoveries that have occurred in Battelle's contract research work or at any of the laboratories where Battelle plays a significant management role, the award-winning team received a \$5,000 education grant to their school of choice.

IEEE International Conference on Data Mining, 2009 Best Paper Award Runner Up

Tina Eliassi-Rad and Brian Gallagher received a best paper runner-up award as part of their LDRD-supported research on role discovery in dynamic semantic graphs (09-ERD-021) to provide computational tools that will help analysts sift through massive amounts of intelligence data for a wide range of national security applications.

James B. Macelwane Medal

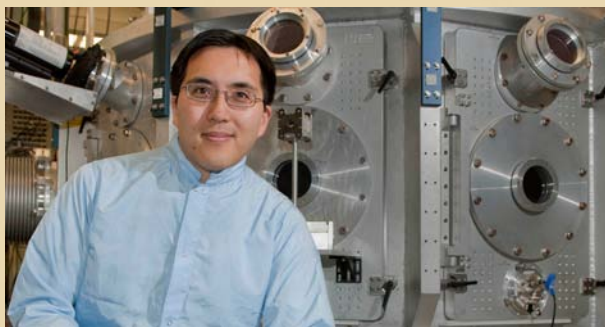
The Macelwane Medal is awarded annually to as many as three or, under exceptional circumstances, up to five individuals "for significant contributions to the geophysical sciences by an outstanding young scientist (less than 36 years of age)." In 2010, David Lobell was cited for his research that "addresses critical problems at the interface between Earth science and society." His contributions span climate change impacts, food and energy security, and agricultural informatics. Lobell was co-investigator for an LDRD project that studied the environmental consequences of large-scale deployment of new energy (05-ERD-047).



The James B. Macelwane Medal

Luis Alvarez Award

The Luis Alvarez Award was given to Cliff Chen, a postdoctoral researcher working on fast ignition at Livermore's Titan laser facility. The award recognizes the best experimental research by a postdoctoral researcher from American Physical Society's California-Nevada Section, and was presented at Caltech. His work was supported by an LDRD project on fast-ignition proof-of-principal experiments (08-SI-001).



Cliff Chen

McKay-Helm Award

John Elmer has been awarded the McKay-Helm Award from the American Welding Society in 2010 for his paper entitled "Heat Transfer and Fluid Flow during Electron Beam Welding of 304L Stainless Steel Alloy," published in the March 2009 issue of *Welding Journal*. The McKay-Helm award is given for the best contribution to the advancement of knowledge of low-alloy steel, stainless steel, or surfacing welding metals involving the use, development, or testing of these materials, as represented by articles published in the *Welding Journal*. Elmer is the principal investigator for the development of high-performance lead-free solders for microelectronics and semiconductor applications (10-LW-002) and co-investigator for a computer-code methodology for thermal forming and joining (96-ERD-037).

Microscopy Today Innovation Award

Recognizing the best new products and methods across the entire field of microscopy, this 2010 inaugural award from *Microscopy Today* cited



The dynamic transmission electron microscope has already produced new levels of scientific understanding of nanostructure growth, phase transformations, and chemical reactions.

Livermore's dynamic transmission electron microscope as one of ten technologies that "will make imaging and analysis more powerful, more flexible, more productive, and easier to accomplish." The dynamic transmission electron microscope captures single molecule images a million times faster than conventional instruments and can capture images during transformations by combining pulsed laser systems with the electron optics of a standard transmission electron microscope. This instrument was initially supported by an LDRD project on time-resolved transitions via dynamic transmission electron microscopy (06-ERD-007).

Optical Society Fellow

Joseph Nilsen was elected a fellow of the Optical Society in October 2010 "for pioneering contributions to the development and understanding of x-ray lasers and their applications." Fellowship is awarded to select society



Joseph Nilsen

members who have made significant contributions to the advancement of optics. Nilsen was a researcher for a number of early LDRD projects related to the development of high-power x-ray lasers (93-ERP-075, 93-SR-043, and 91-LW-005) as well as multilayer mirror technology using scandium-silicon interfaces (03-FS-003).

R. A. Laudise Prize

Livermore physicist Natalia Zaitseva received the R. A. Laudise Prize from the International Organization for Crystal Growth (IOCG) for her work on "creating the technology and scientific basis of rapid growth of perfect crystals from solutions." IOCG, an international federation of regional and national groups and societies, is dedicated to the advancement of the theory and practice of crystal growth, crystal characterization, and allied branches of science. Every three years, it awards the R. A. Laudise Prize for "significant technological contributions to the field of crystal growth." Zaitseva was the principal investigator for an effort examining salicylic acid derivatives, a new class of scintillators for high-energy neutron detection (07-ERD-045), which

performed systematic studies of many single crystals grown by solution techniques to produce scientific results important for developing a deeper understanding of the physics of scintillation processes, especially the composition, physical state, crystallographic structure, and quality of materials.

R&D 100 Awards

In 2010, LDRD-supported technologies garnered four of the six R&D 100 awards presented to the Laboratory by *R&D Magazine*.

- **Software Solution for Radioactive Contraband Detection.** Working at the intersection of commerce and national security, a team of Livermore scientists and engineers led by principal investigator James Candy applied its expertise in radiation science and gamma detection to develop the statistical radiation detection system, an innovative software solution that nonexperts can use to rapidly and reliably detect radionuclides. Along with ICx® Technologies, Inc. in Arlington, Virginia, the team has provided a unique and breakthrough solution to a long-troubling problem, especially in today's climate of terrorist threats. The technology derived early support from an LDRD project on detection, classification, and estimation of radioactive contraband from uncertain, low-count measurements (07-ERD-019).



The statistical radiation detection system is an innovative software solution that can easily be integrated into any gamma-detection system to combat illicit trafficking of radioactive material through customs, border crossings, and limited-access areas. The system identifies radionuclides in low-count situations when measurement time is short and demand for reliability is high.

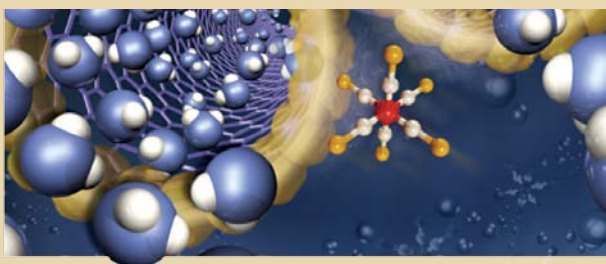
- **High-Speed Imager for Fast, Transient Events at the National Ignition Facility.** Livermore physicists developed the grating-actuated transient optical recorder (GATOR), which is designed to capture and record fleeting, sequential images of x rays and other radiation emitted from the miniature “stars” created in the National Ignition Facility target chamber. An entirely new concept for high-speed imaging, GATOR encodes two-dimensional x-ray or optical images onto coherent light. Because GATOR can convert x rays and other types of radiation to coherent optical radiation, which can be transported and recorded remotely, the instrument can operate in an environment in which copious amounts of neutrons, x rays, and gamma rays are released during ignition experiments. This work was derived from LDRD investigator Bruce Remington’s research into probing extreme high-energy-density states of matter with x rays (09-SI-010).



The grating-actuated transient optical recorder development team: (from left) Steve Vernon, Rick Stewart, Warren Hsing, Mark Lowry, and Paul Steele. (Not shown: Susan Haynes.)

- **Taking the Salt Out of Seawater.** A novel membrane technology developed by Lawrence Livermore in partnership with Porifera, Inc., in Hayward, California could lead to more cost-effective filtration processes for water

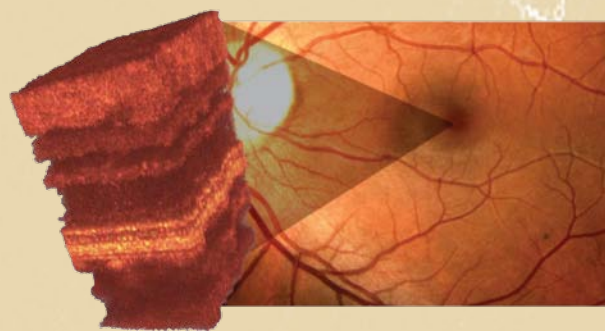
desalination and reclamation than are available today. The highly permeable, chemically inert membranes are composed of carbon nanotubes, which are hollow, seamless cylinders. Extremely smooth interior walls allow liquids and gases to rapidly flow through the nanotubes, while rejecting larger molecules. The team and its partners, including co-investigator Hyung Gyu Park, also received an Editor's Award, signifying the utmost achievement in developing new technology. This research derived early support from LDRD investigator Olgica Bakajin's work on carbon-nanotube permeable membranes (03-ERD-050).



Inside an atomically smooth carbon nanotube, water molecules form linear chains flowing at an ultrafast rate. Shown is an ion being rejected by a carbon nanotube pore. Filtration membranes composed of carbon nanotubes could make water desalination processes more efficient and cost effective. (Rendering by Scott Dougherty.)

- **A Look Inside the Living Eye.** Livermore scientists and engineers, in collaboration with the University of California at Davis, Indiana University, and Boston Micromachines Corporation in Cambridge, Massachusetts, have created a new technology that incorporates micro-electromechanical systems and adaptive optics to noninvasively observe and record ultrahigh-resolution, three-dimensional retinal images in real time. Using this instrument, physicians can see the layers within a living eye in greater detail than ever before. There have been numerous Livermore LDRD investments in the development of adaptive

optics technologies over the years. Most directly relevant to this effort was a project headed by investigator Scott Olivier on diffraction-limited adaptive optics and the limits of human visual acuity (01-LW-036).



Micro-electromechanical systems and adaptive optics enable a three-dimensional image of the cellular layers within the retina. An image of the photoreceptor layers within the eye allows physicians to diagnose sight-threatening diseases, such as macular degeneration, in their earliest stages (inset).

Silicon Valley/San Jose Business Journal Emerging Tech Awards

SecureBox, which is the exclusive licensee of LLNL's ultrawide band intrusion detection technology for cargo tracking, was named a finalist in the security category of the *Silicon Valley/San Jose Business Journal's* Emerging Tech Awards announced in FY10, which seeks to recognize "companies that could completely change technology in their sectors." The technology was an outgrowth of several LDRD projects that explored different detection and communication approaches to monitoring the 11 million cargo containers that arrive in the U.S. each year (02-ERD-064, 03-ERD-025, and 07-ERD-019).

SPIE Fellows

Bruce MacIntosh and Raymond Beach were elected fellows of SPIE, the international society for optics and photonics. SPIE fellows are society members of distinction who have made significant scientific and technical contributions in the

multidisciplinary fields of optics, photonics, and imaging.

- MacIntosh was honored for his work as part of a team of astronomers who produced the first-ever direct images of a planetary system orbiting a star other than our sun using high-contrast, near infrared adaptive optics on the Keck II telescope in Hawaii. He has served as the principal investigator for several LDRD projects including probing other solar systems with current and future adaptive optics (05-ERD-055), tracing the shadows of planetary systems (08-ERD-043), and currently, examining images and spectra of extrasolar planets from advanced adaptive optics (11-ERD-048).



Bruce MacIntosh

- Beach was honored for his work in developing high-average-power diode-pumped lasers. Beach is currently investigating the feasibility of a hybrid rubidium resonance and exciplex pump laser (10-FS-002), and is a member of a team developing precision mono-energetic gamma-ray sources for NNSA missions (09-SI-004). He previously was part of LDRD teams developing cladding-pumped Raman fiber lasers (07-ERD-005) and precision split-beam, chirped-pulse, seed laser technology (05-ERD-061).

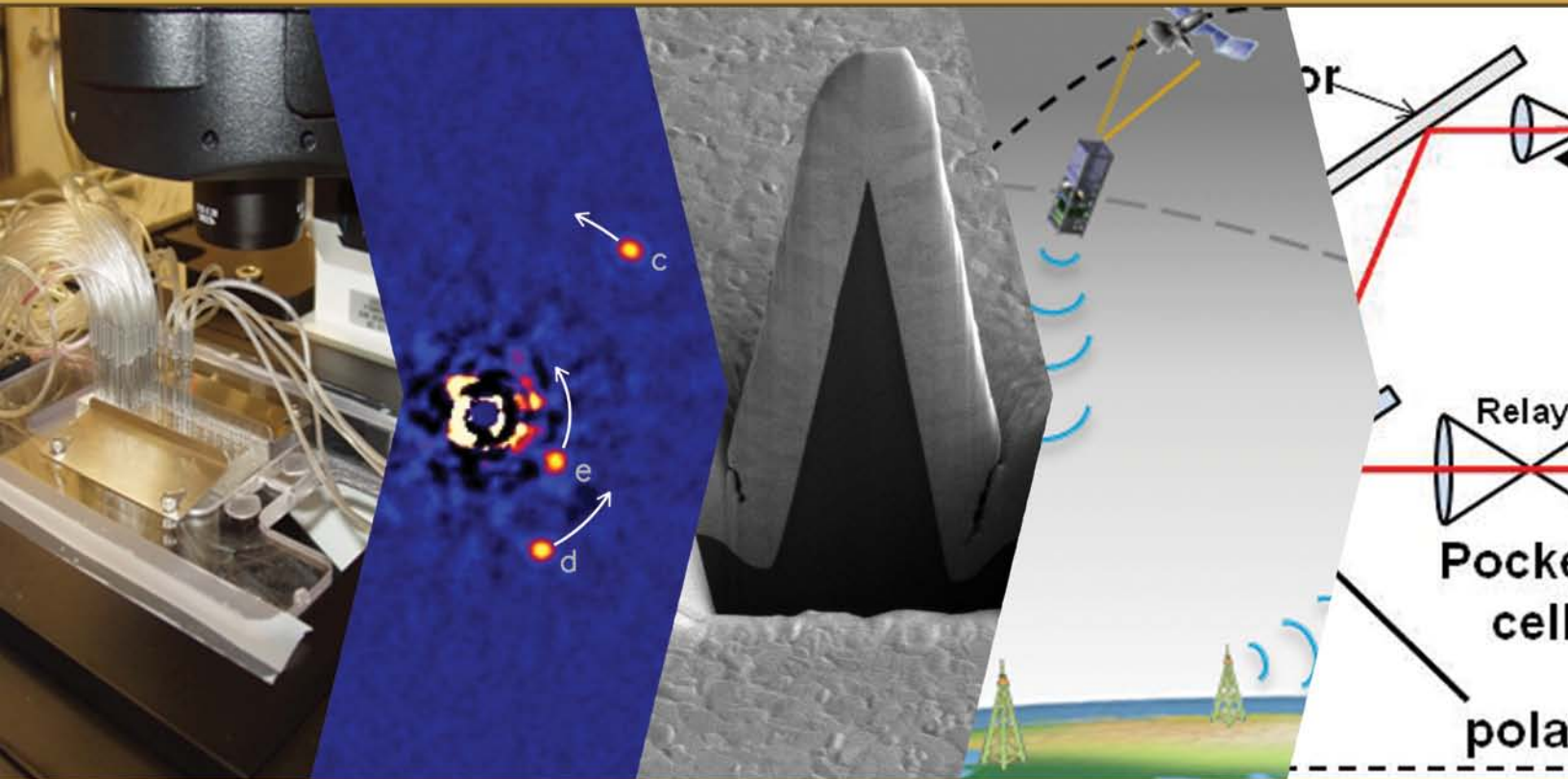
U.S. Frontiers of Engineering Symposium

Klint Rose was selected to take part in the U.S. Frontiers of Engineering Symposium in 2010, an annual gathering of “the nation’s brightest young

engineers.” Rose has participated in several varied LDRD projects as both principal and co-investigator, including a study of maskless, low-cost, high-performance polymer waveguides (09-ERD-057); transparent ceramic optics and advanced armor with nanostructured materials tailored in three dimensions (09-ERD-029); a viral discovery platform (08-SI-002); and a thermal-fluidic system for manipulating biomolecules and viruses (06-ERD-040).

Yoshiaki Arata Award

John Elmer was awarded the Yoshiaki Arata Award by the International Institute of Welding, the largest worldwide network of experts involved in the various areas of welding and joining technology, presented annually to “an individual who has realized extraordinary achievements in fundamental research in welding science and technology and its allied fields.” Elmer has served as both principal and co-investigator for LDRD projects relating to the science of high-performance solder and thermal forming and joining (10-LW-002 and 96-ERD-037).



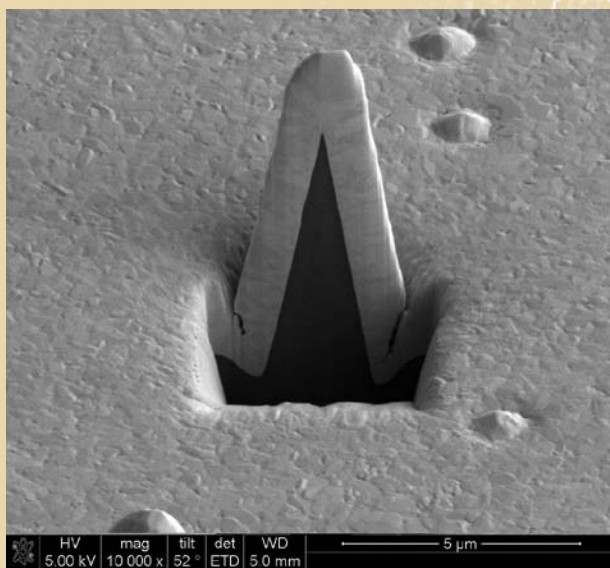
Advanced Sensors and Instrumentation

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

Abstract

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

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



Cross section of a super-lens for infrared light before the aperture is defined by a focused ion beam. The conical silicon core is surrounded by thick gold cladding to enhance photon confinement.

a minimum overhead burden in size, weight, and power. This, in turn, will enable new platform options and applications. At the end of the project we will have demonstrated the key detector components necessary for spectrometer operation at room temperature.

Mission Relevance

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

FY10 Accomplishments and Results

In FY10 we (1) successfully demonstrated the broadband heterodyne spectrometer architecture using a specialized high-speed quantum-well infrared photodetector fabricated by our research partners at the Jet Propulsion Laboratory—our system generated the desired heterodyne signal from infrared light and showed that signals could be obtained under operationally useful conditions with local oscillator performance presently achievable with state-of-the-art components such as quantum cascade lasers; (2) demonstrated, through experiments, ultimate achievable signal levels and showed that, in fact, these could be obtained without a nanostructured antenna; and (3) completed fabrication of sub-wavelength lenses and performed detailed calculations to illustrate the potential of these structures to improve spectrometer performance up to one hundredfold in the mid- to long-infrared wavelength domains. With these results, we have demonstrated the key detector components necessary for useful infrared spectrometer performance at near room temperature, using a broadband heterodyne architecture and a sub-wavelength lens. Records of invention covering this intellectual property have been filed. We will next seek support for full fabrication of this breakthrough instrument from government organizations with interest in remote optical detection of chemical vapor effluents.

Publications

Stevens, C., C. Cunningham, and J. Tringe, 2010. *Broadband infrared heterodyne spectrometer*. LLNL-TR-464192.

Tracing the Shadows of Planetary Systems—Bruce Macintosh (08-ERD-043)

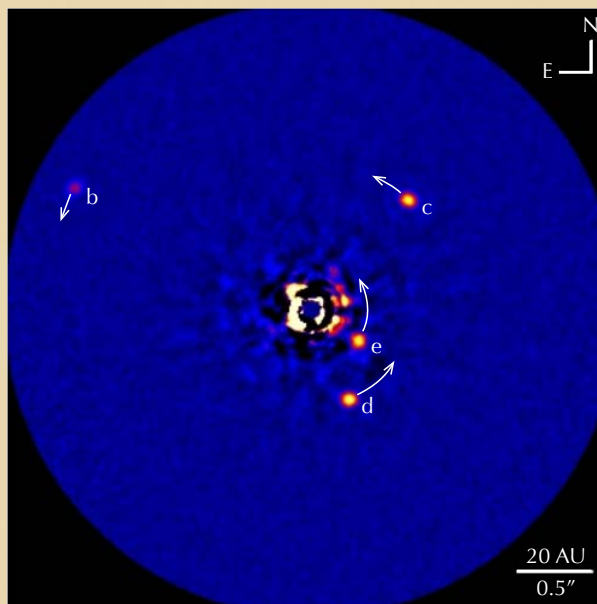
Abstract

The study of other solar systems is driven by the intersection of advanced optical technology and fundamental questions such as how are solar systems formed and are systems like our own common? The next frontier in exploring such systems is characterization through spectroscopy and polarimetry. We will use Livermore expertise in adaptive optics (AO) and image processing to observe interplanetary dust that traces the formation and presence of planets and to search for them using existing AO systems. We propose to develop advanced techniques such as an innovative Fourier-domain predictive controller, which can sharply improve the performance of AO systems for many applications, including remote sensing, microscopy, and lasers.

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

Mission Relevance

A key competency at Livermore, AO is used in applications from astronomy to microscopy and from beam control to surveillance. Advanced techniques benefit all 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 frontier science and technology and employs collaborations that will lead to new, innovative capabilities for LLNL.



Near-infrared adaptive optics image of the HR8799 planetary system showing the newly discovered fourth planet (labeled "e"). Arrows indicate the direction and magnitude of each planet's orbital motion.

FY10 Accomplishments and Results

In FY10 we (1) carried out additional observations of the HR8799 system with the Keck telescope and discovered a completely unanticipated fourth planet in this system, orbiting at the equivalent of the location of Saturn; (2) used more-precise measurements of the planetary orbits, including the new object, and computer models to evaluate the stability and evolution of the system and constrain the planets' masses, proving that these are true planets and not "failed stars;" (3) used the OSIRIS instrument at Keck to obtain spectra of the system's outermost two planets and, together with our collaborators, showed that these planets' atmospheres contain complex cloud structures and nonequilibrium chemistry, thus completing our survey of 90 young massive stars; (4) used AO to demonstrate the optimal modal control of simulated atmospheric turbulence using advanced microelectromechanical-system-deformable mirrors; and (5) developed algorithms for distinguishing and mitigating real and spurious vibration in fast pointing control. In summary, this project produced, in 2008, the first-ever images of an extrasolar planetary system, revealing three planets orbiting HR8799—an epochal result that opens up other solar systems to detailed physical characterization. This achievement was selected as the

runner-up Breakthrough of the Year by the American Association for the Advancement of Science, and the paper describing it was honored with the 2008–2009 Newcomb Cleveland Prize for best paper published in *Science*. Our team is now positioned to lead the scientific use of the Gemini Planet Imager, an instrument funded by the National Science Foundation and being constructed by an LLNL-led team, which will begin scientific operations in 2011.

Publications

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

Konopacky, Q. M., et al., 2010. "High-precision dynamical masses of very low mass binaries." *Astrophys. J.* **711**, 1087. LLNL-JRNL-426167.

Konopacky, Q. M., 2010. *Orbital properties of the HR 8799 planetary system*. 216th American Astronomical Society Mtg., Miami, FL, May 23–27, 2010. LLNL-POST-421514.

Konopacky, Q. M., et al., 2010. *Rotational velocities of very low-mass binaries*. 16th Cambridge Workshop on Cool Stars, Stellar Systems, and the Sun, Seattle, WA, Aug. 29–Sept. 2, 2010. LLNL-POST-450877.

Lunine, J., B. Macintosh, and S. Peale, 2009. "The detection and characterization of exoplanets." *Phys. Today* **62**, 46. LLNL-JRNL-416756.

Macintosh, B., 2010. *Progress and prospects for high-contrast adaptive optics*. SPIE Astronomical Telescopes and Instrumentation 2010, San Diego, CA, June 27–July 2, 2010. LLNL-ABS-423228.

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

Marois, C., et al., in press. "Images of a fourth planet orbiting HR8799." *Nature*. LLNL-JRNL-463073.

Poyneer, L., and J.-P. Véran, 2010. "Kalman filtering to suppress spurious signals in adaptive optics control." *J. Opt. Soc. Am. A* **27**, 223. LLNL-JRNL-426892.

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

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

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

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

Abstract

The timely, effective management of infectious disease—including biothreat agents—requires rapid, scalable, field-operable diagnostics. We will develop a new point-of-care detection capability by designing and characterizing an isothermal assay capable of detecting nucleic acid in clinical samples within 30 minutes. 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 collaborate with the Institute for Animal Health in the United Kingdom.

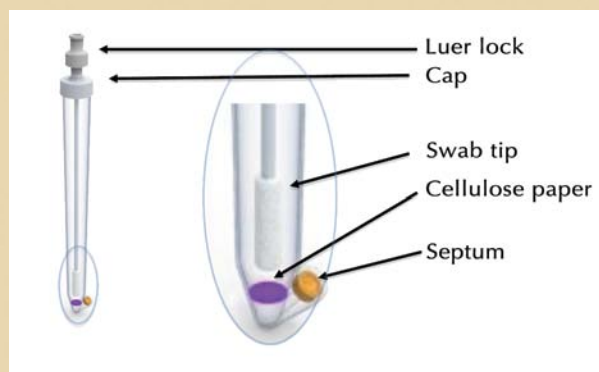
The technology generated by this project will better prepare U.S. first responders to effectively react to infectious diseases and bioterrorism. In the case of foot-and-mouth disease, the technology will reduce the economic impact of an outbreak by (1) providing rapid confirmation of clinical diagnosis, (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, scientifically cutting-edge field.

FY10 Accomplishments and Results

In FY10 we (1) designed and fabricated disposable devices for pathogen detection that integrated sample preparation, nucleic acid amplification, and colorimetric detection into one tube; (2) successfully tested the prototypes and our assay under biosafety level-3 laboratory conditions at the World Reference Laboratory for Foot and Mouth Disease Virus at the Institute for Animal Health at Pirbright in the United Kingdom; and (3) filed three provisional patents related to inventions that resulted from this project and published our findings in an *IEEE Transactions on Biomedical Engineering* special issue dedicated to point-of-care detection. The successful conclusion of this project enabled sample preparation, nucleic acid amplification, and detection all to take place in one disposable tube for detection of live foot-and-mouth disease virus. We are hopeful that we can continue this research with support from the Department of Homeland Security to develop a second-generation, disposable pathogen-detection system.



Schematic rendering of a disposable prototype device developed for point-of-care pathogen detection.

Publications

Bearinger, J. P., et al., in press. "Development and initial results of a low cost, disposable, point-of-care testing device for pathogen detection," *IEEE Trans. Biomed. Eng.* **99**. LLNL-JRNL-463445.

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

Abstract

Detectors to sense nuclear and radioactive weapons concealed in transit across borders 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, but must be operated at cryogenic temperatures. A room-temperature detector is greatly preferred because of cost and ease of use, but the current state of the art 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 better than 1% and operate at room temperature. We will use a band-gap engineered multilayer structure to allow full signal collection while simultaneously rejecting noise to improve detector performance, resulting in a 90% reduction in current leakage 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.

FY10 Accomplishments and Results

We (1) developed finite-element modeling of amorphous CZT hetero-junctions to understand electronic conduction mechanisms; (2) studied amorphous CZT hetero-junctions using current, voltage, and temperature measurements for characterization of Schottky barrier height; (3) fabricated amorphous selenium and CZT and amorphous silicon hetero-junction detectors that reduced leakage current by a factor of 100, resulting in an effective resistivity of greater than 10^{12} ohm-cm in a bulk material otherwise too conductive for typical CZT gamma detectors; and (4) demonstrated proof-of-principle detectors with improved energy resolution. In summary, this project enabled the development of novel hetero-junction contacts for the reduction of noise in CZT-based gamma ray detectors. The Defense Threat Reduction Agency will support further work aimed at understanding the effect that CZT surfaces have on the performance of CZT radiation detectors.



Schematic diagram of the amorphous selenium-cadmium-zinc-telluride-amorphous silicon (a-Se-CZT-a-Si) hetero-structured gamma ray detector, with aluminum (Al) and platinum (Pt) electrodes, developed with this project.

Publications

Conway, A. M., et al., 2009. *Amorphous semiconductor blocking contacts on CdZnTe gamma detectors*. 2009 Intl. Semiconductor Device Research Symp., College Park, MD, Dec. 9–11, 2009. LLNL-ABS-461411.

Conway, A. M., et al., 2010. *Amorphous semiconductor blocking contacts on CdZnTe gamma detectors*. 2010 Materials Research Society Fall Mtg., Boston, MA, Nov. 29–Dec. 3, 2010. LLNL-ABS-416278.

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

Nelson, A. J., et al., 2010. "X-ray photoemission analysis of passivated $\text{Cd}_{(1-x)}\text{Zn}_x\text{Te}$ surfaces for improved radiation detectors." *Mater. Lett.* **63**, 180. LLNL-PROC-400091.

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

Voss, L. F., et al., 2010. "Surface current reduction in (211) oriented CdZnTe crystals by Ar bombardment." *J. Appl. Phys.* **108**, 014510. LLNL-JRNL-426884.

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

Abstract

DNA microarrays for genetic testing identify hybridization patterns and signatures ideal for environmental and clinical monitoring, but 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 the (1) chemical and physical changes that occur during the processes of in vitro DNA hybridization; (2) stabilities of different chemical couplings between DNA molecules and surfaces; (3) controlling mechanisms between DNA in solution and DNA affixed to a solid support in hybridization experiments; (4) influence of optical, thermal, and fluidic effects on the intrinsic binding or stringency for DNA targets on probes; and (5) analysis of individual spots to eliminate the complex background signal.

Mission Relevance

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

FY10 Accomplishments and Results

In FY10 we (1) developed and demonstrated high-sensitivity, off-line detection of eluted DNA oligonucleotides for selective release; (2) upgraded the selective-release optical system to give a smaller heating area and better penetration; (3) performed our first integrated flow-cell hybridization experiment with a biological sample using the LLNL virulence array; and (4) began experiments to reduce hybridization times. We deferred regeneration work planned for this LDRD because of a reduced funding level. In addition, we originally proposed to demonstrate selective release on the microarray

in FY10. However, because of technical challenges that included developing laser system controls and selecting the correct buffer chemistry to ensure that only selective release occurred (instead of eluting everything off the chip), this task was not completed. A surface chemist joined our team at the end of FY10 to help solve the buffer issue in FY11.

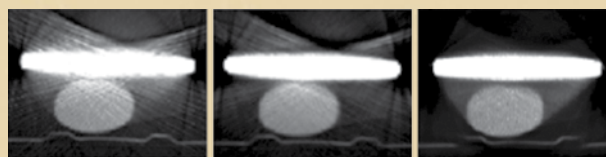
Proposed Work for FY11

In FY11 we will (1) perform initial demonstrations of selective release, then shift focus to characterizing the effects of laser power schedule and fluid flow conditions on release selectivity and yield; (2) perform initial characterization of hybridization rates using an artificial kinetics array, then conduct hybridization experiments to determine rates using biological samples on the virulence array; and (3) collect the remaining characterization data required to produce manuscripts on selective release and hybridization.

Optimized Volumetric Scanning for X-Ray Area Sources—Angela Foudray (09-ERD-045)

Abstract

Our goal is to perform a systematic study to determine optimal scanning geometries for x-ray area sources and provide a roadmap for area-source imaging in field applications such as explosives detection and weapons inspection. Area sources are typically implemented through the use of an array of standard “point” x-ray sources. Area sources have a much greater spatial coverage than the traditionally used point sources, enabling a more accurate volumetric scanning of an object. This capability is of high importance in many key efforts at Lawrence



Comparison of reconstruction algorithms for a traditional fan beam system, showing how the application of algorithms (center and right) significantly reduces streak artifacts.

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

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

Mission Relevance

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

FY10 Accomplishments and Results

In FY10 we (1) developed an understanding of the physics for modeling and for data collection in collaboration with Triple Ring Technologies, a company that designs and manufactures an x-ray imaging system based on an x-ray array, which is a form of area source; (2) designed, manufactured, and imaged various objects of interest; (3) designed and applied data-collection methods and techniques for instances in which the source and detector are parallel, generating full-angle, limited-angle, and

sparse-angle data sets; (4) identified, developed, and utilized iterative algorithms—the Kallman conjugate gradient algorithm and randomized subset expectation maximization algorithm—that significantly reduce streak artifacts in the image obtained with an area source; and (5) identified and utilized figures of merit to evaluate system performance.

Proposed Work for FY11

In FY11 we will collaborate with Triple Ring Technologies and Stanford University to investigate acquisition geometries and increase acquisition speed by experimenting with variable source-detector distance and with a source and detector not parallel to each other. In addition, we propose to further increase reconstruction speed by extending the two iterative reconstruction algorithms we investigated in FY10 to graphical processor units.

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

Abstract

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

In addition to enabling rapid and sensitive biological organism detection, this work will provide the first proof of concept for the integration of photonic and plasmonic crystal-based signal transduction and separation. This new class of extremely compact and sensitive flow-through sensors will enable real-time detection of known organisms for counterterrorism, environmental, and medical applications, and enable future work focused on generating

fingerprints for detecting unknown organisms. Novel design and nanofabrication approaches for integrating photonics and spectroscopy transduction will also be developed, enabling next-generation multi-functional biosensing platforms and paving the way for new membrane-based devices.

Mission Relevance

This project directly supports Livermore's efforts in the rapid detection of threats in support of the biosecurity mission by developing a novel class of platforms for identifying biological particles. Current techniques are based on polymerase chain reaction, which is not easily carried out in the field. The project takes an innovative approach to nanofabrication challenges encountered when creating multi-functional platforms. It will advance the science of functional nanostructures, signal transduction, and organism detection, which will be of interest to both national security and health agencies.

FY10 Accomplishments and Results

In FY10 we (1) optimized the instrumental setup for measuring optical transmission spectra of photonic crystals and for fabricating flow-through

photonic crystal devices to enable integration with fluidics; (2) performed finite-difference time-domain modeling simulations to guide the integration of SERS structures with the photonic crystal devices; (3) determined the detection limits of defect-free photonic crystal devices, using both experimental data and simulations and demonstrating that the devices could be used for size-selective particle detection; and (4) developed a fundamental understanding of the geometric and materials requirements for integrating fluid flow, sensitive photonic crystal transmission measurements, and SERS. Our work on the detection of bio-organism simulants was featured on the cover of *Applied Physics Letters*.

Proposed Work for FY11

In FY11 we plan to (1) complete fabrication of the flow-through photonic crystal membranes and integrate them with a fluidic assembly for real-time organism simulant-binding studies; (2) integrate optical transmission measurement and Raman measurement on the same device, using either plasmonic crystal or nanoscale gold-ring geometry to provide for SERS enhancement of the Raman signal while maintaining the photonic bandgap; and (3) incorporate these design elements into a prototype device that will be functionalized for selective organism simulant capture.

Publications

Baker, S. E., et al., 2010. "Detection of bio-organism simulants using random binding on a defect-free photonic crystal." *Appl. Phys. Lett.* **97**, 113701. LLNL-JRNL-432541.

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

Baker, S. E., et al., 2010. *Silicon filtration membranes for organism capture, detection, and identification*. 2010 Materials Research Society Spring Mtg., San Francisco, CA, April 5–9, 2010. LLNL-POST-426522.



A paper describing this work—"Detection of bio-organism simulants using random binding on a defect-free photonic crystal"—was featured on the cover of the September 13, 2010 issue of *Applied Physics Letters*.

Antibiotic Heteroresistance in Methicillin-Resistant *Staphylococcus Aureus*: Microchemostat Studies at the Single-Cell Level—Raymond Lenhoff (09-LW-112)

Abstract

The development of new antibiotics is outpaced by the emergence of antibiotic-resistant bacterial strains, making it crucial to understand the genetic mechanisms of antibiotic resistance. At the center of this mystery is heteroresistance—the concurrent existence of multiple bacterial subpopulations with varying degrees of antibiotic resistance. We propose to leverage a novel microchemostat technology at LLNL to probe heteroresistance in bacteria, with the aim of restoring the efficacy of existing antibiotics that have lost potency. We will use a clinically important bacterium, methicillin-resistant *Staphylococcus aureus* (MRSA), as our test case.

If successful, we will experimentally determine the mechanism of heteroresistance, including constructing protein–protein fusions with other heteroresistance candidates: *hmrA*, the operon *vraSR* (already known to be necessary for methicillin resistance), and a global regulator of cell-wall biosynthesis that is activated by oxacillin and vancomycin.

Mission Relevance

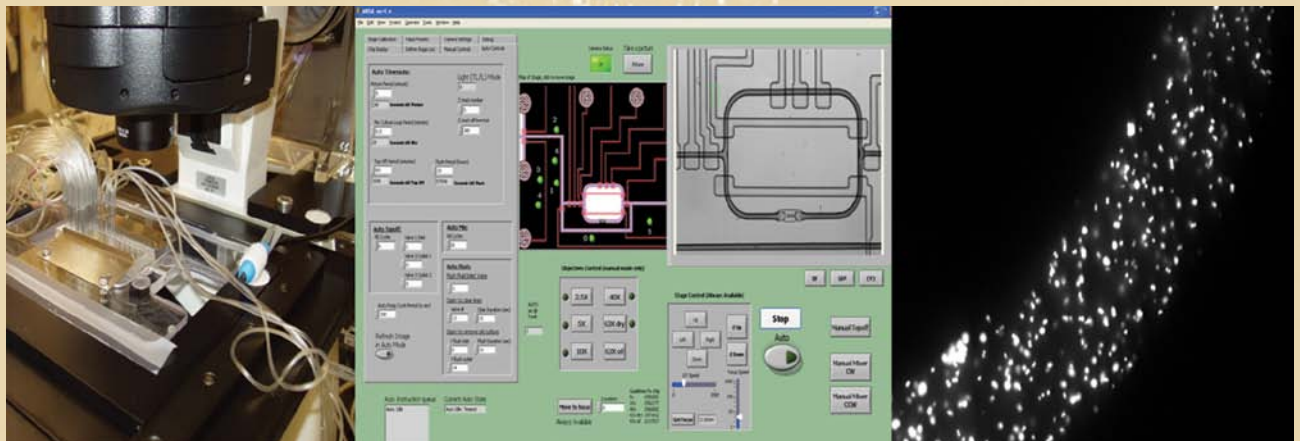
By elucidating the genetic mechanisms of antibiotic resistance and potentially helping to restore the potency of existing antibiotics against both clinically significant bacteria and potential bioterror pathogens, this project supports the Laboratory's missions in homeland and national security. It additionally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

FY10 Accomplishments and Results

In FY10 we (1) grew MSRA cultures in our microchemostat to a steady state and at a fixed dilution rate, (2) performed preliminary fluorescence distributions of the gene expression for *mecA* bacteria that was fused with green fluorescent protein, and (3) examined the role of *mecA* in heteroresistance. We are hopeful this research will be continued with support from the Defense Advanced Research Projects Agency for a project on prediction of virus evolution.

Publications

Lenhoff, R., 2010. *Antibiotic heteroresistance in methicillin-resistant Staphylococcus*. LLNL-TR-463636.



Microfluidic culture project for analysis of antibiotic-resistant *Staphylococcus aureus*. The microfluidic chip is shown on the microscope stage (left), with software interface (middle) and fluorescent *S. aureus* in the microfluidic bioreactor (right).

Real-Time Space Situational Awareness— Scot Olivier (10-SI-007)

Abstract

More than 80 countries have joined the space community, making Earth orbit an increasingly congested piece of aerial real estate. Hundreds of active satellites as well as thousands of pieces of space debris orbit Earth. We propose to develop and demonstrate advanced capabilities for “space situational awareness” that will result in enhanced safety for space operations. We will leverage three relevant key capabilities: extensive experience with numerous operational sensor systems, sophisticated analysis tools for interpreting data from multiple sensor systems, and unparalleled expertise in simulation and modeling of complex systems using the world’s largest computers.

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

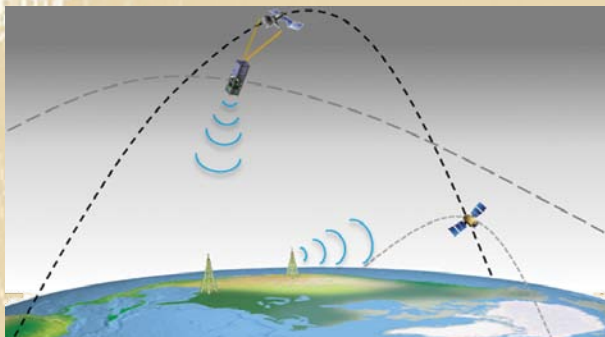
Mission Relevance

Freedom of operation in a crowded space environment is crucial to U.S. interests, and maintaining space flight safety is a key component of this freedom. Utilizing unique Laboratory technical resources to help address this issue directly supports core LLNL missions in national and global security. Through this project, Livermore has an opportunity

to establish a major new business area, to enhance core competencies important for basic scientific research, and to provide leadership for the U.S. in an area of intense national interest and enduring importance.

FY10 Accomplishments and Results

In FY10 we (1) developed advanced techniques for high-performance computer modeling and simulation of signatures, observables, and sensor responses from threats to space operations, including improved physics models for satellite collisions, detailed models of radar and optical sensor physics, advanced orbital propagation and orbit determination algorithms, and satellite conjunction analysis and collision-probability algorithms; (2) incorporated these simulation and modeling techniques into a comprehensive space situational awareness simulation framework, including the ability to process feedback from sensor and analysis modules; (3) demonstrated techniques for synthesizing data from multiple sources using simulated data; (4) used our simulation framework to develop requirements for new sensor systems to improve space flight safety; and (5) designed a new prototype sensor system for satellite collision avoidance using a mission concept named Space-Based Telescopes for Actionable Refinement of Ephemeris (STARE).



Space-Based Telescopes for Actionable Refinement of Ephemeris (STARE) will help prevent satellite collisions with improved sensor systems for monitoring and modeling satellite orbits and collisions, along with efficient synthesis of data from multiple sources.

Proposed Work for FY11

In FY11 we will (1) develop additional advanced techniques for modeling and simulating threats to space operations, including computationally efficient models for satellite collisions and radar reflectivity calculations, detailed models of radar and optical sensor operation and data processing, and techniques for modeling and determining the orbits of tumbling objects; (2) incorporate these additional techniques into our comprehensive space situational awareness simulation framework, including upgrading sensor and analysis modules to provide feedback; (3) demonstrate the synthesis of real data from multiple sources; (4) demonstrate sensor-cueing techniques; and (5) continue to develop improved sensor systems by building and testing the prototype designed in FY10.

Publications

de Vries, W., and D. Phillion, 2010. "Monte Carlo method for collision probability calculations using 3D satellite models." *Proc. 11th Ann. Advanced Maui Optical and Space Surveillance Technologies Conf.* LLNL-CONF-454474.

Henderson, J. R., et al., 2010. "Intelligent sensor tasking for space collision mitigation." *Proc. SPIE* **7691**. LLNL-TR-427454.

Horsley, M., 2010. "A Bayesian approach to multi-sensor track correlation." *Proc. 11th Ann. Advanced Maui Optical and Space Surveillance Technologies Conf.* LLNL-CONF-454076.

Horsley, M., and B. Fasnfest, 2010. "A parallel, high-fidelity radar model." *Proc. 11th Ann. Advanced Maui Optical and Space Surveillance Technologies Conf.* LLNL-CONF-454075.

Jefferson, D., and J. Leek, 2010. "Application of parallel discrete event simulation to the Space Surveillance Network." *Proc. 11th Ann. Advanced Maui Optical and Space Surveillance Technologies Conf.* LLNL-CONF-454938.

Jiang, M., et al., 2010. "A scalable visualization system for improving space situational

awareness." *Proc. 11th Ann. Advanced Maui Optical and Space Surveillance Technologies Conf.* LLNL-CONF-455073.

Phillion, D., et al., 2010. "Large-scale simulation of a process for cataloging small orbital debris." *Proc. 11th Ann. Advanced Maui Optical and Space Surveillance Technologies Conf.* LLNL-CONF-454931.

Springer, H., et al., 2010. "Satellite collision modeling with physics-based hydrocodes: Debris generation predictions of the iridium-cosmos collision event and other impact events." *Proc. 11th Ann. Advanced Maui Optical and Space Surveillance Technologies Conf.* LLNL-CONF-454151.

Compact, Efficient Lasers for Inertial Fusion-Fission Energy—Robert Deri (10-SI-010)

Abstract

To mitigate the challenges of nuclear energy and to advance the timescale for availability of fusion sources, the Laboratory envisions a novel once-through, closed fusion-fission nuclear fuel cycle based upon the Laser Inertial Fusion Energy (LIFE) concept. We propose to develop a compact, economically viable laser system that can drive the LIFE power plant. Current laser designs required for LIFE are large and expensive. Eliminating these impediments is critically important to enabling practical fusion energy, providing abundant clean power without nuclear waste disposal, safety, or proliferation issues. We will develop key, enabling optical technologies and use them to design a laser with performance, footprint, and costs suitable for LIFE, leading to a laser architecture and design that will guide further development. We will test key technology elements of this laser to validate our approach.

We expect to deliver an advanced laser system architecture and baseline design for LIFE that is compact and cost effective, accompanied by experimental results for key technology elements that validate our approach. Relative to today's baseline, the design could reduce the length of the optical

beam path by more than fivefold, leading to a similar reduction in the building size required to house a LIFE power plant. We will develop system concepts and technology that enable a significant improvement in system costs required for the diode laser pumps. Because these components account for over 90% of LIFE laser system cost, as calculated with current technologies, this represents a significant reduction in the overall cost. These results will define a clear path forward for realizing the laser system required.

Mission Relevance

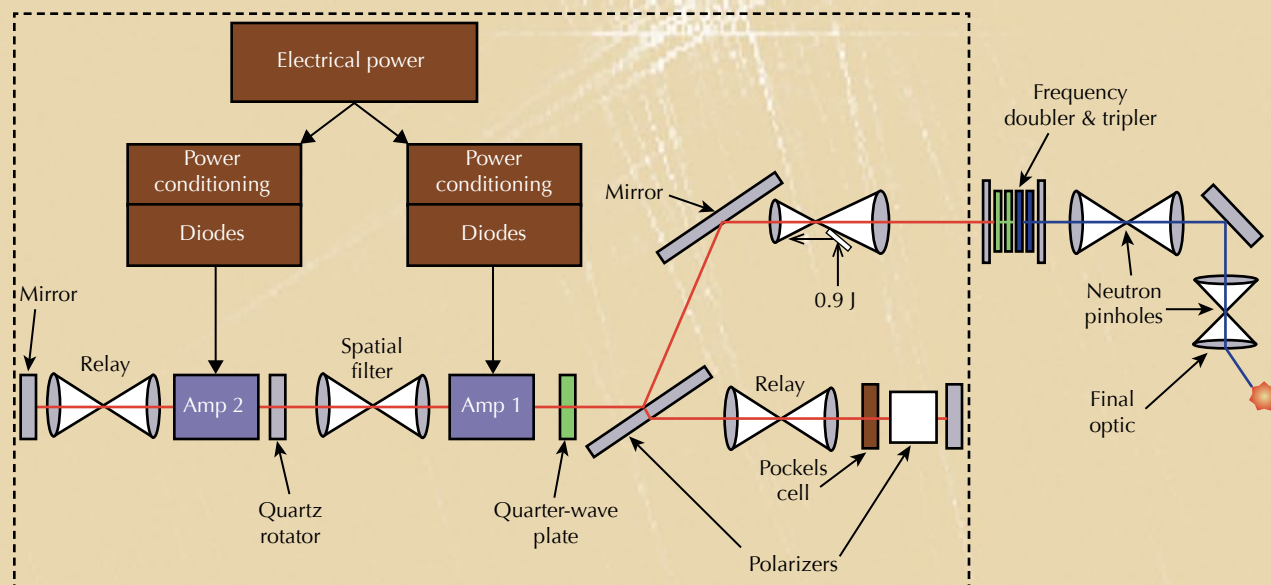
This project supports LLNL's mission of enhancing energy security for the nation and builds directly upon the Laboratory's world-class capabilities in inertial-confinement fusion and laser technologies. Resolving key issues for practical, cost-effective laser inertial-fusion energy plants also supports the Laboratory mission in environmental security by eliminating nuclear waste disposal. In addition, high-power laser advances achieved by this work will enable widespread deployment of laser-driven mono-energetic gamma-ray sources, which provide unique advantages for detecting nuclear devices and reducing the threat posed by nuclear terrorism, in support of LLNL's national and homeland security missions.

FY10 Accomplishments and Results

We (1) developed simulation methods to assess the impact of new laser media and thermal birefringence on laser system performance; (2) applied these tools to develop a laser architecture concept with an associated pump cavity design that is compact, efficient, and robust to thermal birefringence—a less than 16-m³ “beam-line in a box” based on a neodymium-doped glass gain medium; (3) verified that the beam line provides greater than 6-kJ infrared output pulses with a wall-plug efficiency (i.e., the efficiency of converting electrical to optical power) greater than 10%; and (4) began applying our methods to investigate the potential advantages of alternative gain media, achieving results that guided several laser subsystems—notably diode pumps and a Pockels cell—and leading to new designs for these components that we hope to further develop in FY11.

Proposed Work for FY11

In FY11 we will continue to explore architectural paths to even greater performance gains. Specifically, we will (1) build subscale prototypes of novel spatial filters and evaluate their performance at high fluences, (2) investigate the gain saturation behavior of neodymium-doped glass for diode pumping and circularly polarized light, (3) build prototype Pockels cell electrodes that eliminate the



The 1-W optics that can be folded into a single, transportable unit are shown within the dashed line of this laser architecture schematic.

need for plasmas and test their ability to withstand high fluences, and (4) explore bonding technologies that can enable high-intensity diode arrays.

Publications

Bayramian, A. J., et al., 2010. "A laser technology test facility for laser inertial fusion energy." *J. Phys. Conf.* **244**, 032016. LLNL-PRES-416506.

Bayramian, A. J., et al., 2010. *Fusion energy: Laser systems required to harness the power of the sun*. 2010 Conf. Lasers and Electro-Optics/Quantum Electronics and Laser Science Conf. (CLEO/QELS), San Jose, CA, May 16–21, 2010. LLNL-PRES-432679.

Bayramian, A. J., et al., 2010. *Heat capacity laser*. HEC DPSSL 6th Workshop High Energy Class Diode Pumped Solid State Lasers, Versailles, France, Sept. 8–10, 2010. LLNL-PRES-452893.

Bayramian, A. J., et al., 2010. *LIFE laser system update*. HEC DPSSL 6th Workshop High Energy Class Diode Pumped Solid State Lasers, Versailles, France, Sept. 8–10, 2010. LLNL-PRES-452916.

Bayramian, A. J., et al., 2010. *LLNL DPSSL activities*. HEC DPSSL 6th Workshop High Energy Class Diode Pumped Solid State Lasers, Versailles, France, Sept. 8–10, 2010. LLNL-PRES-452915.

Bayramian, A. J., et al., 2010. *NIF update*. HEC DPSSL 6th Workshop High Energy Class Diode Pumped Solid State Lasers, Versailles, France, Sept. 8–10, 2010. LLNL-PRES-452971.

Caird, J. A., et al., 2009. *DPSSL design for LIFE*. 6th Intl. Conf. Inertial Fusion Sciences and Applications (IFSA 2009), San Francisco, CA, Sept. 6–11, 2009. LLNL-PRES-416598.

Rubenchik, A. M., et al., 2010. "Modulation instability in high power amplifiers." *Optic. Express* **18**(2), 1380. LLNL-JRNL-431613.

Embedded Sensors for Monitoring Complex Systems—Jack Kotovsky (10-ERD-043)

Abstract

As the nation's nuclear stockpile is reduced in size, stockpile surveillance approaches must change significantly to increase safety, security, and cost effectiveness. This project will explore broad-spectrum sensing technologies for this purpose. Several embedded sensing methods that have not been previously explored will be pursued. Broad-spectrum sensors most efficiently address the surveillance challenges and deliver the greatest overall impact. For this reason, this effort pursues the broad-sensing technology of gas sensing. Techniques for assessing noble and non-noble species will be considered using methods that are compatible with actual stockpile applications.

If successful, several new sensing capabilities will be produced for stockpile surveillance. Specifically, optic-fiber-based surface-enhanced Raman scattering (SERS), photo-acoustic spectroscopy, and ionization techniques will be considered for detection of unknown gas mixtures. Novel materials, fabrication processes, and designs will be explored for their applicability to the difficult constraints of in situ state-of-health stockpile monitoring.

Mission Relevance

If successful, this project will lay the groundwork for a game-changing, comprehensive sensor suite that will dramatically enhance stockpile surveillance and significantly advance the entire nuclear weapons complex, in support of the Laboratory's national security and stockpile stewardship missions.

FY10 Accomplishments and Results

In FY10 we pursued SERS and photo-acoustic spectroscopy gas sensing. Specifically, we (1) constructed a dedicated gas cell with a cooling and heating apparatus for SERS experiments; (2) tested and collected data on pure oxygen using SERS assisted by temperature control; (3) performed initial tests on toluene detection with SERS; (4) devised a novel laser excitation scheme that will compensate for system noise, allowing continued shrinking of the overall system for photo-acoustic spectroscopy; and

(5) experimentally tested photo-acoustic devices, successfully measuring atmospheric carbon dioxide.

Proposed Work for FY11

In FY11 we propose to (1) improve SERS detection limits for toluene vapor to less than 0.1%; (2) perform qualitative and quantitative SERS measurements of single and mixed gases; (3) evaluate the adsorption properties of SERS substrates, such as adsorption and desorption rates and sticking probability; (4) fabricate an optical acoustic detector and test it with carbon dioxide mixtures; and (5) characterize and miniaturize the acoustic detection cell.

Publications

Bond, T. C., et al., 2010. *Large-area nanopillars SERS arrays*. 38th Ann. Conf. Federation of Analytical Chemistry and Spectroscopy Societies (FACSS 2010), Raleigh, NC, Oct. 17–21, 2010. LLNL-POST-433531.

Bora, M., et al., 2010. “Plasmon-resonant cavities in vertical nanowire arrays.” *Nano Lett.* **10**, 2832. LLNL-JRNL-425128.

Bora, M., et al., 2010. *Vertical pillar arrays as plasmon nanocavities*. 2010 Solid-State Sensors, Actuators, and Microsystems Workshop (Hilton Head 2010), Hilton Head, SC, June 6–10, 2010. LLNL-ABS-420921.

Passive, Standoff Detector of High-Density Masses with a Gravity Gradiometer Based on Atom Interferometry— Stephen Libby (10-FS-003)

Abstract

Each year, millions of cargo containers from around the world are shipped to U.S. ports. Monitoring the contents in such a vast volume of containers poses a significant challenge to homeland security and emergency response experts. Determining the mass of containers is key to identifying which containers require further scrutiny for security and for monitoring treaty compliance. For the security, emergency response, and treaty

verification communities, passive methods of determining shipping container mass are highly desirable. We propose to test the feasibility of a completely new passive method to determine the mass of high-density material in a closed container, without moving or otherwise manipulating the container. We will apply an atomic fountain, an interferometric gravity gradiometer developed at Stanford University, to perform differential gravity measurements around the container and infer the overall mass configuration present as a function of distance and integration time.

If the demonstration of relevant mass determination as a function of distance and integration time is successful, we will obtain the fundamental scientific understanding required to envision a portable system for use in security, emergency response, and treaty verification, as well as extend the ability to image density distributions. This capability has the potential to replace aspects of x-ray radiography with a completely passive technique.

Mission Relevance

Passive methods to determine masses in shipping and other containers used in commerce are highly desirable and would supply complementary information to nuclear methods, relevant to the Laboratory's mission in nuclear threat elimination, as well as efforts for homeland security.

FY10 Accomplishments and Results

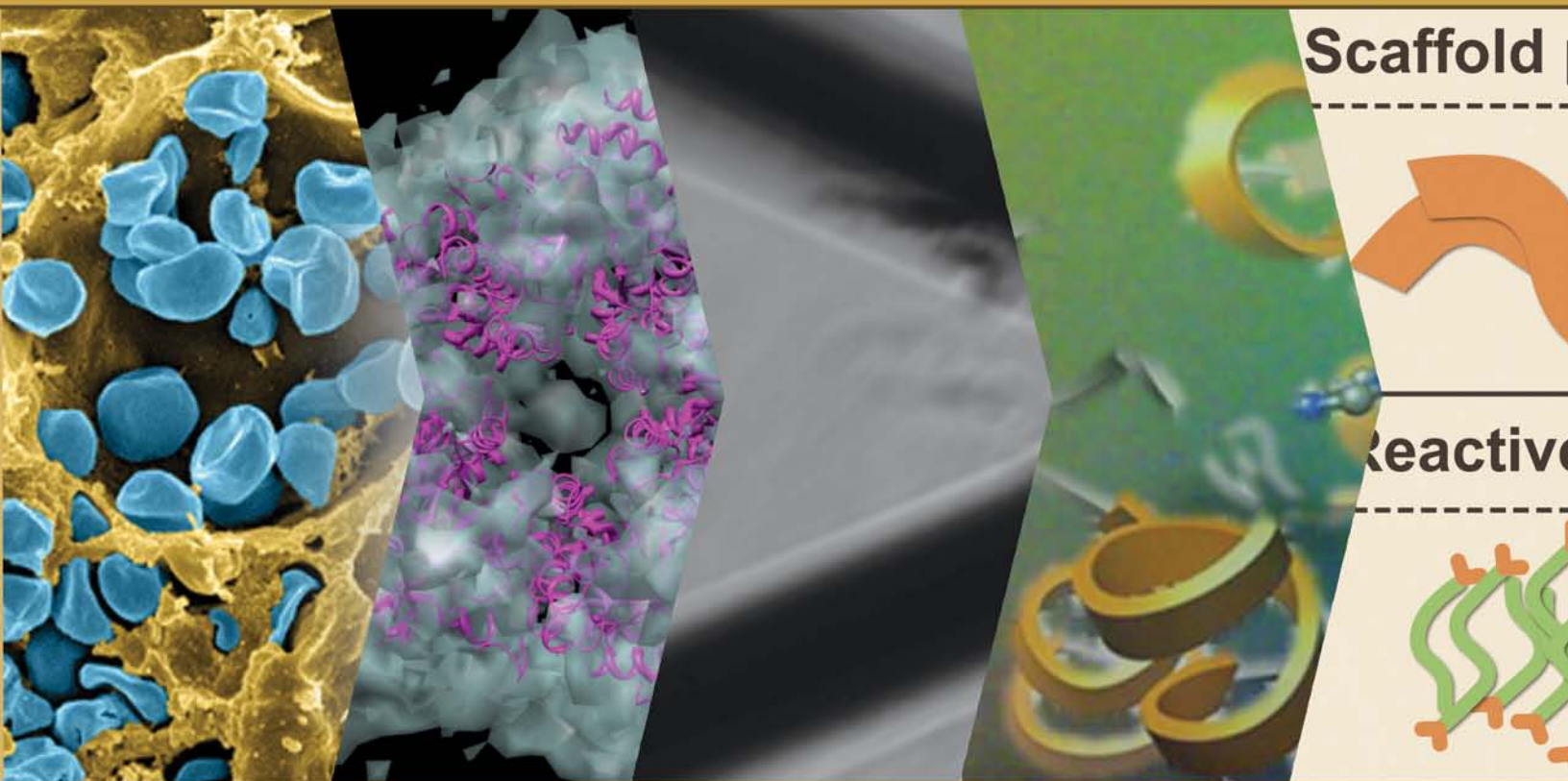
In FY10 we successfully used a cold-atom fountain gravity gradiometer to demonstrate relevant mass and mass-distribution detection at standoff distances of up to 1 m and in times as short as 800 s. Specifically, we (1) built a blind box containment system coupled to a mass translator to collect position-dependent data, (2) accurately matched detailed atomic interferometer data to our new computational models of the perturbing masses, (3) measured and quantified in detail the detector Allan noise characteristics to develop relative probability models for distinguishing mass-distribution hypotheses, and (4) verified that the model quantifies the gravity gradient interferometer response as a function of source mass distribution, location, and integration time for application to a mobile sensor. A record of invention was submitted for this new capability. In summary,

we successfully demonstrated the ability to detect and distinguish high-density masses relevant to emergency response with a cold-atom interferometer gravity gradiometer and new computational sensor response models. With the data obtained and modeling tools established in this feasibility study, our next step will be to approach DOE and the Department of Homeland Security to develop a prototype, practical mobile sensor system for use in emergency response, treaty monitoring, and other security-related applications.

Publications

Brady, K., S. B. Libby, and V. Sonnad, in press.

"Towards density imaging with atomic-interferometry-based gravity gradiometry." *J. Undergrad. Res.* LLNL-JRNL-451331.



Biological Sciences

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

Abstract

The recent ban on use of antibiotics when manipulating bacteria designated as select-agent pathogens has severely hampered research in this important area and created an urgent and unaddressed need for molecular genetic technologies involving non-antibiotic selectable markers. The main objective of this project is to advance basic and applied research on bacterial pathogens by developing a genetic engineering technology that will enable manipulation of these pathogens without the use of antibiotics. Our specific goals 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 relevant pathogens.

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

Mission Relevance

By developing biodefense capabilities and furthering our understanding of mechanisms of virulence in select-agent pathogens, our project supports LLNL's homeland and national security missions by anticipating and meeting the challenges of mitigating the evolving biosecurity threat.

FY10 Accomplishments and Results

In FY10 we (1) successfully introduced genetic material into the *Yersinia pestis* (plague) chromosome

and selected for the genetically altered strains, though we could not confirm that the new strains had the intended genetic mutation; (2) constructed a mild toxin that could be transformed, in a plasmid, into bacteria such that the bacteria could propagate in the presence of a plasmid; (3) successfully produced strains of bacteria that express red fluorescent protein; and (4) introduced antitoxin into a bacterial chromosome by recombination, but were unable to couple the toxin–antitoxin system such that we were able to select for specifically engineered genetic mutations. We were not able to reach a publishable endpoint for this project, although we successfully completed all but one of the interim proof-of-principle tasks, but we hope to continue this research through the publications stage via a follow-on collaboration with colleagues at California State University, Fullerton.

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

Abstract

Currently, the pharmaceutical industry is not actively pursuing development of antimicrobial compounds from natural products. This is because of 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* (plague), which delivers virulence proteins into host cells using a macromolecular protein complex called the injectisome. Specifically, we will (1) provide new antibacterial

compounds and increase potential countermeasures against select-agent bacterial and opportunistic drug-resistant pathogens, (2) determine the plague injectisome's full complement of protein components and detailed information of its self-assembly, and (3) characterize effective natural products in collaboration with the pharmaceutical or biotechnology industry. Identified proteins will be available for targeting in biodetection and therapeutic strategies.

Mission Relevance

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

FY10 Accomplishments and Results

In FY10 we completed testing of 450 drugs approved by the Food and Drug Administration against 21 strains of bacteria, including 12 multi-drug-resistant clinical isolates of the pathogenic bacterium *Acinetobacter baumannii* using two different endpoint screens. There were 36 compounds shown to be effective in one of two biological assays—of these, 17 were effective in both. Minimum inhibitory concentrations were determined for four rifamycin-family antimicrobials against all bacteria, which suggest these may be useful as broad-spectrum antimicrobials. In addition, we continued to employ protocols to further subdivide the plague proteome. Our seminal work in single-cell host–pathogen interactions in real time will enable the study of temporal and kinetic aspects of the type III secretion system. The successful conclusion of this project enabled several studies in drug discovery and produced a novel technique for study of host–pathogen interactions. Our research has fostered follow-on LDRD and programmatic projects at LLNL as well as related projects at the University of California at Davis and the University of Washington.

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.

Chromy, B. A., T. A. Laurence, and P. Pauzauskie, 2010. "Revealing the secrets of a deadly disease." *Sci. Tech. Rev.*, Mar. 2010. UCRL-TR-52000-10-3.

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

Laurence, T. A., and B. A. Chromy, 2010. "Efficient maximum likelihood estimator fitting of histograms." *Nat. Methods* 7, 338. LLNL-JRNL-420247.

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

Abstract

We will focus on detecting viable bacterial pathogens in complex environmental samples relevant to biosecurity by developing RNA signatures of pathogens using reverse transcriptase polymerase chain reaction (RT-PCR) and employing novel RNA extraction technology and RNA signatures. 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 samples to develop automated protocols for rapid, high-throughput processing and PCR analysis.

If successful, this project will deliver rapid, robust RNA extraction protocols and specific RNA amplification assays to determine the presence of viable *Bacillus anthracis* (anthrax) and *Yersinia pestis* (plague) in environmental samples. Results from RT-PCR or isothermal RNA amplification analysis should be well correlated with culture-based methods and rapid-viability PCR methods. This technology will be transferable to other sample types and pathogens. We expect to produce publications for peer-reviewed journals, form collaborations

for method validation and application, and enable next-generation development of biodetection technologies.

Mission Relevance

This project will advance 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.

FY10 Accomplishments and Results

In FY10 we evaluated RT-PCR assays for *B. anthracis* spores and *Y. pestis* cells. Specifically, we (1) demonstrated rapid, consistent detection at the level of 10^2 colony-forming units; (2) verified the speed of RNA-based methods, obtaining data within 8 hours of sample receipt, compared to days for culture-based techniques; (3) found no RNA background in dead *B. anthracis* spores, showing the utility of RNA-based viability methods, although *Y. pestis* cells killed with different methods, such as bleach, desiccation, and ultraviolet light, did show RNA persistence, pointing to limitations for use with cells; (4) found protocols for RNA extraction and RT-PCR analysis to be compatible with semi-automated sample processing for surface and environmental samples; (5) investigated the enrichment of *Y. pestis* cells prior to RT-PCR analysis to improve detection limits and possibly mitigate the dead-cell RNA background, finding that *Y. pestis* cells incubated with live, non-target bacterial cells showed either no growth inhibition or a negative effect on RT-PCR analysis, whereas testing with debris showed inhibition; and (6) conducted a brief survey of immuno-magnetic separation techniques that could extract *Y. pestis* cells from complex backgrounds prior to RT-PCR analysis, finding the potential for removing inhibitors and confirming the techniques' compatibility with RT-PCR methods. In summary, this project's results on RNA-based viability methods demonstrate the feasibility of applying

specific RT-PCR assays to germinated *B. anthracis* spores, along with potential limitations for application to *Y. pestis* cells unless the RNA background can be mitigated. The Environmental Protection Agency has expressed interest in supporting follow-on work to develop rapid viability methods for *B. anthracis* spores.

Publications

Létant, S., et al., 2010. *Rapid viability methods for biothreat agents on surface and environmental samples: DNA- and RNA-based approaches*. 4th Natl. Bio-Threat Conf., New Orleans, LA, Dec. 7–9, 2010. LLNL-ABS-462185.

Important Modes to Drive Protein Molecular-Dynamics Simulations to the Next Conformational Level—Babak Sadigh (08-ERD-037)

Abstract

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

We will design a novel Monte Carlo algorithm—the projected importance-sampling Monte Carlo scheme. Integrating this new algorithm into existing molecular dynamics codes, we expect to prove the efficacy of our method by calculating binding energies and kinetic barriers. This project will provide illustrative predictions of how biological enzymes, receptors, and transmembrane ion channels alter their conformation to perform their function and determine the atomic structures of transition and active states of these proteins.

Mission Relevance

This project supports LLNL's efforts to produce breakthroughs in fundamental science and technology and in the bioscience and biotechnology disciplines. By creating a tool applicable to predicting membrane protein response to stimuli, this approach could also be applied to efforts to counter the effects of biological terrorism in support of national and homeland security.

FY10 Accomplishments and Results

In FY10, we made significant progress toward our goal of speeding up by at least an order of magnitude the calculation of protein reaction rates and conformational free-energy differences through innovative choices of steering coordinates, as we had previously demonstrated with our liquid–solid free-energy difference calculations. Specifically, we (1) found a novel pathway that can allow for calculation of the free energy of the freezing of protein degrees of freedom in a solvent, using a non-trivial renormalization of the potential energy landscape for the frozen degrees of freedom; (2) implemented this technique into the massively parallel bio-molecular dynamics code NAMD; (3) successfully used this method to calculate the binding free energy of a ligand to the protein BChE; and (4) calculated the solvation entropy of BChE. The next step would be to prove the applicability of our technique to the calculation of the absolute solvation entropy of protein–water solutions, taking explicit account of interactions with solvent molecules. If successful, this would enable a small revolution in computation of protein reactions and functions.

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

Abstract

We propose to develop new molecular tools to detect and monitor key plant and fungal cell wall polymers. Conventional biochemical reagents such as polysaccharide-specific antibodies are not adequate for biofuel processing or pathogen recognition. We will enable the development of molecular probes that recognize target molecules sought in

bioenergy, medicine, forensics, and biosensor applications. Novel nucleic acid aptamer sequences will be created using a combinatorial synthesis approach. Natural polysaccharides will be the targets in affinity selection of specific DNA sequences. These will be amplified, purified, and characterized for their utility.

Aptamers are short strands of DNA that bind with high affinity to specific molecules. We are developing several new aptamers for assays of specific polymeric components of microbial and plant cell walls. Aptamers that recognize and bind to key polysaccharides will be valuable, not only in plants for biofuel processing but also in detecting certain fungal pathogens. We anticipate that the aptamers will be patented and used in other projects at LLNL and in collaborations with the DOE Joint BioEnergy Institute. In addition, we will characterize the progression of a region-specific combinatorial library of aptamers that bind to a polymer found in both plants and fungi.

Mission Relevance

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

FY10 Accomplishments and Results

We used the polysaccharides beta-1,3 glucan and alpha-1,4 glucuronic acid to select substrate-specific DNA aptamers. Specifically, we (1) synthesized aptamer libraries, each with randomized 40-nucleotide sequences flanked by distinct 20-nucleotide sequences—one containing a 5'-biotinylated residue and the other 3'-tagged with a fluorescent nucleotide; (2) incubated our libraries with the individual polysaccharides immobilized on columns, then selected the aptamers using an amplification-enrichment regimen based on the systemic evolution

of ligands by exponential enrichment; (3) eluted, sequenced, and tested the aptamers for specificity in binding polysaccharide-coated beads by fluorescence microscopy, achieving negative or inconclusive results—sequencing indicated the absence of conservation in sequence elements that would point to successful selection; and (4) conducted further tests of the methodology using a carbohydrate-binding module protein as the target, which we greatly improved by monitoring successive rounds of PCR, although no specific carbohydrate-binding module aptamers were found. The results of this project's many experiments indicated that the technique for aptamer selection is fraught with many pitfalls, each of which require troubleshooting before proceeding to the next steps, and that polysaccharides are poor binding substrates for DNA aptamers, making it difficult to follow up the methods developed here with similar targets. Although aptamers are potentially powerful molecular tools and, once identified, can be easily synthesized in quantity, further work in this area requires the development of reproducible and facile aptamer-selection technologies.

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-ABS-408636.

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

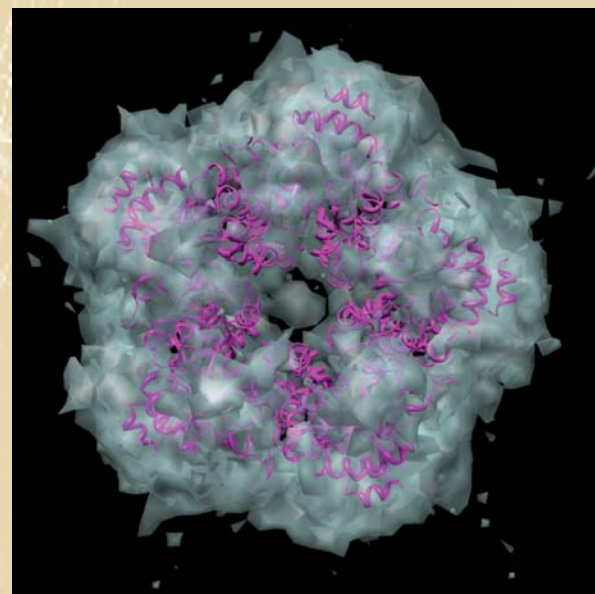
Siebers, A. K., and M. Thelen, 2009. *DNA as a probe for bioenergy research*. LLNL-ABS-408526.

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

Abstract

Our objective is to combine advancements in aberration-corrected cryo-electron microscopy with high-performance computing to rapidly determine biomolecular structures and their function. We plan to be the first to use aberration-corrected electron microscopy to image a protein at atomic resolution while avoiding the current limitation of protein crystallization. Specifically, we will (1) adapt ion mobility to improve sample preparation and deposit more homogeneous populations of proteins on a clean substrate, (2) obtain aberration-corrected electron microscopy data on protein, (3) develop image-processing techniques to reconstruct the three-dimensional (3D) image and model, and (4) apply high-performance computing to simulate the protein to predict its function.

If successful, we will be the first to use aberration-corrected electron microscopy to image a protein complex at atomic resolution, which will



An x-ray-imaged structure docked into a three-dimensional electron-microscopy reconstruction, confirming the size and decamer assembly of the protein LsrF.

revolutionize the biological field by eliminating the need to crystallize samples prior to structural determination. Ultimately we will develop a single-molecule method for determining biomolecular structures at resolutions conducive to rational drug design. To achieve this goal, we will make advancements in each step necessary for 3D reconstructions of proteins, including sample preparation, high-resolution imaging, and algorithms for image analysis. By utilizing constraints revealed from the solved structure with high-performance-computing simulations, we will also begin to probe the predicted function of the protein.

Mission Relevance

The national and homeland security missions of Lawrence Livermore include developing new countermeasures to combat chemical- and biological-warfare threats. Our success will enable a new capability to determine structures and functions of unknown proteins in host-pathogen pathways, which will provide rational approaches that can be applied to developing new therapeutics and pre-treatments and can be applied to many fields of biology.

FY10 Accomplishments and Results

In FY10 we (1) developed an improved sample-preparation method for increasing the homogeneity of purified protein deposited on a microscopy grid, (2) tested the ion mobility method with fluorescent polystyrene beads and applied it to purified LsrF protein, (3) successfully imaged transmission electron microscopy grids containing size-segregated samples with cryo-electron microscopy and worked to optimize sample preparation to achieve atomic-resolution conditions, (4) developed novel algorithms to improve the signal-to-noise ratio of cryo-electron microscopy images with a 1D and 2D adaptive noise-canceling filter—preliminary results suggest its continued usage will significantly improve the quality of 3D protein structures generated from cryo-electron microscopy data, and (5) ran high-performance-computing simulations of LsrF structures.

Proposed Work for FY11

In FY11 we will (1) continue to optimize sample preparation and apply it to inhomogeneous protein complexes, (2) collect the aberration-corrected cryo-electron microscopy data on LsrF and the LsrF-LsrG protein complex, (3) implement the full 2D noise-canceling algorithm and test it with a variety of data sets, (4) complete the performance-measurement algorithm implementations and compute quantitative performance, (5) implement and test iterative image-restoration algorithms to mitigate image distortion, (6) create and test statistical machine-learning algorithms for further signal-to-noise improvement, (7) reconstruct the 3D protein structures and quantitatively determine improvement of structural resolution, and (8) simulate the LsrF protein and LsrF-LsrG protein complex using high-performance computing.

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

Abstract

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

We expect to develop automated, high-throughput extraction and culturing techniques for processing existing libraries of marine natural products and

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

Mission Relevance

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

FY10 Accomplishments and Results

In FY10 we continued developing network-analysis computational tools incorporating systems biology, structural informatics, and docking studies. We also used our computational tools to identify and prioritize relevant genes for promising drug targets. For the pathogenic bacterium *Francisella tularensis*, we identified, crystallized, and annotated a novel cysteine protease drug target from seven identified virulence factors. For *Yersinia pestis*, we worked to identify a previously unknown phosphatase

and essential metabolic pathways that may reveal vulnerability for therapeutic intervention against the pathogen. Finally, we began drug-drug interaction studies using caffeine and ciprofloxacin and started generating data for physiologically based pharmacokinetic simulations.

Proposed Work for FY11

In FY11 we will (1) screen computationally identified compounds for binding to the protein rep24 to determine a candidate inhibitor, (2) finish determining the structure of *F. tularensis* and *Y. pestis* targets and inactivated homologues, (3) conduct gene knockout and binding studies to validate our predictions on the *Y. pestis* flavin biosynthesis pathway phosphatase and thereby confirm identity of the novel target, (4) conduct protein-protein validation studies for proteins in the *Y. pestis* lsr operon, and (5) complete the drug-drug interaction studies of caffeine and ciprofloxacin at both therapeutic and microdose levels to generate physiologically based pharmacokinetic models.

Publications

Segelke, B. W., et al., 2010. *Structure-function of Y. pestis LsrG, a protein involved in AI-2 quorum sensing*. LLNL-JRNL-427462.

Wheeler, K. E., et al., 2010. "Functional insights from computational modeling of orphan proteins



Steps in the drug development process include: characterization of pathogen entry into a host, crystal structure determination, high-throughput screening in conjunction with high-performance computing and accelerator mass spectrometry, and drug production.

expressed in a microbial community." *J. Proteomics Bioinform.* **3**, 266. LLNL-JRNL-421048.

Zemla, A., and B. W. Segelke, 2008. *Practical applications of structural genomics technologies for mutagen research*. 39th Ann. Mtg. Environmental Mutagen Society, Rio Grande, PR, Oct. 18–22, 2008. LLNL-PRES-407861.

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

Abstract

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

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

Experimentally derived fluxes will be compared to fluxes predicted by the existing flux model for yeast and used to experimentally constrain and validate the model.

Mission Relevance

By developing advanced flux-modeling technology with biodefense and bioenergy applications, this project supports LLNL's missions in national and energy security by assisting efforts in the rapid detection and characterization of emerging and unknown biothreats as well as efforts to deliver clean energy systems.

FY10 Accomplishments and Results

In FY10 we (1) developed methods to extract polar metabolites from *S. cerevisiae* cells and optimized metabolite-labeling protocols for detection of metabolites belonging to the glutamate family using accelerator mass spectrometry, (2) developed high-performance liquid chromatography techniques and used them to separate and quantify yeast amino acids, (3) labeled cellular amino acids using glutamate and glutamine labeled with carbon-14 and successfully measured metabolic fluxes terminating in glutathione production using high-performance liquid chromatography in conjunction with accelerator mass spectrometry, and (4) began applying the generated data to constrain the existing yeast flux-balance model.

Proposed Work for FY11

In FY11 we will (1) use the yeast-labeling protocols and techniques for metabolite extraction and separation developed in FY10 to measure additional fluxes in amino acid and related metabolic pathways to constrain our computational model of yeast metabolism; (2) use the data acquired in FY10 to further constrain, test, and validate the existing yeast flux-balance model; (3) use these computational results to design and perform additional iterative experiments; and (4) insert the resulting measurements into our yeast flux-balance model to significantly reduce uncertainty and validate or correct the model.

Publications

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

Stewart, B. J., et al., 2010. *Yeast metabolic flux measurement by accelerator mass spectrometry*. American Chemical Society National Mtg., San Francisco, CA, March 23, 2010. LLNL-POST-425375.

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

Abstract

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

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

Mission Relevance

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

FY10 Accomplishments and Results

We (1) localized the stage at which pathogenic *F. tularensis* strains disrupt the phagosomal pathway in dendritic cells by comparing the trafficking of pathogenic and nonpathogenic strains, (2) analyzed cytokine profiles of dendritic cells infected with pathogenic and nonpathogenic strains to determine if *F. tularensis* suppresses T-lymphocyte responses by interfering with cytokine production, and (3) optimized the imaging capabilities of amoeba-infected host cells and created new state-of-the-art images.

Proposed Work for FY11

Our goals for FY11 are to (1) complete the elucidation of endosomal pathway disruption by pathogenic *F. tularensis* strains, (2) isolate bacterial phagosomes from infected cells and identify the bacterial proteins present, and (3) isolate and identify host proteins that interact with the bacterial proteins that we identified. Both bacterial and host proteins identified are likely to be involved in pathogenesis and would represent targets for developing countermeasures against tularemia.

Publications

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

Verges, L., A. Rasley, and S. H. El-Etr, 2010. *Differential endosomal trafficking of pathogenic and nonpathogenic Francisella tularensis strains in human dendritic cells*. American Society of Microbiology 110th General Mtg., San Diego, CA, May 23–27, 2010. LLNL-POST-432756.

Effect of Aging on Chondrocyte Function— Gabriela Loots (09-LW-072)

Abstract

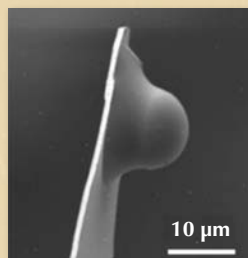
Age is a risk factor associated with skeletal degenerative diseases such as osteoporosis and osteoarthritis. More than 20 million Americans are affected by osteoarthritis, incurring over \$30 billion in medical costs annually. We hypothesize that age-dependent changes in molecular and biochemical content of skeletal tissue affect the binding of individual cells to the extracellular matrix, resulting in the understimulation of cells and altering the cell's metabolic activity. We will examine mechanisms by which aged cells become less responsive to mechanical loading to determine if the decrease in cell synthetic

activity with age is caused by reduced cell–matrix interaction. For this project, we will leverage LLNL's capabilities in molecular biology, bioengineering, atomic force microscopy, and microfabrication.

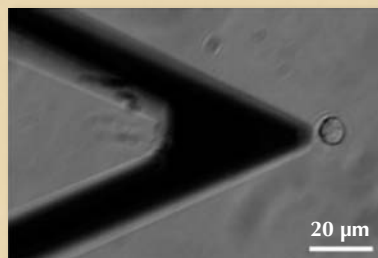
If successful, we expect to find that aged cells have impaired gene expression and are less responsive to mechanical loading because of weaker adhesion to the surrounding extracellular matrix, and that this weakened interaction shields the cells from the normal physiological loading that healthy young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



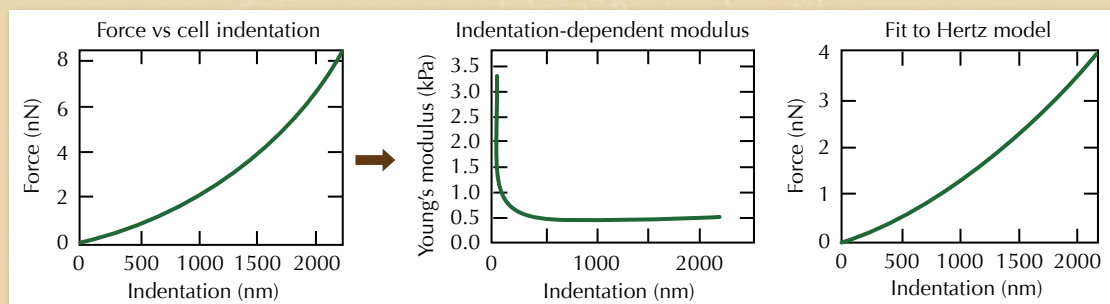
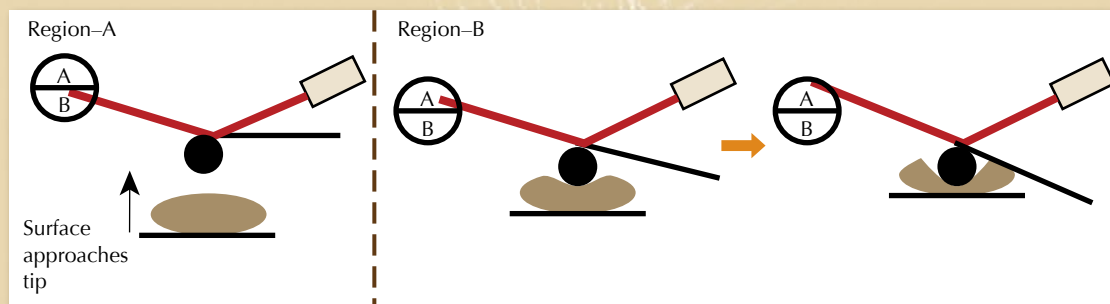
AFM/optical microscope



10 µm PS/AFM tip



Align AFM/10 µm probe over cell



A combined atomic force microscopy (AFM) and optical microscope was used to measure the mechanical response of chondrocyte cells to loading. Force versus deformation plots using indentation-dependent and Hertz analyses are shown in the bottom row.

amenable to pharmaceutical treatment or gene therapies to retard or reverse the onset of osteoarthritis.

Mission Relevance

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

FY10 Accomplishments and Results

In FY10 we (1) determined that cellular stiffness in chondrocytes is dependent on the magnitude of the mechanical force; (2) determined that stiffness is a result of two structural proteins, actin and vimentin; (3) isolated chondrocyte RNA from young and aged cells and carried out microarray experiments; (4) depolymerized the actin and vimentin cytoskeleton and determined that vimentin depolymerization is a key contributor to cellular stiffness from large loads; and (5) determined that stiffness is not affected by aging. The successful conclusion of this project enabled novel techniques of measuring cellular biomechanical properties in single cells that were cartilage derived.

Publications

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

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

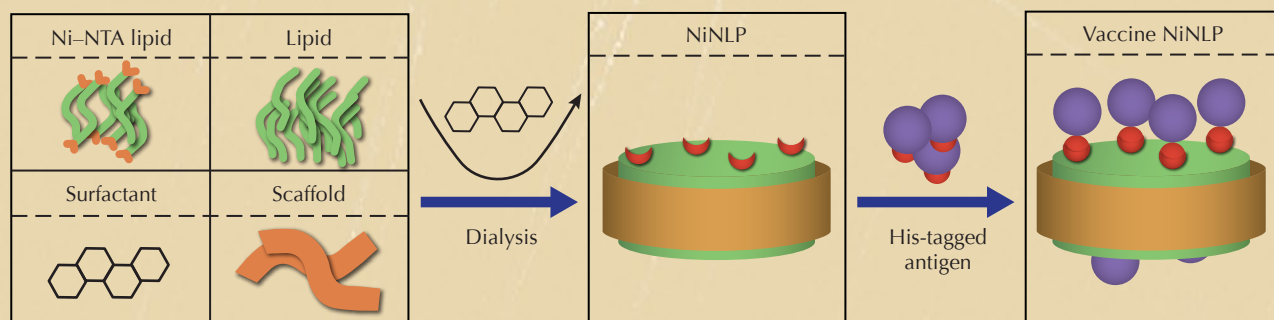
Abstract

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

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

Mission Relevance

Our proposed work is crucial to developing potent vaccines for both disease prevention and increased biodefense capabilities, in support of



Schematic of vaccines based on nickel-nanolipoprotein (NiNLP) constructs. One of the inputs is a nickel-nitrilotriacetic (Ni-NTA) lipid.

Laboratory missions in homeland and national security.

FY10 Accomplishments and Results

In FY10 we (1) successfully measured the immune response to optimized nanolipoproteins in mice using an antigen from the *Yersinia pestis* bacterium, using our nickel–nanolipoprotein vaccine platform; (2) added the secondary adjuvants lipid A and cholesterol CpG into the nanolipoprotein constructs; (3) developed new methods of attaching antigens to nanolipoprotein particles; and (4) published manuscripts on nanolipoprotein stability and protein-binding kinetics and nanolipoproteins for vaccine delivery.

Proposed Work for FY11

For FY11 we will (1) clone, express, and purify potential polyhistidine-tagged *Francisella tularensis* and *Y. pestis* antigens in *Escherichia coli* bacterial expression systems; (2) test the immune-stimulating properties of nickel–nanolipoproteins alone and in combination with lipid A and cholesterol CpG at different concentrations in cell-based assays; and (3) test the efficacy of the nanolipoprotein *F. tularensis* and *Y. pestis* vaccines using the optimized adjuvant compositions in animal models with live pathogens in Livermore's new Biosafety Level 3 laboratory.

Publications

Blanchette, C. D., et al., 2010. "Kinetic analysis of His-tagged protein binding to nickel-chelating nanolipoprotein particles." *Bioconjugate Chem.* **21**, 1321. LLNL-JRNL-425115.

Fischer, N. O., et al., 2010. "Conjugation to nickel-chelating nanolipoprotein particles increases the potency and efficacy of subunit vaccines to prevent West Nile encephalitis." *Bioconjugate Chem.* **21**, 1018. LLNL-JRNL-420436.

Fischer, N. O., et al., 2010. "Isolation, characterization, and stability of discretely-sized nanolipoprotein particles assembled with apolipoprotein-III." *PLoS ONE* **5**, e11643. LLNL-JRNL-427664.

Genomics of Cell-to-Cell Communication: Identification of DNA Sensors in Humans—Gabriela Loots (10-ERD-020)

Abstract

Communication between individual cells is an essential process in all living organisms. Although several signal transduction pathways have been identified, we do not yet know how a signal from the cell surface is interpreted at the genomic level to control transcription. Furthermore, tumor formation is a direct result of the failure to carry out normal intercellular communication. We propose to undertake a genomic approach to identify non-coding regions in the human genome that are activated in a receiver cell by signals from a cancer cell. We will use the metastasis of prostate cancer to bone as a model for testing our hypothesis and for identifying genomic signals that are activated in response to prostate cancer cells.

Our experiments will address the consequences of intracellular communication and identify changes in gene expression that are induced either in osteoblasts (cells responsible for the synthesis and mineralization of bone) or prostate cancer cells that are grown in mixed co-cultures. We will elucidate gene expression changes in prostate cells in response to osteoblasts, as well as changes in osteoblasts because of cancer response. The goal of these experiments is to gain insight into how osteoblasts respond to the presence of cancer cells in an in vitro, co-culture system as a first approximation of changes in gene expression that may be involved in early stages of bone metastasis. This study will be the first global genomic survey of gene expression in response to intracellular communication in the context of bone metastasis.

Mission Relevance

We will use cancer metastasis as a model of intracellular communication to develop novel genomic tools and methods that will help us understand what regulatory elements are critical for sensing tumors, which would comprise a significant advancement in basic biology in support of LLNL's mission in frontier science. These tools can then be applied

to understanding how cells recognize pathogens, including potential bioterror pathogens, in support of the Laboratory's national security mission area of countering bioterrorism.

FY10 Accomplishments and Results

We (1) identified optimal prostate cancer cell lines with different metastatic potential, (2) optimized the in vitro expression of fluorescent proteins that can be co-expressed in co-cultures to monitor reporter cell activity, (3) examined the RNA expression of bone morphogenetic protein antagonists and antagonists of the protein Wnt in various lines of prostate cancer cells, and (4) established an immunosuppression protocol to enable prostate cancer delivery to the bone marrow of genetically modified strains of mice.

Proposed Work for FY11

In FY11 we will (1) isolate RNA from osteoblasts from a primary immortalized cell line and carry out control microarray experiments, (2) isolate RNA from prostate cancer cells and conduct control microarray studies on four cell lines with different metastatic potential, (3) optimize the formaldehyde-assisted isolation of regulatory elements for enriching non-coding sequences in prostate cancer cell lines, (4) isolate high-molecular-weight human DNA using standard methods, and (5) create a human expression library.

Understanding the Role of Virus Evolution in Interspecies Transmission Events— Monica Borucki (10-LW-020)

Abstract

We propose to investigate the role of genetic mutation in the generation of bovine coronavirus variants that acquire the ability to adapt to human laboratory cell lines. This will allow us to assess the likelihood of a host-jumping event. Data obtained from this work will be analyzed using advanced pattern recognition and other bioinformatics techniques to identify genomic markers applicable to future studies of adaptation of a zoonotic virus to

human cells. This research will lay the foundation for virus evolutionary and forensic studies that further the development of a framework for understanding and ultimately predicting natural emerging infectious diseases and for differentiating these from man-made pathogens.

This project will advance our understanding of host-pathogen interactions, predictive biology, and forensic microbiology. The results of these experiments will provide the first systematic, controlled data set that can be used to develop models that predict the likelihood of pathogen emergence. In addition, these experiments will provide information that may be valuable for forensic identification of intentional pathogen introductions, because they will allow us to test the hypothesis that viral genomes undergo predictable changes when transferred in cell cultures, and these differences can be used to distinguish naturally occurring strains from those propagated via passage in cell culture.

Mission Relevance

By developing a framework for understanding and ultimately predicting natural emerging infectious diseases and differentiating these from man-made pathogens, this research will lay the foundation for future studies of virus evolution and forensic work in support of Livermore's missions in national and homeland security.

FY10 Accomplishments and Results

We focused on passing bovine coronavirus in human and bovine cells and characterizing the resultant viruses using pyrosequencing and phenotypic assays. Specifically, we (1) collected over 200 bovine nasal samples and identified over 20 samples infected with bovine coronavirus, (2) identified the necessary human and bovine cell lines and tested them for the ability to be infected with bovine coronavirus, (3) developed protocols for identifying the presence of other common infecting viruses and for titering bovine coronavirus so that replication rate can be determined, (4) passed four viruses serially in five different cell lines, and (5) established controls for sequence analysis. We used 16 polymerase chain reaction primer sets

designed from conserved regions of the genome to sequence approximately 12 kb of the genome for ultra-deep 454 sequence analysis.

Proposed Work for FY11

We propose to investigate the role of both point mutations and recombination in the generation of bovine coronavirus variants able to adapt to human cell lines. Specifically, we will (1) determine mutational dynamics by serial passage in both human and bovine cell culture, (2) sequence and phenotypically analyze the resultant quasispecies, (3) compare the genomes of cell-passaged isolates to the genome of non-passaged isolates to identify genetic changes characteristic of laboratory passage in human cells as compared to bovine cells, (4) investigate the propensity of the bovine coronavirus to recombine with other coronaviruses, and (5) genetically and phenotypically characterize the resultant recombinant viruses.

Establishing Cancer Stem Cell Longevity and Metastatic Potential—Bruce Buchholz (10-LW-033)

Abstract

We propose to demonstrate that cancer stem cells in human cancers are long-lived, resistant to conventional therapies, and are prime suspects in metastasis and relapse. Our goal is to advance cancer treatment and to initiate transformation in cancer research by targeting these stem cells. We intend to use the spike in carbon-14 that occurred as a result of atmospheric nuclear testing to date stem cells isolated from actual tumors and produce highly labeled cells as a tool for research. Techniques we developed for DNA dating of healthy tissue using the carbon-14 spike will be used for cancer stem cells, and we will grow cancer cell lines on highly labeled DNA precursors to produce labeled cells. The stem cells will then be isolated from other cancer cells for use as indicators of metastatic potential.

We expect DNA dating of cancer stem cells to clearly establish that they are long-lived cells that exist well before tumors occur. Producing highly

labeled cancer stem cells in cell culture will provide a tool for measuring the metastatic potential of any cell line and will potentially lead to a clinical tool to assess biopsied tissue. We believe our results will provide clear evidence that cancer stem cells are cancer initiators and need to be the targets of all cancer therapies. Because most cancer deaths are associated with metastasis, changing the targets of therapy to metastatic cells will revolutionize the treatment of cancer and potentially reduce cancer deaths.

Mission Relevance

This project supports the Laboratory's efforts in exploring the forefronts of science and technology, as well as bringing specialized expertise and Livermore's unique measurement capabilities to bear on problems of national and international interest. If successful, measuring the longevity of cancer stem cells and their metastatic potential will focus future cancer research to target these cells for eradication of metastatic cancer.

FY10 Accomplishments and Results

In FY10 we (1) established a set of cell markers to identify cancer stem cells in multiple bladder tumor cell lines, each with different sensitivities to chemotherapy and different metastatic potential; (2) began using these cell lines to develop protocols for cell sorting and DNA purification specific to bladder tumors; (3) began applying our new protocols to human tumor cells; and (4) began laboratory preparations necessary to produce cancer stem cells labeled with carbon-14 for FY11 tasks.

Proposed Work for FY11

In FY11, we will (1) isolate cancer stem cells from other tumor cells in collaboration with researchers at the University of California at Davis, (2) date DNA separated from these samples using our established techniques to determine the longevity of cancer stem cells, (3) finish producing highly labeled stem cells in culture and establish protocols for growing labeled cancer stem cells, and (4) perform initial measurements of metastatic potential and determine viable tracing studies.

Publications

Sarachine, M. J., B. A. Buchholz, and R. W. de Vere White, 2010. *An investigation of stem-like cancer cells in three bladder cancer cell lines*. 15th Ann. Cancer Research Symposium, Sacramento, CA, Oct. 28, 2010. LLNL-POST-461177.

Sarachine, M. J., et al., 2010. *Establishing cancer stem cell longevity in bladder cancer*. LLNL Postdoc Symp., Livermore, CA, May 27, 2010. LLNL-POST-433311.

Radiation Biodosimetry Using Loop-Mediated Isothermal Amplification— Paul Wilson (10-LW-041)

Abstract

We propose to develop rapid radiation biodosimetry assays using loop-mediated isothermal amplification (LAMP)—a novel DNA amplification technology—to detect abnormal blood cells with chromosomal translocations induced by exposure to ionizing radiation and other agents. As proof of principle, we will use LAMP to amplify the messenger RNA (mRNA) transcripts resulting from the Philadelphia chromosome translocation breakpoint in chronic myelogenous leukemia cells. We will then focus on a genomic “hot spot” on a chromosome associated with radiotherapy-induced acute myelogenous leukemia. Identification of low-frequency precancerous cells provides an opportunity for early therapeutic intervention and medical triage following an unanticipated radiological event.

We expect to develop LAMP assays to detect the primary mRNA transcripts resulting from Philadelphia chromosome translocation using chronic myelogenous leukemia cell lines, which could yield a patentable, clinically deployable laboratory-based assay for detecting and staging these leukemia patients. We will optimize LAMP assays to detect normal cells carrying radiation-induced mRNA transcripts and chromosome translocations in acute myelogenous leukemia cells to determine the assay’s sensitivity, dynamic range, and radiation dose response for applications in medical triage of a

radiological event as well as in radiotherapy clinics. We also propose to integrate the LAMP assay into handheld point-of-care devices in development at LLNL for microbial pathogen detection.

Mission Relevance

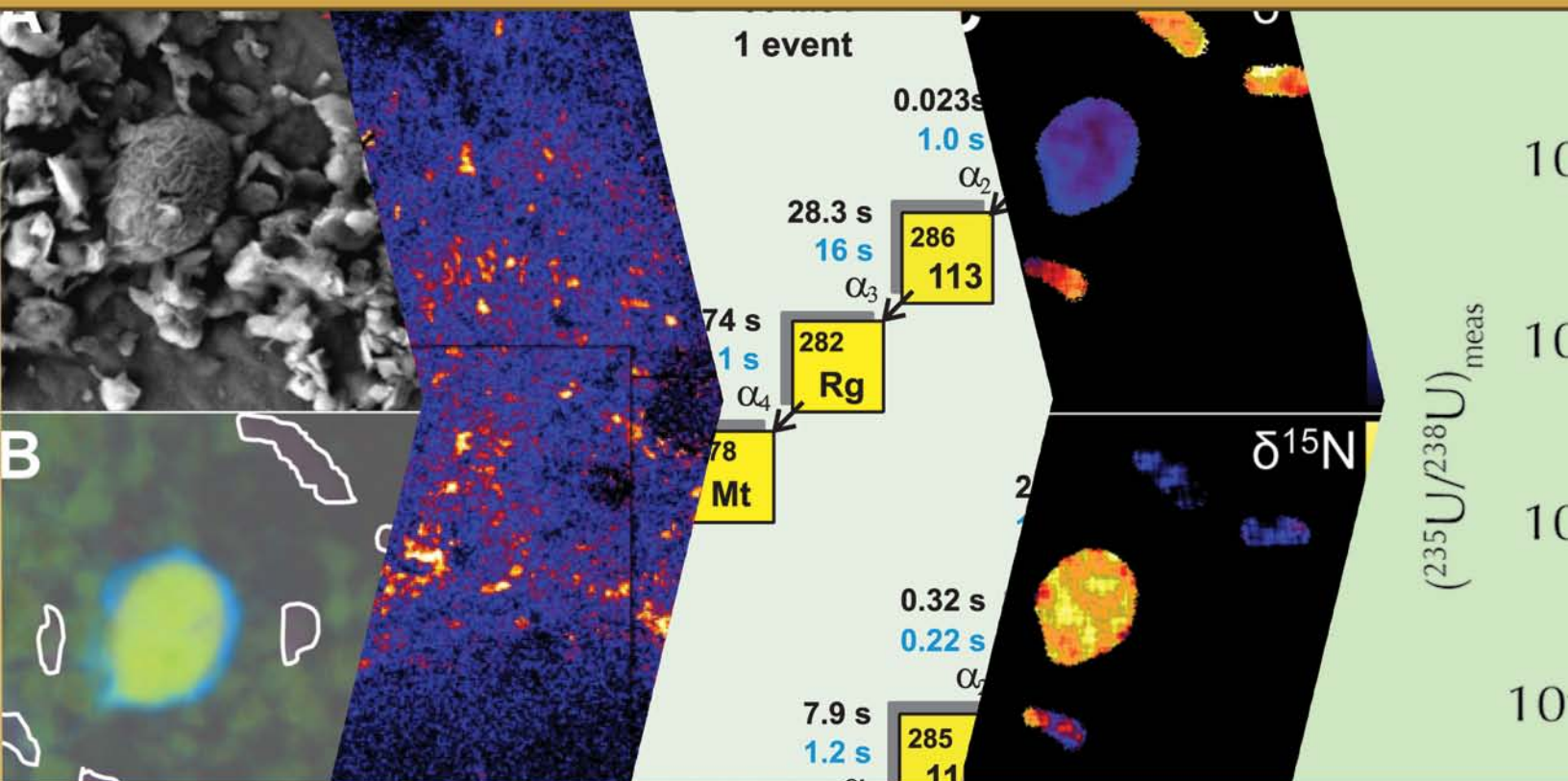
Our LAMP assay supports the Laboratory mission to ensure national security by aiding medical efforts in the event of a radiological attack. Further development of LAMP-based DNA detection assays at Livermore will benefit current efforts to develop assays to detect other chemical and biological threats, and may also provide valuable patient information for clinical oncologists to individualize therapy regimens and identify at-risk individuals earlier, when treatment may be far more effective for controlling disease progression.

FY10 Accomplishments and Results

We developed chronic myelogenous leukemia LAMP assays tailored to detect primary Philadelphia chromosome mutations in chronic myelogenous leukemia patients. Specifically, we (1) verified mutations from nine Philadelphia-positive chronic myelogenous leukemia cell lines using quantitative reverse transcription polymerase chain reaction and LAMP primers designed to positively identify Philadelphia mutations in less than an hour; (2) determined that combining reverse transcriptase with LAMP alleviated issues of genetic heterogeneity in individual translocation breakpoints by allowing LAMP amplification of conserved mRNA transcripts resulting from alternative splicing; (3) began developing in situ protocols to detect Philadelphia-positive cells with immunofluorescence, an essential step in clinical assay development; (4) developed “radiation LAMP” assays to detect radiation-responsive mRNA transcripts routinely used in reverse transcription polymerase chain reaction-based biodosimetry panels, which is more attractive than the originally envisioned 11q23 translocation assay, because radiation LAMP technology is more adaptable to point-of-care devices being developed at LLNL; and (5) began development of an acute myelogenous leukemia LAMP assay by addressing technical issues with flow cytometry and procuring cell lines.

Proposed Work for FY11

In FY11 we will (1) continue to optimize LAMP assays to detect mutant transcripts in chronic myelogenous leukemia cells and develop a clinical assay, (2) develop and optimize LAMP assays to detect specific ionizing-radiation-induced mRNA transcripts in normal cells and establish a multiplex LAMP-based assay for radiological emergency triage, (3) develop and optimize assays to detect chromosome translocations in acute myelogenous leukemia cell lines and radiotherapy patient samples in collaboration with researchers at the University of California Davis Cancer Center, (4) establish dose response for radiation-induced chromosome translocations by irradiating TK6 human lymphoblastoid cells with cesium-137 gamma rays, and (5) integrate the LAMP assays into handheld point-of-care devices currently in development at LLNL for microbial pathogen detection.



Chemistry

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

Abstract

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

We expect to (1) develop and experimentally validate the first-ever bioinformatic system to design multiplexed primer sets for rapid identification of all viruses; (2) provide design parameters and analysis for next-generation microarrays; (3) optimize short primer sets to generate expected family-specific signatures for identifying known and unknown threats; (4) demonstrate microfluidic isolation of virus particles in complex biological samples; (5) develop systems for precise fluid manipulation, droplet sorting, and polymerase chain reaction (PCR); and (6) develop the first-ever comprehensive, automated sample-preparation system for sorting all components in clinical samples.

Mission Relevance

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

FY10 Accomplishments and Results

In FY10 we designed, fabricated, and tested the third generation of the microbial discovery array. Unlike previous generations, this array contains bacterial and fungal probes in addition to viral probes, providing a unique all-pathogen detection device. It was tested on a variety of samples from around the world, including those from sick sea lions from local coastal waters and paralyzed

children from Pakistan. We used the array, along with sequencing, to check the purity of a commercially available rotavirus vaccine. Contamination by a porcine virus was discovered, causing the suspension of sales of the vaccine until it could be proven safe for human use. In addition, we continued development of our droplet analysis system and collaborated with Raindance Technologies to increase throughput—their commercial technology met our capacity needs and we began using their chips and emulsion chemistry for our emulsion PCR experiments. We incorporated additional dielectrophoretic and isotacophoretic microfluidic modules into our sample preparation system to remove bacterial and nucleic acid contamination, and for the dielectrophoresis module, we developed a unique design that will confine bacteria to areas where the dielectrophoresis is strong but will still allow the high flow rates needed for our sample-throughput requirements. We continued our work with bioinformatic approaches to viral discovery by developing efficient algorithms for design of probes for both microarrays and PCR assays for more comprehensive sets of viruses. Finally, we completed Primux software for multiplex, degenerate primer and probe prediction and designed signatures for numerous viruses and bacterial virulence factors, which have been tested in the laboratory. With this project we achieved a number of goals for the identification of viruses including (1) fast, efficient PCR amplification of single viral genomes; (2) algorithms for designing new sets of viral-discovery PCR reagents; (3) breakthrough automated sample-preparation techniques for isolation of biological constituents in complex samples; and (4) design, fabrication, and testing of a unique microbial discovery microarray. We have licensed our technology on emulsion PCR to two commercial companies and the microbial discovery array is being deployed in an increasing range of public health and national security applications. We expect to receive support from the Department of Homeland Security and the Department of Defense to expand and further develop our sample preparation technology for forensics applications.

Publications

Beer, N. R., K. A. Rose, and I. M. Kennedy, 2009. "Monodisperse droplet generation and rapid trapping for single molecule detection and

reaction kinetics measurement." *Lab Chip* **9**, 841. LLNL-JRNL-405725.

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

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

Heredia, N. J., 2010. "In vitro double transposition for DNA identification." *Anal. Biochem.* **399**, 78. LLNL-JRNL-413261.

Jaing, C., et al., 2008. "A functional gene array for detection of bacterial virulence elements." *PLoS One* **3**, e2163. UCRL-JRNL-236055.

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

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

Victoria, J. G., et al., 2010. "Viral nucleic acid in live attenuated vaccines: Detection of minority variants and adentitious virus." *J. Virol.* **84**, 6033. LLNL-JRNL-426582.

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

Abstract

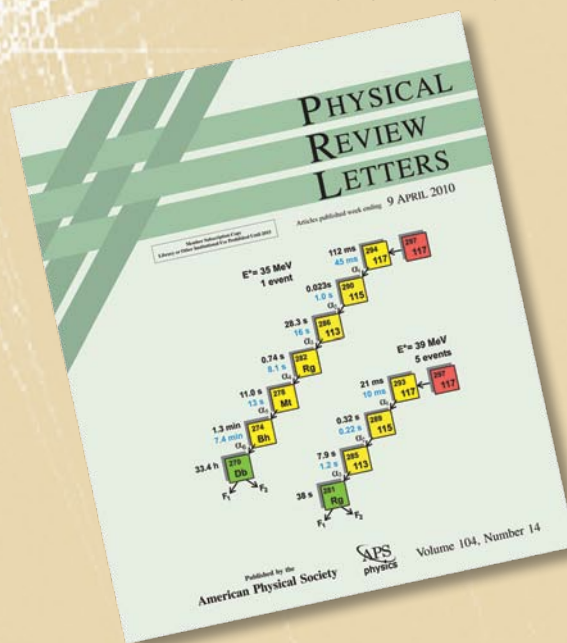
Producing heavy elements brings us closer to the "Island of Stability," where nuclei are postulated to have longer half-lives. The location of this island and the chemical properties of the transactinides are largely unknown. We will investigate chemical and physical properties of heavy elements and develop chemical separations and automated techniques to determine if transactinides behave like their lighter

homologues or if relativistic effects induced by nuclear charge alter predicted chemistry. The combination of physics and chemistry will potentially result in discoveries of new elements and isotopes. A search for undiscovered element 117 using the reaction of calcium-48 and berkelium-249 will be performed along with chemical identification of its decay daughters.

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 elements' chemical properties. The automated chemistry apparatus we develop will be capable of rapid sample processing with minimal dose exposure to personnel, used in accelerator-based online experiments with element 104 and 105 homologues, and have applications in nuclear forensics and attribution, environmental monitoring, and diagnosis of fusion-laser capsule performance. A search for element 117 will be performed and either its discovery or upper limit on production rate will be reported. The chemical properties of element 117 and its decay daughters will also be investigated.

Mission Relevance

This project supports the Laboratory's missions in national and energy security by furthering the



Cover of *Physical Review Letters* showing the two new element-117 decay chains discovered during bombardment of berkelium-249 with calcium-48 at the Joint Institute for Nuclear Research in Dubna, Russia.

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. Our achievements in automated chemistry will have applications in nuclear forensics and attribution and in fusion-laser capsule diagnostics.

FY10 Accomplishments and Results

In FY10 we (1) performed a calcium-48 and berkelium-249 experiment at the Joint Institute for Nuclear Research in Dubna, Russia, and reported the discovery of element 117—we found that the observed decay chains were shorter than predicted, which precluded performing chemical separations on the decay daughters; (2) completed work on use of DGA resin for separation of elements 104 and 105 and began modification of our automated system for future experiments; and (3) performed gas-phase chemistry of element 117 decay daughters (specifically element 113) and evaluated the data. Over the course of this project we reported the discovery of a new chemical element, number 117; participated in the first gas-phase chemistry of elements 113 and 114; and designed a new separation scheme for isolation of elements 104 and 105.

Publications

Eichler, R., et al., 2010. "Indication for a volatile element 114." *Radiochim. Acta* **98**, 133. LLNL-JRNL-409594.

Henderson, R. A., 2010. *Discovery of element 117*. Interlaboratory Working Group (ILWOG) 42, Los Alamos, NM, May 25, 2010. LLNL-PRES-432557.

Henderson, R. A., et al., 2009. *Automated chemistry efforts at LLNL using Eichrom's DGA resin*. 7th Workshop Chemistry of the Heaviest Elements, Mainz, Germany, Oct. 11–13, 2009. LLNL-PRES-406833.

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

Henderson, R. A., et al., 2010. *Electrodeposition of U and Pu on thin C and Ti substrates*. Intl. Target Development Society 2010 Conf., Vancouver, BC, Canada, Sept. 12–17, 2010. LLNL-PROC-454691.

Henderson, R. A., et al., 2009. *Recent developments in heavy element separation methods using DGA resin*. Asia-Pacific Symp. Radiochemistry (APSORC) 09, Napa, CA, Nov. 29, 2009. LLNL-ABS-414573.

Henderson, R. A., et al., 2009. *Recent updates in heavy element production from LLNL*. Asia-Pacific Symp. Radiochemistry (APSORC) 09, Napa, CA, Nov. 29, 2009. LLNL-ABS-414572.

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

Oganessian, Y. T., et al., 2010. "Synthesis of a new element with atomic number $Z = 117$." *Phys. Rev. Lett.* **104**, 142502. LLNL-JRNL-462051.

Rykaczewski, K., et al., 2009. *Search for a new element $Z = 117$ among the $249\text{Bk} + 48\text{Ca}$ reaction products*. American Physical Society HAW09 Mtg., Waikola, HI, Oct. 13–17, 2009. LLNL-ABS-414574.

Shaughnessy, D. A., K. J. Moody, and R. A. Henderson, 2010. *Synthesis and observation of new chemical element number 117*. American Physical Society April Mtg., Washington, DC, Feb. 13–17, 2010. LLNL-ABS-462040.

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

Wittwer, D., et al., 2010. "Gas phase chemical studies of superheavy elements using the Dubna gas-filled recoil separator—stopping range determination." *Nucl. Instrum. Meth. Phys. Res. B* **268**, 28. LLNL-JRNL-462091.

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

Abstract

The objective of this research is to provide new insight into the mechanisms of cell membrane organization. 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. We will provide the first direct evidence of the role of lipids in cell organization. Our approach combines molecule-specific stable isotope and antibody labeling with nanoscale secondary-ion mass spectrometry (nanoSIMS) to probe membrane organization.

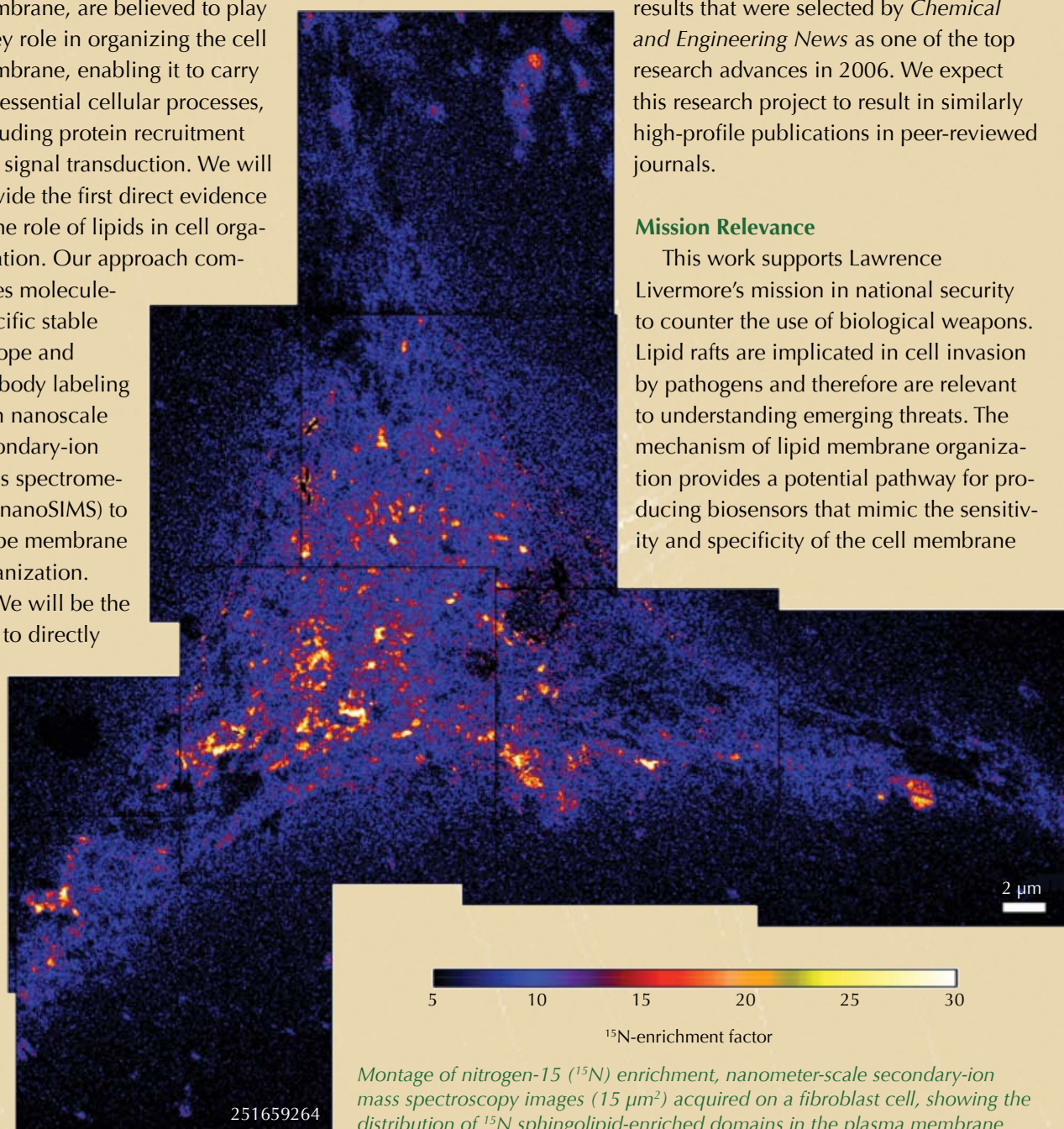
We will be the first to directly

image and quantify lipid rafts, and we 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 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.

This project will build on previous proof-of-concept results that were selected by *Chemical and Engineering News* as one of the top research advances in 2006. We expect this research project to result in similarly 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 provides a potential pathway for producing biosensors that mimic the sensitivity and specificity of the cell membrane



Montage of nitrogen-15 (¹⁵N) enrichment, nanometer-scale secondary-ion mass spectroscopy images (15 μm²) acquired on a fibroblast cell, showing the distribution of ¹⁵N sphingolipid-enriched domains in the plasma membrane.

and could be applicable to characterizing nanoscale lipoproteins for such sensors. In addition, the project will advance our capability for nanoSIMS analysis of bioweapon agents.

FY10 Accomplishments and Results

In FY10 we continued our innovative experiments on the membranes of intact cells—the most exciting outcome was demonstrating the segregation of lipids in these cell membranes. We conducted extensive experiments to test these results, including changes in our metabolic modeling method and fixation methods. In summary, this project has established a new approach to cell membrane research and provided direct imaging evidence of the formation of lipid rafts as compositionally distinct lipid domains. The methods developed under this project have been adopted for virus research, genomics research, and other thin-film research. We expect interest from the National Institutes of Health, DOE, and the National Science Foundation in future work that continues this research.

Publications

Anderton, C. R., et al., 2010. “Correlated AFM and NanoSIMS imaging to probe cholesterol-induced changes in phase behavior and non-ideal mixing in ternary lipid membranes.” *BBA Biomembranes* **1808**(1), 307. LLNL-JRNL-463216.

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

Frisz, J. F., et al., 2010. *High-resolution chemical imaging of sphingolipid distribution in the plasma membrane*. LLNL-JRNL-463256.

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

Nuclear Forensics: An Integrated Approach for Rapid Response— Ian Hutcheon (10-SI-016)

Abstract

This project develops a robust and responsive nuclear forensics capability, providing the technical basis to enable the U.S. to reconstruct a nuclear incident quickly and with high fidelity, even in a crisis situation. We will integrate LLNL world-class capabilities in radiochemistry, analytical and forensic science, and weapon physics to achieve scientific and technological breakthroughs critical to nuclear counterterrorism. The proposed research leverages LLNL’s ability to meet national security requirements for accurate and timely nuclear forensics and attribution, providing a powerful deterrent to potential adversaries. Focusing initially on the challenges of post-detonation, the advances will also be useful in assessing pre-detonation events and signatures.

We expect to achieve breakthroughs in experimental science to increase the speed and fidelity of nuclear forensic analysis by meeting the following challenges: (1) develop resonance ionization mass spectrometry to provide isotope-specific, definitive information on fuel composition in post-detonation scenarios within hours, without chemical separation; (2) develop a cavity ion source to increase mass spectrometry sensitivity 10 to 25 times; (3) develop accelerator mass spectrometry to measure activation products at ultralow concentrations; (4) apply in situ Raman and infrared spectrometry to evaluate actinide chemical behavior at high temperature; (5) synthesize uranium oxides by precipitation, hot pressing, and sintering to interpret material signatures; and (6) characterize nanometer-scale particles in fallout to provide the “ground truth” for evaluating new experimental techniques.

Mission Relevance

This project supports LLNL’s national security mission by developing nuclear forensics and attribution capabilities for reducing the threat of the

proliferation and use of weapons of mass destruction. It will also help cultivate the next generation of scientific leaders necessary to ensure the nation's ability to safeguard nuclear weapons and respond to nuclear threats.

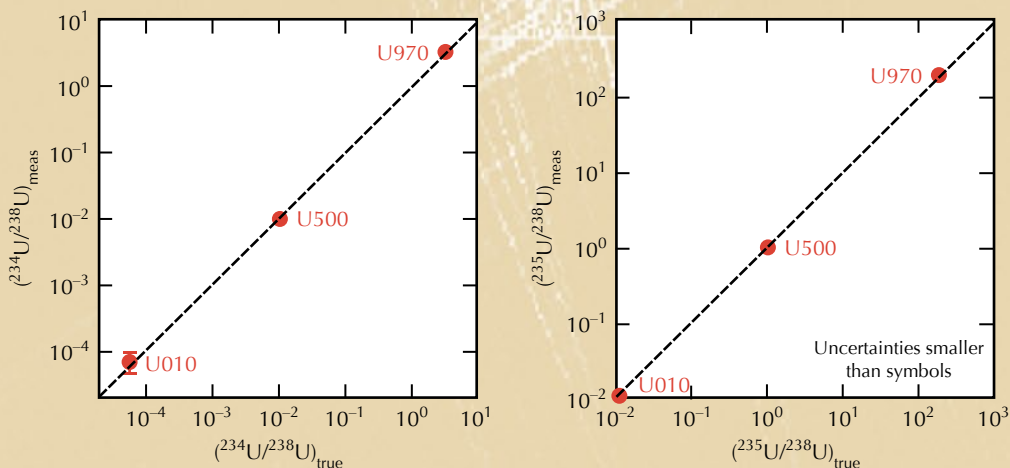
FY10 Accomplishments and Results

In FY10 we (1) achieved precision exceeding 0.5% for measuring the ratios of uranium-234 and uranium-235 to uranium-238 in uranium oxides containing between 1 and 98% uranium-235 using resonance ionization mass spectrometry, which was completed in less than an hour and demonstrated for the first time that the technology can rapidly and accurately measure uranium isotopes in debris samples containing as little as 10 $\mu\text{g/g}$ uranium; (2) completed a modeling study of the ion optics of a cavity ion source using the SIMION charged-particle optics simulation software, evaluating critical parameters necessary to achieve greater than 20% ionization efficiency; (3) designed a new detector for LLNL accelerator mass spectrometry to optimize isobaric resolving power for the key transition-metal activation products chromium, iron, and nickel; (4) expanded our studies of uranium dioxide, using x-ray absorption spectroscopy to determine electronic structure in the region of the band gap, and carried out, for the first time, a parameter-free

first-principles calculation of the electronic structure—this work shows unequivocally that the lowest lying state above the Fermi energy has an f-character; (5) completed initial fabrication of a suite of uranium oxides at the University of Nevada, Las Vegas, using three precipitation methods to produce uranium-oxide compounds with different base compositions; and (6) developed, using these samples, new scanning electron microscopy methods for signature evaluation including quantification of grain morphology at the micrometer scale, and began to apply these methods to commercial fuel samples.

Proposed Work for FY11

To build a robust, forward-looking nuclear forensic capability, we will (1) develop resonance ionization mass spectrometry for uranium and plutonium with an accuracy of 0.5% for the target uranium isotope ratios and with an elemental discrimination greater than 10,000; (2) create a cavity ion source to increase the sensitivity of actinide mass spectrometry by a factor of 10; (3) use accelerator mass spectrometry to measure transition-metal activation products at ultralow concentrations (fewer than 1,000 atoms in gram-size samples); (4) develop thermal chromatography for ultrafast separation of actinides from debris; (5) study uranium compounds at high



Comparison of uranium isotope ratios measured by resonance ionization mass spectrometry (shown in red) against true values (line). This is the first systematic study of precision and accuracy using resonance ionization mass spectrometry for any isotope system.

temperatures using Raman and infrared spectroscopy to evaluate the volatilities of uranium and refractory fission products; and (6) synthesize uranium compounds under controlled conditions to understand their signatures.

Publications

Gostic, R. C., et al., 2010. *Evaluation of fallout debris for nuclear forensic applications*. Intl. Chemical Congress of Pacific Basin Societies (Pacifichem 2010), Honolulu, HI, Dec. 15–20, 2010. LLNL-ABS-427582.

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

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

Isselhardt, B. H., et al., in press. "Improving precision in RIMS: The influence of laser bandwidth in uranium isotope ratio measurements." *Anal. Chem.* LLNL-JRNL-458116.

Klingsporn, J. M., et al., 2009. *Predicting the activity distribution of nuclear fallout*. LLNL-POST-415301.

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

Knight, K. B., et al., 2009. *A world without sample preparation: Developing rapid uranium isotope measurement capabilities by resonance ionization mass spectrometry (RIMS)*. Asia-Pacific Symposium on Radiochemistry (APSORC) 09, Napa, CA, Nov. 29–Dec. 4, 2009. LLNL-POST-413953.

Knight, K. B., et al., in press. "Uranium resonance ionization mass spectrometry in natural U-silicate." *Radiochim. Acta*. LLNL-JRNL-422855.

Levine, J., et al., 2009. "First four-isotope measurements of chromium in presolar grains." *Lunar Planet. Sci.* **40**, 1982. LLNL-ABS-409961.

Levine, J., et al., 2009. "Resonance ionization mass spectrometry for precise measurements of isotope ratios." *Int. J. Mass Spectrom.* **288**, 36. LLNL-JRNL-414068.

Siekhaus, W., and J. Crowhurst, 2010. "Optical properties of a mechanically polished and air equilibrated [111] UO₂ surface by Raman and ellipsometric spectroscopy." *IOP Conf. Series: Materials Science and Engineering*, vol. 9, issue 1, p. 012055. IOP Publishing, Ltd., Bristol, U.K. LLNL-PROC-415099.

Microbes and Minerals: Imaging Carbon Stabilization—Jennifer Pett-Ridge (10-ERD-021)

Abstract

Understanding the mechanisms and persistence of interactions between organic molecules and minerals is crucial to the maintenance of sustainable organic matter levels in soils, especially in systems stressed by climate change and intensive agriculture. We propose to study the interactions between organic molecules, soil minerals, and microbes by marrying high-resolution spectroscopy and imaging mass spectrometry, which will allow us to map organic carbon distribution and image associations of organic material with specific minerals in soil. We will develop new preparation techniques for complex organic and mineral samples, new ways to navigate and relocate analyses, and mechanistic explanations for the carbon saturation behavior of soil fractions crucial to long-term soil carbon stabilization.

We propose to develop advances in sample preparation and imaging analysis by combining scanning

transmission x-ray microscopy and nanoscale secondary-ion mass spectrometry (NanoSIMS) to address the stability of relationships between organic molecules and minerals. Specifically, we intend to determine specific preferential sorption relationships, whether sorption processes amplify over time, and the effects of microbes. Our technology will have great potential for applications in industrial chemistry, geochemistry, and cosmochemistry, as well as for terrestrial carbon sequestration.

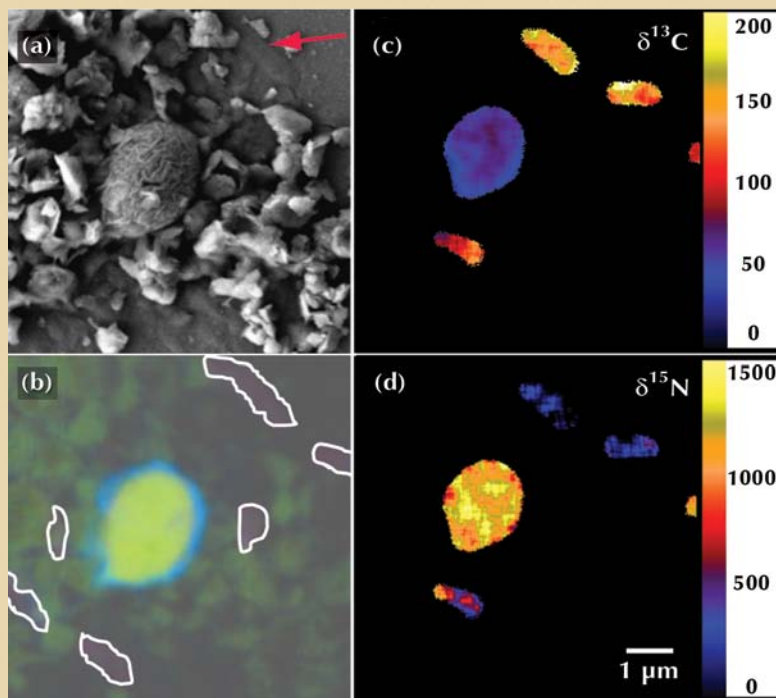
Mission Relevance

Our approach will allow us to characterize highly complex associations of biological and mineral materials and contribute to an improved understanding of carbon stabilization in soils, which supports

the Laboratory's mission of enhancing the nation's environmental security. With our unique combination of high-sensitivity and high-resolution imaging for coupled analyses of organic, mineral, and isotopic distributions, this research advances LLNL measurement science and technology efforts for a strong foundational science and engineering base. Our technology is also relevant to a primary mission area in the DOE's Genomic Science Program.

FY10 Accomplishments and Results

In FY10 we developed novel techniques to prepare complex organic–mineral samples and new ways to navigate and relocate analysis sites using scanning electron microscopy, scanning transmission x-ray microscopy (STXM), and NanoSIMS.



Scanning electron microscopy, scanning transmission x-ray microscopy (STXM), and nanometer-scale secondary-ion mass spectroscopy (NanoSIMS) images of a microbe–mineral microstructure. (a) Electron micrograph of a yeast nucleus in the center, surrounded by montmorillonite quasicrystals and bacteria surrounded by montmorillonite quasicrystals and bacterial cells (red arrow). (b) Color composite of quantitative component maps of proteins, amino sugars, and phospholipids obtained by spectral fitting of reference compounds to STXM and near-edge x-ray absorption fine-structure image sequences using linear regression. (c) Carbon-isotope-ratio NanoSIMS image, in which the scale indicates the ratio of ^{13}C – to ^{12}C –. (d) Nitrogen-isotope-ratio NanoSIMS image, in which the scale indicates the ratio of $^{12}\text{C}^{15}\text{N}$ – to $^{12}\text{C}^{14}\text{N}$ –.

Specifically, we (1) set up microcosm incubations with minerals, nitrogen-15 and carbon-13 substrates, and microbial inocula; (2) conducted test analysis of analysis sites with both STXM and NanoSIMS in which we examined the necessary size of particles and the effects of gold and iridium coating, as well as the effects of pure yeast bacterial cultures labeled with carbon-13 and nitrogen-15 before and after mixing with minerals, soils after long-term addition of nitrogen-15-labeled leaf litter, organic layer soils after addition of labeled chitin (as a fungal hyphae surrogate), and the interior and exterior of subsoil aggregates exposed to labeled chitin—in all cases performing extensive scanning electron microscopy characterization before and after analyses; (3) assessed STXM and NanoSIMS analytical effects using a combination of before-and-after secondary electron microscopy imaging; and (4) began a suite of multifactorial soil incubations with combinations of isotope-labeled bacteria and fungi, pure manganese oxide minerals, and field soils.

Proposed Work for FY11

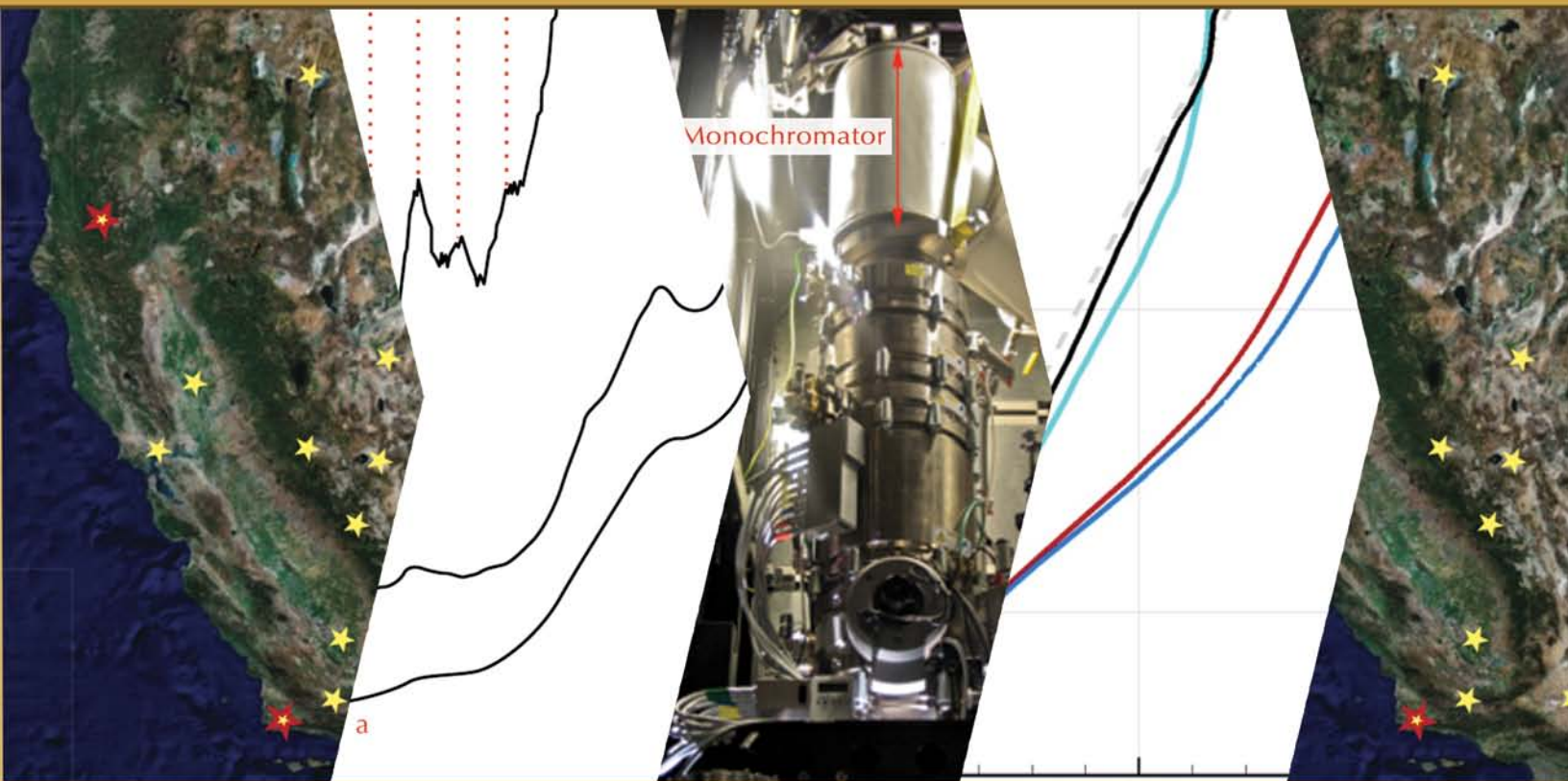
In FY11 we will (1) start a series of multifactorial soil-incubation experiments with “synthetic soil”—mineral mixtures incubated with organic functional groups—both with and without microbial catalysts; (2) collect soil samples at the peak and nadir of soil organic carbon respiration; (3) analyze the samples for carbon-13 dioxide production using both bulk characterization and microanalysis—namely, STXM to elucidate spatial association of the key elements of interest including carbon, nitrogen, oxygen, and transition metals within microaggregates, and NanoSIMS to make high-resolution correlated maps of the distribution of isotopically labeled organic matter relative to the STXM mapping; and (4) use the results of analyses to determine the stability of sorption relationships formed between organic functional groups and components of the soil, identify groups with preferential sorption to various mineral phases, and understand whether sorption processes amplify over time and what the physio-spatial effects of the microbes are.

Publications

Keiluweit, M., et al., 2010. *The chemistry of environmental interfaces: A joined x-ray spectromicroscopy and NanoSIMS approach*. Microscopy and Microanalysis 2010 Mtg., Portland, OR, Aug. 1–5, 2010. LLNL-PRES-435974.

Pett-Ridge, J., et al., 2010. *C and N dynamics in soil microstructures: A joined STXM–NEXAFS and nanoSIMS approach*. Goldschmidt 2010, Knoxville, TN, June 13–18, 2010. LLNL-PRES-435974.

Pett-Ridge, J., et al., in press. “Joining NanoSIMS and STXM/NEXAFS to visualize biotic and abiotic processes at the nanoscale.” *Environ. Sci. Tech.* LLNL-PRES-435974.



Earth and Space Sciences

Coordinated Analysis of Geographic Indicators for Nuclear-Forensic Route Attribution—M. Lee Davisson (08-ERD-065)

Abstract

We propose to develop a scientific foundation for determining the route of smuggled nuclear materials via nuclear forensics by exploring which types of signatures are viable over what timescales and why. The pathways and means of transport are key to uncovering the smuggling routes and potential distribution sites of illicit nuclear material. Environmental and geological particulates and surficial deposits will be analyzed in coordinated studies by x rays, electron and ion microscopy, and gas chromatography–mass spectrometry to extract geographically specific signatures such as molecular and trace-element chemistry and stable isotope abundances. Accuracy and limitations will be analyzed using real-world materials.

This work will improve our understanding of which, why, and how geographically specific clues identify their environment and can be used as measurable, meaningful signatures of the route of smuggled radioactive and associated materials. We anticipate the first-ever demonstration of isotope signatures for route attribution. The analytical methods and technical capabilities we develop will significantly impact the scientific foundations for more efficient and effective route attribution. This project will leverage, enhance, and expand LLNL's capabilities and expertise in nuclear forensics; produce publications; and establish core technical capabilities that can address future programmatic needs in nonproliferation and nuclear attribution.

Mission Relevance

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

FY10 Accomplishments and Results

In FY10 we (1) completed packaging material exposure experiments, demonstrated the value of exposure data as forensic evidence, and presented the results at a conference; (2) exposed pollen samples to carbon-13-labeled dodecane compounds and analyzed the results (including depth of penetration) with nanometer-scale secondary-ion mass spectroscopy to test the compounds' utility as a chemical forensic substrate and showed that hydrophobic surface adsorption dominated; (3) expanded our geographic database for oxidation layer studies by initiating rust collection at different elevations; (4) performed controlled oxidation experiments to determine the contribution of oxygen from water (globally variable) and air (not variable) in oxide formation; and (5) explored double oxidations with different isotopic compositions and showed that different generations of rust form distinct isotopic (oxygen-18) zones at the microscale.

Proposed Work for FY11

In FY11 we will (1) complete a set of iron oxidation experiments with water of different oxygen-stable isotope compositions using combined scanning electron microscopy and nanometer-scale secondary-ion mass spectrometry, (2) test our predictive ability with actual environmental samples collected from a range of elevations that map stable isotope variation, (3) measure mineralogy and isotope compositions as well as oxidation layers in actual samples acquired from transported nuclear material, and (4) submit a paper on the use of oxidation (corrosion) layers as a route attribution indicator.

Publications

Davisson, M. L., H. A. Ishii, and R. N. Leif, 2010. *Potential route evidence from fugitive chemicals adsorbed to packaging materials and metal oxides*. 51st Mtg. Institute of Nuclear Materials Management, Baltimore, MD, July 11–15, 2010. LLNL-CONF-434293.

Davisson, M. L., R. N. Leif, and H. A. Ishii, 2010. *Potential for detecting fugitive chemicals sorbed to packaging material*. LLNL-JRNL-461054.

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

Abstract

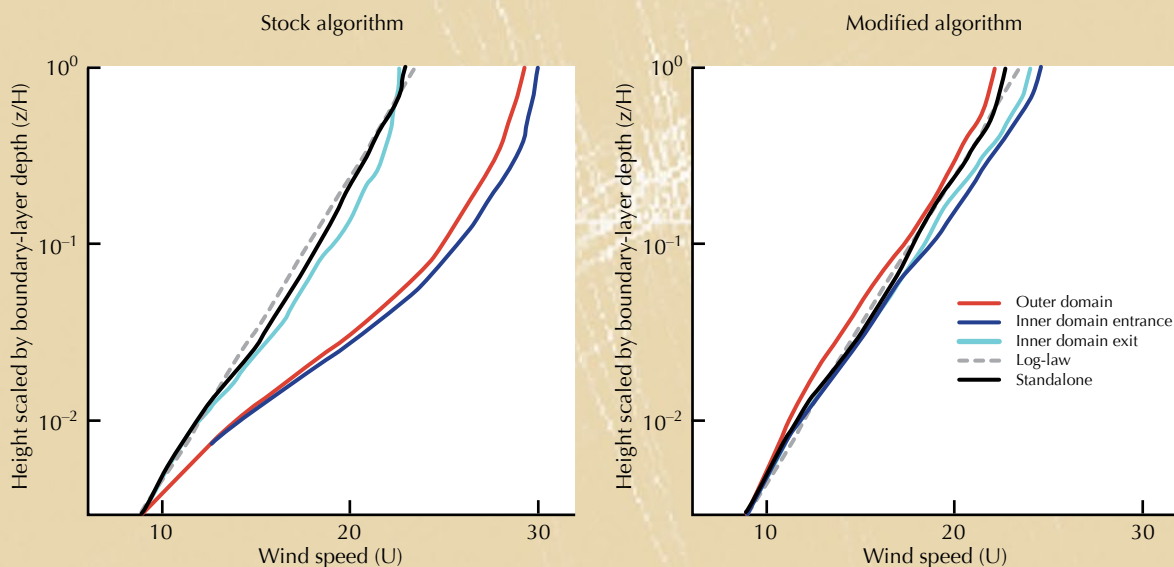
A significant problem in simulating atmospheric flow in the lower atmosphere is how to accurately represent the entire spectrum of flow features, from the large scales of weather to the small scales of turbulence, that influence near-surface flow. To overcome this problem, we must fill an important knowledge gap involving modeling flow at intermediate scales—that is, those between the large- and small-scale endpoints that we understand more fully. In this project, we aim to fill this gap by developing both the physical models and the technical expertise required to achieve an accurate multiscale flow simulation and prediction capability. Filling this

knowledge gap is critical to many important scientific thrusts, including wind energy, climate modeling, and emergency preparedness and response.

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

Mission Relevance

By extending the ability to simulate and predict complex atmospheric flows, this work directly benefits efforts in risk and response management in support of the national security mission. In addition, wind-resource characterization and



Improvement in vertical wind speed profiles as a function of height normalized by boundary-layer depth for nested simulation of atmospheric flow using an improved near-surface turbulence algorithm. Grey dashed lines show the expected solution, while black lines show solution from non-nested, stand-alone simulation, demonstrating optimal performance for this model. Other colors represent a nested simulation: blue lines show profiles at the inlet and outlet planes of the inner domain, while red lines are from the outer domain solutions that drive the inner domains. The simulation employing the standard algorithm (left) shows significant departures from the expected behavior, whereas the modified algorithm simulation (right) more closely matches the expected solutions at all locations within both domains.

dynamic downscaling approaches address regional climate adaptation and mitigation in support of the Laboratory's missions in energy security and regional climate modeling.

FY10 Accomplishments and Results

In FY10 we (1) examined flow transition at nest inflow interfaces and implemented dynamic subfilter stress models that reduce the length scale of flow equilibration and better match non-nested (truth) simulations, (2) continued multiple nested simulations of air flow over an isolated hill and compared the results with observational data, (3) validated new turbulence models in stable and convective simulations, and (4) examined the transition between large-scale and large-eddy turbulence models in multiple nested simulations.

Proposed Work for FY11

In FY11 we will (1) continue to improve algorithms for turbulent flow exchange at mesh interfaces and extend the algorithms to multiple nests, (2) continue extending nesting beyond turbulence-resolving scales to larger scales, (3) investigate some simple approaches to modeling turbulence that span length scales from mesoscale to large-eddy scale, (4) continue using data from previous experiments and LLNL's wind-energy industry partners to validate progress in modeling the effects of complex terrain and wind park environments, and (5) investigate mesoscale turbulence interactions involving breaking waves and low-level jets.

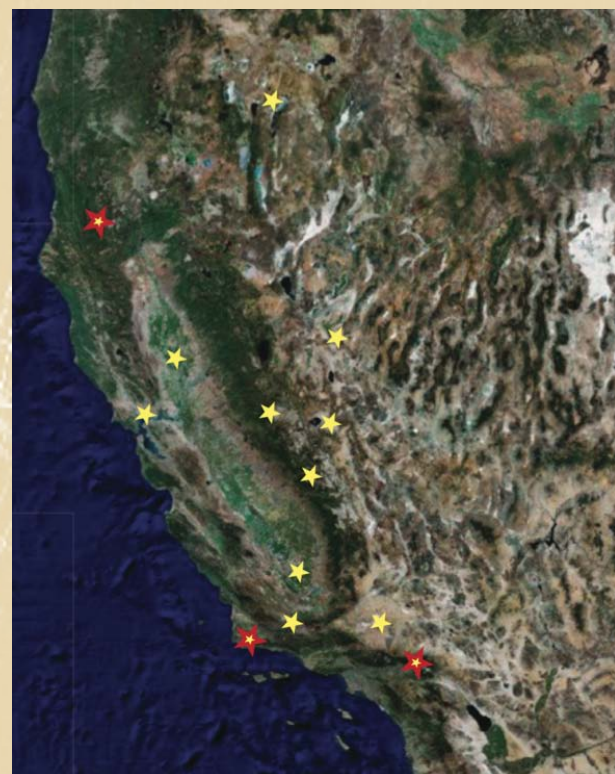
Publications

Kirkil, G., and J. Mirocha, 2010. *Nested high-resolution mesoscale/large eddy simulations in WRF: Challenges and opportunities*. 5th Intl. Symp. Computational Wind Engineering (CWE2010), Chapel Hill, NC, May 23–27, 2010. LLNL-PRES-432948.

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

Abstract

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



A network of high-resolution, well-dated records of past climate change from California lakes will improve our understanding of Earth's climate system and the prediction of future climate changes. Yellow stars indicate sites where dating work was done for the project. Red-yellow stars mark the four sites that are the focus of mapping and spectral analysis because of the quality of paleoclimate records: Fish and Ogarmtoc and neighboring lakes in the north; Zaca Lake in the south coast; and Big Bear Lake in the mountains east of Los Angeles.

and twigs from outcrop and core samples for which collaborators have climate records under development. The goal is to create high-resolution, high-precision radiocarbon and calendar chronologies for these climate events.

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

Mission Relevance

Creating drought records for California supports the Laboratory's mission in energy security and climate. We will ultimately provide diagnostic tools in support of LLNL work to modify the Weather Research and Forecasting Model for regional climate prediction, which will enhance collaborations between Lawrence Livermore and outside organizations and support programs at DOE and various other federal agencies.

FY10 Accomplishments and Results

In FY10 we (1) produced working age models for Zaca and Klamath lakes; (2) significantly improved the resolution of a previous age model for Big Bear Lake; (3) dated Big Soda Lake climate records; (4) collected a new core from Mono Lake, because sediment sequences from Crooked Meadows and Mono Lake did not contain sufficient datable material for high-resolution chronologies; and (5) demonstrated that Anodonta shells from Mojave lake beds are a reliable matrix for radiocarbon dates.

Proposed Work for FY11

In FY11 we will (1) complete high-resolution records from Zaca, Big Bear, and Fish and Frog lakes, as well as for the Sequoia cores recovered in FY10,

the Mojave sites, and the San Francisco Bay and Big Soda Lake cores; (2) study several other potential sites, including Lake Moran, San Francisco shell mounds, and Soda Lake; (3) complete four to six high-resolution records; and (4) generate California drought maps and spectral analysis for these data sets.

Publications

LeRoy, S. L., et al., 2009. *Radiocarbon constraints on fossil thinolite tufa formation in the Mono Basin, CA*. American Geophysical Union 2009 Fall Mtg., San Francisco, CA, Dec. 14–18, 2009. LLNL-POST-421330.

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

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

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

Abstract

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

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

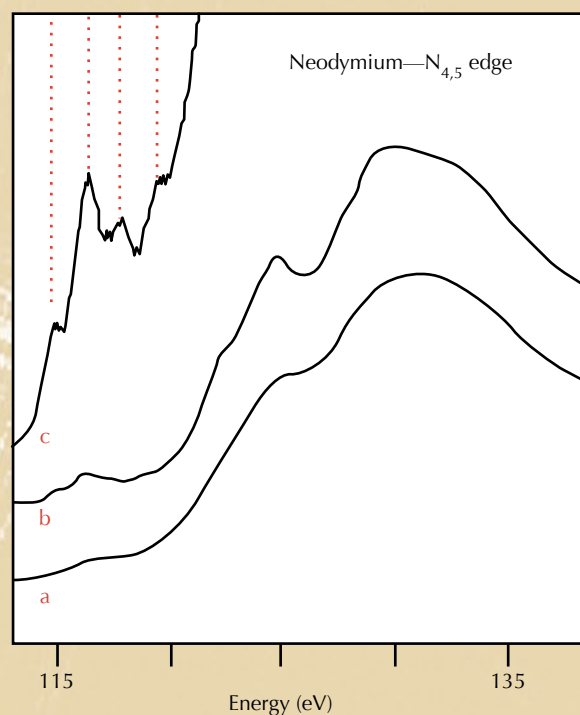
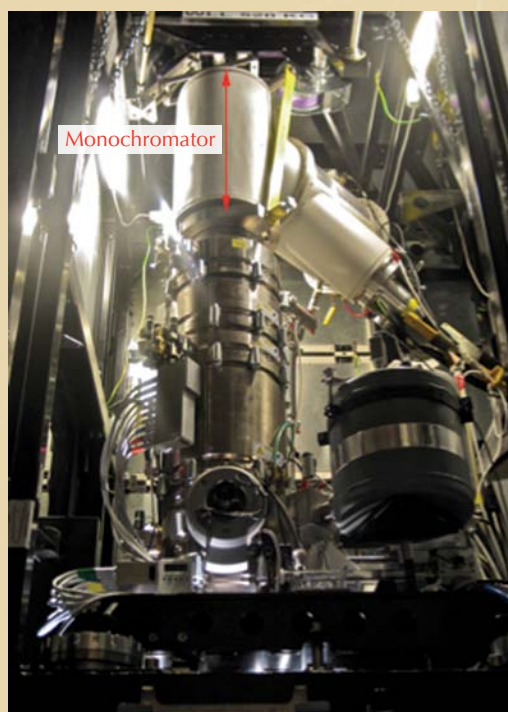
Mission Relevance

This project supports the Laboratory's national security mission by gaining insight into an important

material for radiation detection. Other aspects of the project support efforts in breakthrough science by addressing fundamental planetary science questions and the properties of these and other materials at atomic or near-atomic level. The proposed research will also attract top young scientists to the Laboratory.

FY10 Accomplishments and Results

In FY10 we (1) identified a design flaw in the Titan scanning transmission electron microscope and proposed and implemented an engineering modification that resulted in an increased energy resolution of about twofold, (2) continued to publish our results from studies of Stardust samples and other meteoritic materials in the peer-reviewed literature, (3) gained fundamental insight about radial transport of materials during the earliest (pre-planetary) phase of early solar system evolution, and (4) expanded the range of projects and samples examined using Titan with



Livermore's 80- to 300-keV Titan scanning transmission electron microscope is shown in its vibration isolation chamber (left). The monochromator we helped develop, used for isolating a narrow portion of a spectrum, enables electron energy-loss measurements with significant improvement in signal-to-noise and atomic-scale spatial resolution. Recent energy-loss spectra measured at Titan for the lanthanide element neodymium (a surrogate for the actinide elements) are shown on the right. The $N_{4,5}$ edge is shown in (a) with the monochromator deactivated and in (b) with the monochromator activated. In (c), the spectrum from (b) has been expanded vertically by about tenfold. The features (highlighted by red dotted lines) encode information about the localization of f orbitals in neodymium. Subtle changes in these features as a function of temperature and chemical doping provide direct insight into the character of the f -electron localization and delocalization transition.

emphasis on emerging programmatic needs such as actinide analogues, steels for reactor containment vessels, and experimental semiconductor materials for nonproliferation technologies.

Proposed Work for FY11

We will continue to perform basic scientific research on extraterrestrial and other materials and publish the results to focus international attention on LLNL as a center for world-class analytical science. Our activities will also serve as a powerful tool for recruiting young scientists to important research areas. We will also seek to attract internal and external users of the Titan and other analytical assets, both for mission-relevant activities and basic scientific research, and seek to develop a wide range of applications.

Publications

Aguiar, J. A., et al., 2010. "Detection of organic compounds with one-nanometer spatial resolution." *41st Lunar and Planetary Science Conf. (2010)*, 1901.pdf. LLNL-PRES-425121.

Bonal, L., et al. 2010. "Highly ^{15}N -enriched chondritic clasts in the CB/CH-like meteorite Isheyevo." *Geochim. Cosmochim. Acta* **74**(22), 6590. LLNL-JRNL-410057.

Bradley, J. P., and Z. R. Dai, 2010. "Analytical SuperSTEM for extraterrestrial materials research." *Meteorit. Planet. Sci.* **44**(10), 1627. LLNL-JRNL-416911.

Chi, M., et al., 2009. "The origin of refractory minerals in comet 81P/Wild 2." *Geochim. Cosmochim. Acta* **73**(23), 7150. LLNL-JRNL-410054.

Ishii, H. A., et al., 2010. "Nitrogen carrier identified in ^{15}N extreme hotspots in the Isheyevo (CH/CB)." *Meteorit. Planet. Sci. Suppl.*, 5406.pdf. LLNL-ABS-431240.

Matzel, J. E. P., et al., 2010. "Constraints on the formation age of cometary material from the NASA Stardust mission." *Science* **328**(5977), 483. LLNL-JRNL-420385.

Matzel, J., et al., 2009. "Mg isotope measurements of a Stardust CAI: No evidence of ^{26}Al ." *Meteorit. Planet. Sci. Suppl.*, 5373.pdf. LLNL-PRES-414494.

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

Abstract

Ammonium perchlorate and other perchlorate salts can be found in a number of commercial, industrial, and military applications. This use has resulted in environmental releases of the substance, which were first discovered in the surface and groundwater around the U.S. in the late 1990s. Subsequent human exposure is a human health concern, because perchlorate has been found to reduce iodine uptake by the thyroid gland and can affect hormone secretion. A first step in characterizing the anthropogenic sources of perchlorate and their impact is to arrive at an understanding of the natural abundance and occurrences of perchlorate in the environment. To this end, we will measure perchlorate isotope systematics in groundwater having no known anthropogenic perchlorate sources. We will do this by exploiting the ubiquitous natural presence of the rare chlorine-36 isotope to determine the source, formation mechanisms, and fate of groundwater perchlorate. Samples will be dated and assessed for recharge conditions, improving our ability to identify and characterize the source and environmental disposition of groundwater perchlorate. This project will leverage LLNL's unparalleled technical capabilities in accelerator mass spectrometry and noble gas mass spectrometry.

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

Mission Relevance

This project supports LLNL's security mission by developing a new method for assessing sources and mobility of groundwater contamination and has applications in regional climate modeling. Our research will help answer important basic questions about the source of perchlorate contamination in pristine wells, thereby elucidating historic perchlorate exposure. This helps determine scientifically defensible regulations and provides insight into the storage and release of perchlorate during expected changes in the nation's water supply caused by climate change.

FY10 Accomplishments and Results

During FY10 we (1) completed sample preparation protocols and collected well water samples for testing isotope-ratio mass spectrometry techniques; (2) developed novel methods for isolation and purification of groundwater-derived perchlorate samples, with an emphasis on chlorine isotopes for accelerator and isotope-ratio mass spectrometry; and (3) began two publications that will document the results of this project. Continued research will involve performing a selected set of specialized analyses in collaboration with hydrologists from the U.S. Geological Survey.

An Adaptive, Coupled Regional Climate and Hydrologic Modeling System for Accurate Wind-Power and Water-Resource Simulation—Carol Woodward (10-ERD-011)

Abstract

We propose to research algorithms necessary for an adaptive subsurface simulation capability for the coupled ParFlow and Weather Research and Forecasting (PF-WRF) regional climate and hydrologic modeling system. We intend to apply the system to a site in California's Central Valley to further knowledge about this area's water resources and demonstrate applicability of the model for wind-resource assessment. Proposed work includes research in numerical discretizations and solvers for coupled, nonlinear flow and refined grids. Model applications will address wind-energy forecasting

and deployment and water-resource questions related to regional climate change.

If successful, this project will provide the necessary discretization and solver algorithms required for solving nonlinear parabolic equations posed on adaptive spatial grids. These algorithms are necessary for implementing an accurate and efficient spatial adaptive capability within the subsurface portion of the coupled PF-WRF model. We will analyze a site in the California Central Valley to answer wind-energy deployment and water-resource vulnerability and reliability questions related to regional climate change. The proposed work will allow development of a significant and efficient computational capability not achieved by any other wind-power simulator.

Mission Relevance

Our modeling system for wind-energy deployment and water-resource availability supports the Laboratory mission in energy and environmental security. The proposed capability will provide a significant tool for the strategic mission thrust of regional climate modeling and impacts, with the goal of providing for wind-energy deployment, simulation, and boundary-layer physics.

FY10 Accomplishments and Results

In FY10 we (1) completed a literature search and identified two potential schemes for use in discretization of the coarse-fine boundaries of an adaptive grid within the ParFlow Richards equation model; (2) documented these schemes, including potential advantages and disadvantages; (3) developed and implemented a spline fit and lookup table for efficiently computing relative permeabilities within the Richards equation model, which is essential for efficient running of the Central Valley site model; (4) developed a heuristic method for subcycling the WRF model relative to ParFlow, also giving significant potential efficiency benefits; (5) completed an initial specification of the Central Valley site model, including surface topography, geological models, and atmospheric forcing specification; and (6) conducted initial runs of the PF-WRF model to identify solver difficulties and computational bottlenecks. In summary, this project enabled simulations of the Central Valley site using the PF-WRF model, including investigations of surface and subsurface

water interactions. Follow-on support for additional work with this PF-WRF capability will be sought from DOE's Office of Biological and Environmental Research, other Federal agencies, and the State of California.

Publications

Kollet, S. J., et al., 2010. "Proof of concept of regional scale hydrologic simulations at hydrologic resolution utilizing massively parallel computer resources." *Water Resour. Res.* **46**, W04201. LLNL-JRNL-462006.

Maxwell, R. M., et al., in press. "Development of a coupled groundwater-atmospheric model." *Mon. Weather Rev.* LLNL-JRNL-423133.

Enhancing Climate Model Diagnosis and Intercomparison—Karl Taylor (10-ERD-060)

Abstract

Current capabilities in global climate modeling and evaluation lack information about why models differ in their projections. They also fail to incorporate carbon cycle and atmospheric chemistry information. It is not understood how uncertainties in cloud feedbacks and other key mechanisms vary over different timescales, and simplistic metrics are used for model performance. We intend to conduct innovative research that would address these needs. We will develop concepts for globally distributed and synthetic data sets, as well as advanced metrics for model simulations of ocean, land-surface, and sea-ice processes. We will also provide new analysis and diagnostic methods for cloud and other feedbacks and new measures of model performance.

This project will result in the most comprehensive and scientifically meaningful set of climate modeling and evaluation tools available to the scientific community to date. Specifically, the enhancements over existing global climate modeling and evaluation approaches are expected to (1) improve the ability to constrain climate model projection uncertainties related to the structural uncertainties in the models themselves (e.g., in the physics and parameterizations); (2) improve the ability to constrain

inter-model feedback differences on the century timescales that are of most interest; (3) increase our understanding of model differences and reliability; and (4) maintain and strengthen LLNL's national and international preeminence in climate model diagnosis and intercomparison.

Mission Relevance

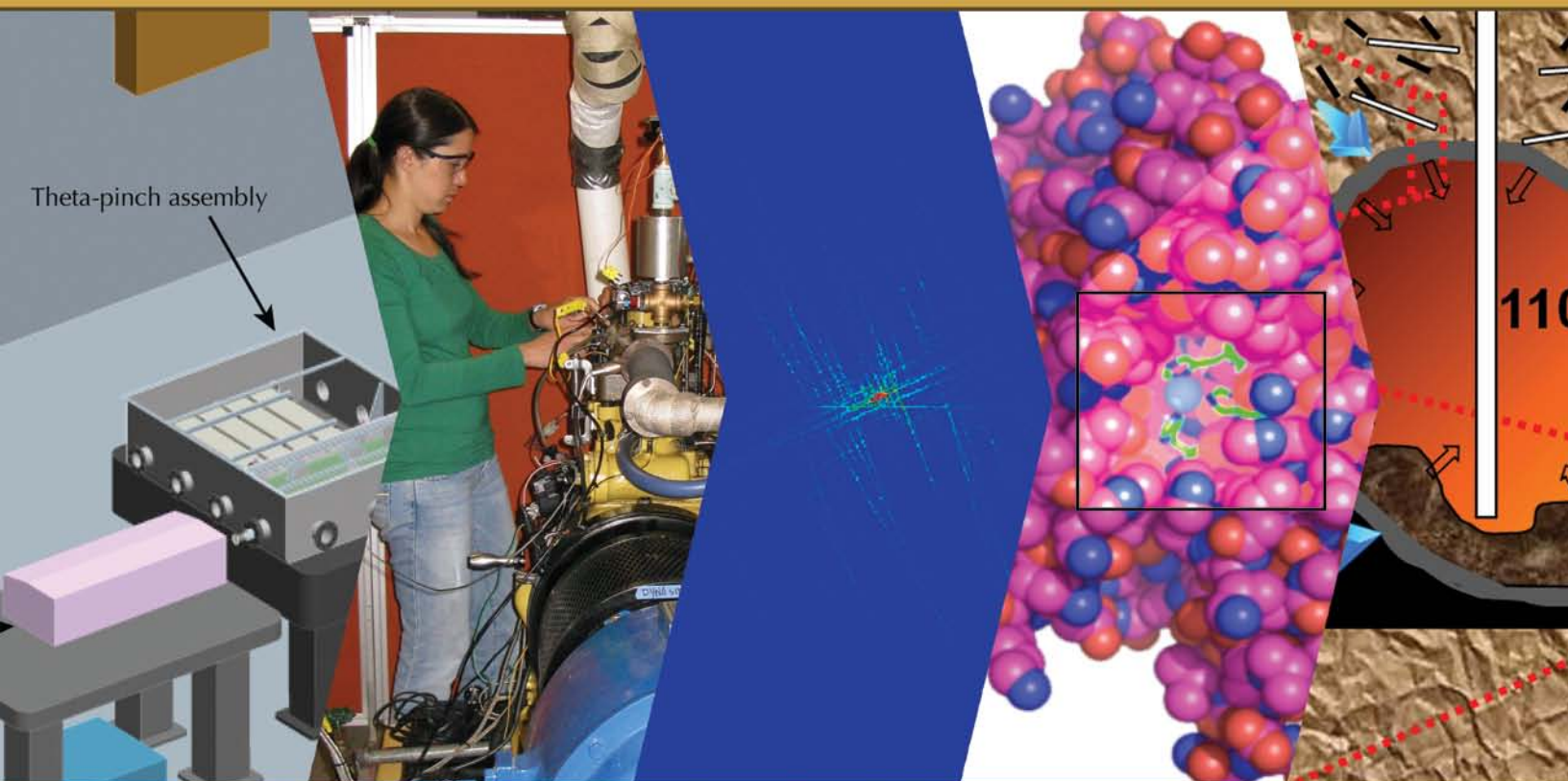
This work supports LLNL's mission focus area in energy and climate by furthering regional and global climate predictive capabilities, and it is directly relevant to DOE's mission in understanding and mitigating global climate change. It will address scientific questions that underpin the upcoming Coupled Model Intercomparison Project, a flagship activity of DOE's Climate Change Prediction Program.

FY10 Accomplishments and Results

In FY10 we (1) completed development of an enhanced capability for rewriting model output in conformance with community-accepted data standards, (2) provided our software library to modeling groups worldwide to prepare data for analysis by thousands of researchers, and (3) developed a new code to produce what are termed "synthetic microwave sounding unit" temperatures from standard climate model output. This will make it possible to routinely compare Coupled Model Intercomparison climate model microwave sounding unit temperature trends directly to observations, which is a significant addition to our model evaluation capabilities.

Proposed Work for FY11

We will (1) develop new analysis techniques for cloud- and carbon-cycle feedbacks that will lead to new understanding of the sources of model uncertainty, (2) explore the advantages of multivariable and multiple timescale approaches for detecting and attributing observed climate change to specific causes, (3) develop methods for estimating uncertainty in climate projections based on a combination of multimodel simulations and perturbed-physics ensembles, and (4) continue to develop innovative concepts for data management and analysis for globally distributed data sets.



Energy Supply and Use

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

Abstract

The capability to quantify and verify carbon emissions to ensure adherence to emission limits is vital to California as well as to national and global environmental management and energy security efforts. Expertise in carbon isotope analysis, atmospheric modeling, and computational physics make Lawrence Livermore uniquely qualified to supply independent verification of emissions of carbon dioxide (CO₂) resulting from burning of fossil fuels. Accurate assessment of fossil-fuel carbon emissions requires 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 CO₂ emissions in California. Issues we will address include solving the inversion problem and numerically estimating the emission magnitude and distribution of chemical species, given measurements of chemical concentrations at various locations.

This project will create a simulation-based framework for locating and tracking fossil-fuel emissions for California and will document the needs for an independent emissions estimate using conventional CO₂ concentrations and carbon isotope (carbon-14 dioxide) analyses. These results will also further our understanding of other inert trace greenhouse gases in the atmosphere. California is a challenging test bed for this potential tool, and federal agencies are looking to California as a model for a possible future national program.

Mission Relevance

This project supports LLNL's missions in regional climate modeling and energy security by promoting advancements in predicting, understanding, and monitoring climate and energy systems.

FY10 Accomplishments and Results

In the final year of our project we expanded our synthetic retrievals in the time domain, using meteorological data for a full 30 days of simulations in both January (nominal winter) and July (nominal summer). For the network design problem, we treated fossil-fuel CO₂ as a passive tracer in the atmosphere—that is, equivalent to an idealized anthropogenic nonreactive emission. Simulations were run in ensemble mode, including the use of an ensemble Kalman averaging filter, and the retrieval mean and uncertainty of the ensemble was consistent with the prescribed emissions field. Not surprisingly, individual model runs with poor representation of the planetary boundary layer and its mixing into and with the free troposphere had poorer retrievals. Additionally, we instituted a formal cost-benefit analysis of network design and retrieval error using Pareto analysis, which allows us to determine tradeoffs between the retrieval error and the cost of making additional observations. Our modifications allow for the simultaneous transport of multiple fossil-fuel CO₂ tracers emitted from different surface regions. With our idealized tracer transport and retrieval system, we have shown that fossil-fuel CO₂ emissions (or other surface-emitted trace gases) can be reliably retrieved via a top-down transport and inversion model. Exploration of the cost-benefit relationship via the use of Pareto analysis quantifies that, for California, the network is finite and tractable. Similar analysis could be done for a larger national or global network to assist in network design and uncertainty quantification in support of treaties and protocols. We are continuing to work with DOE and related sponsors in developing a roadmap for a greenhouse gas information system.

Publications

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

Delle Monache, L., et al., 2008. "Toward regional fossil fuel CO₂ emission verification using WRF-CHEM." *EOS Trans. AGU* **89**(53), A53H-03. LLNL-ABS-406850.

Lucas, D. D., et al., 2010. "Multi-objective design of optimal greenhouse gas observation networks." *EOS Trans. AGU Supp.*, GC13D-0729. LLNL-ABS-452333.

Direct Simulation of Dynamic Fracturing during Carbon Storage and Prediction of Potential Storage Failures—Scott Johnson (08-ERD-039)

Abstract

Large-scale carbon dioxide (CO₂) storage projects are required to reduce greenhouse gas emissions. Integrity of the caprock overlying storage reservoirs is critical to safe and effective long-term subsurface CO₂ storage. This project seeks to develop and apply a new simulation capability for predicting the stability of geologic carbon storage. Specifically, we will leverage existing LLNL codes to simulate the possibility of dynamic fracture and reactivation of existing fractures and faults in caprock in response to CO₂ injection. To achieve this goal, we will modify LDEC (an existing LLNL finite-difference element code with dynamic fracture and fully coupled fluid-flow capabilities) to directly simulate potential damage within caprock. A reservoir-scale fracture network simulator will evaluate the large-scale consequences of these events.

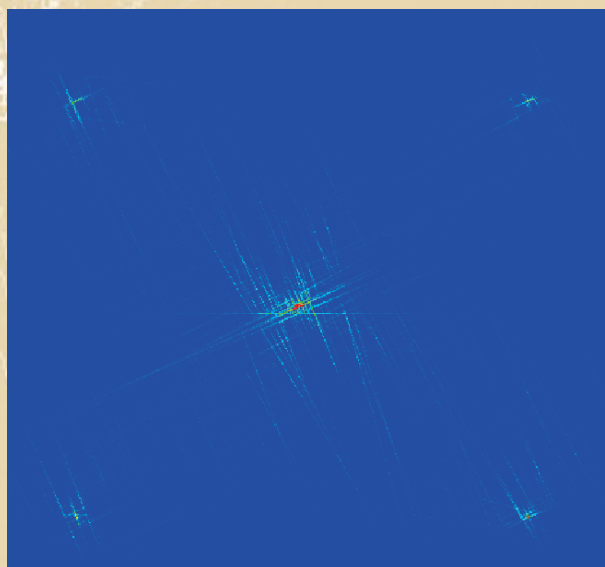
To date, little attention has been dedicated to either geomechanical deformation of caprock or fault and fracture reactivation. If successful, the project will deliver a versatile tool for simulating permeability change at the field scale in response to dynamic fracture activation and from changes in pore fluid pressure. We will perform a parameter study investigating the response of caprock to typical CO₂ 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 CO₂. The tools developed can also be used for other energy-related activities such as optimization of gas recovery from shale and the engineering of geothermal systems, which both use 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 of the geomechanical sources of risk in CO₂ storage.

FY10 Accomplishments and Results

In FY10 we (1) extended the capabilities of LDEC to accommodate massively fractured rock masses containing up to several thousand fractures of arbitrary length, orientation, and aperture; (2) demonstrated this capability for analyzing large, reservoir-scale systems; and (3) demonstrated the ability of LDEC to capture flow and evolving fracture network topology for highly fractured systems, positioning the capability to provide improved site characterization as new data becomes available from existing geologic carbon sequestration sites. In summary, this project provided enhanced capabilities for simulating fluid-rock interaction in a number of crystalline geologic systems, thus enabling not only prediction of caprock integrity for geologic carbon sequestration, but also capabilities for applications such as enhanced oil recovery, enhanced geothermal



The flow field in a heterogeneous, fractured, low-matrix-permeability rock mass with a five-spot well configuration, with the injector in the center and production wells in the corners.

systems, and induced seismicity from subsurface engineering operations. The next step needed will be to enhance these numerical techniques across a range of energy applications by increasing numerical stability, extending the code to accommodate matrix permeability directly—thereby extending the geologic range of applicability—and continuing verification and validation.

Publications

Johnson, S. M., and J. P. Morris, 2010. *Caprock integrity in carbon sequestration and study of geomechanics in engineered geothermal systems*. 44th U.S. Rock Mechanics Symposium, Salt Lake City, UT, June 27–30, 2010. LLNL-ABS-418846.

Johnson, S. M., and J. P. Morris, 2008. *Coupled finite-volume and discrete-finite element methods for modeling hydraulic fracturing in geologic formations*. 2008 Fall Mtg. American Geophysical Union, San Francisco, CA, Dec. 15–19, 2008. LLNL-ABS-406675.

Johnson, S. M., and J. P. Morris, 2009. *Hydraulic fracturing mechanisms in carbon sequestration applications*. 43rd U.S. Rock Mechanics Symposium, Asheville, NC, June 28–July 1, 2009. LLNL-ABS-407776.

Johnson, S. M., and J. P. Morris, 2009. *Modeling of hydraulic fracturing for geologic carbon sequestration applications*. Intl. Conf. Rock Joints and Jointed Rock Masses, Tucson, AZ, Jan. 4–10, 2009. LLNL-CONF-406622.

Johnson, S. M., S. Ezzedine, and Y. Hao, 2010. *Study of geomechanics in engineered geothermal systems*. 44th U.S. Rock Mechanics Symposium, Salt Lake City, UT, June 27–30, 2010. LLNL-PRES-438711.

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

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., and S. M. Johnson, 2009. *Permeability evolution in a fractured rock mass in response to fluid injection*. Intl. Conf. Rock Joints and Jointed Rock Masses, Tucson, AZ, Jan. 4–10, 2009. LLNL-CONF-406303.

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, Pittsburgh, PA, May 5–8, 2008. LLNL-PROC-403056.

Morris, J. P., S. M. Johnson, and S. J. Friedmann, 2008. *Geomechanical simulations of CO₂ storage integrity using the Livermore distinct-element method*. Intl. Pittsburgh Coal Conference, Pittsburgh, PA, Sep. 29–Oct. 2, 2008. LLNL-CONF-405398.

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 a hydrogen engine with the potential to deliver the highest 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 approximately 80% and in practice to approximately 50% after heat transfer and friction losses. Our goal will be accomplished by conducting fundamental research on basic issues such as ignition, flame propagation, and detonation that control efficiency at the operating conditions of this engine.

Demonstrating the most efficient internal combustion engine in history demands fundamental understanding of combustion and engine operation in a brand 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. In this project we will conduct basic research to characterize the relevant processes to deliver optimum efficiency. On the road to characterizing this engine, we will explore the uncharted territory of combustion science for hydrogen, oxygen, and argon at high pressures.

Mission Relevance

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

FY10 Accomplishments and Results

In FY10 we (1) successfully operated the engine at a maximum efficiency of 46% without knock, and explored spark timing, relative amounts of argon, and engine speed to achieve maximum efficiency; (2) added a second spark plug to the combustion chamber to increase burn rate and decrease the time for knock to occur; (3) validated use of the KIVA-3V engine modeling code for this application with

experimental data from our project, achieving good agreement between the two; (4) used the validated KIVA-3V model to examine engine physics and improve the operating parameters of our experimental engine; and (5) demonstrated that operating the engine on hydrogen and air at the same fueling rate produced an efficiency of only 36%. Our improvement in performance over hydrogen–air operation shows the promise of utilizing a hydrogen–oxygen–argon mixture. Our project resulted in the successful demonstration of extremely high efficiency with a hydrogen–oxygen–argon internal combustion engine that produces zero harmful emissions.

Publications

Killingsworth, N. J., et al., 2010. "Characteristics of knock in hydrogen–oxygen–argon SI engine." *Proc. Spring Mtg. Western States Section of the Combustion Institute*, vol. 1. LLNL-CONF-424554.



University of California at Berkeley graduate student Vi Rapp (left) and Lawrence Livermore National Laboratory post-doctoral researcher Nick Killingsworth (right) examine the hydrogen–oxygen–argon cooperative fuel research engine.

Killingsworth, N. J., et al., 2010. "Increased efficiency in SI engine with air replaced by oxygen in argon mixture." *Proc. Combustion Institute*, vol. 33. LLNL-CONF-422515.

Toward More Intrinsically Secure Nuclear Fuel Cycles—Keith Bradley (08-ERD-056)

Abstract

The rapid growth in nuclear energy production worldwide poses dramatic risks for the proliferation of nuclear weapons materials. The objectives of this project are to assess and enhance the utility of spent nuclear fuel in numerous fuel recycle schemes being considered worldwide, and use this understanding to conceptualize approaches that hinder the misuse of spent fuel. We expect to determine the dynamic and nuclear properties of sub-mixtures of partitioned spent fuel, assessing the potential for weaponization of such mixtures, and identify and evaluate approaches to mitigating their utility as a nuclear explosive. Lastly, we will demonstrate a proof of principle for one very promising engineering approach to making spent fuel resistant to misuse.

We expect to develop and demonstrate a methodology for assessing the attractiveness of formerly unaddressed nuclear materials. We will identify and study one method to degrade the explosive utility of attractive mixtures. In addition, we will seek solutions that make misuse of nuclear fuel more difficult, in particular by non-state adversaries such as terrorist organizations. Building on a knowledge base that we have developed so far, we will demonstrate the viability of a concept that will re-engineer morphology of the fuel, significantly hindering extraction while allowing for compatibility with existing light water as well as other future reactor designs. Because spent fuel throughout the world is largely under-protected—such a solution should serve to make nuclear fuel more secure.

Mission Relevance

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

FY10 Accomplishments and Results

Our project goal was to develop a class of fuel that is intrinsically resistant to conventional solvent-based extraction methods—unfortunately, any fuel material with a chemically protective coating would be susceptible to defeat by common mechanical means such as crushing or milling. We hypothesized that nanosized fuels may be markedly less susceptible to such attrition methods. Therefore, in FY10 we studied surrogate nanosized samples ranging in size from 20 to 100 nm, a regime where we expected, from theoretical considerations, that samples may begin to exhibit mechanical toughness. Specifically, we studied aluminum oxide and found that it exhibits two key properties after heavy attrition: average particle diameter remains approximately unchanged and the originally faceted surfaces appear to have been rounded. These properties support the concept that particles appear to reach an asymptotic size beyond which they do not decrease in size, but do not resolve the question of whether a surface coating would remain intact or be damaged. Overall, this project has generated an enhanced understanding of numerous fuel cycles used throughout the world and enabled the conceptualization of approaches to hinder misuse of spent fuel, with the last year of the project focused on exploring a promising novel engineering approach for intrinsically securing fuel. We have briefed the Assistant Secretary of Nuclear Energy on our results, and are hopeful for future support for this research through DOE's program for Materials Protection, Accounting and Control for Transmutation within the Office of Nuclear Energy.

Dynamic Chamber Processes for LIFE: Simulations and Experiments on Beam Propagation and Chamber Clearing—Jeffery Latkowski (10-SI-009)

Abstract

To mitigate the challenges of nuclear energy and to advance the timescale for availability of fusion sources, the Laboratory envisions a novel once-through, closed fusion-fission nuclear fuel cycle based upon the Laser Inertial Fusion Energy (LIFE)

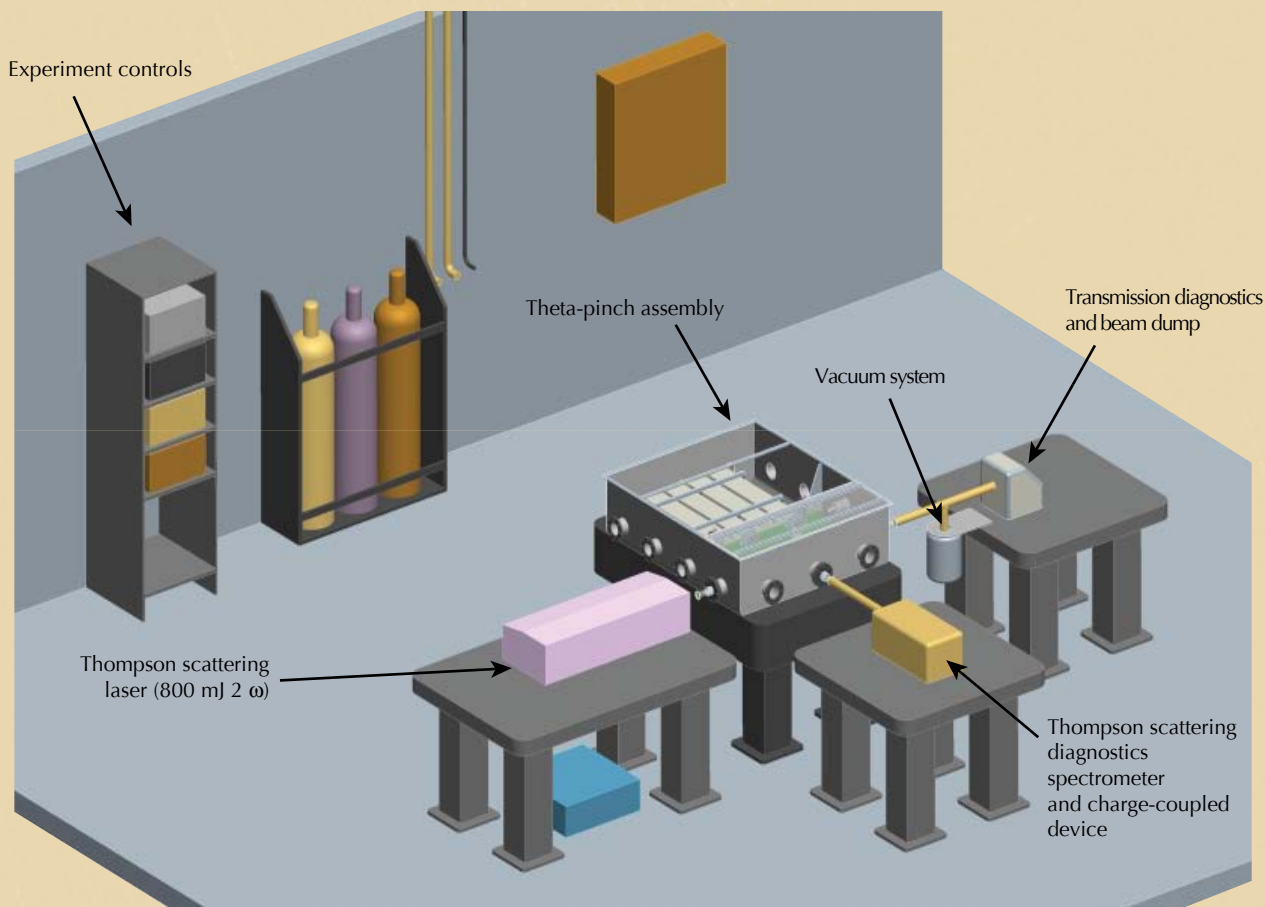
concept. We propose to couple modeling and experiments to explore and resolve fundamental issues for the LIFE chamber, including gas clearing between rapid (10-Hz) shots and laser beam propagation. Radiation-hydrodynamics modeling will predict the chamber-gas state after a LIFE shot and support scaled experiment design, while computational fluid dynamics will be used to explore the clearing of hot gas and debris from the chamber. Scaled experiments using existing kilojoule-class lasers will be used to observe chamber clearing and beam propagation.

We expect to achieve experimental proof of principle for chamber clearing and beam propagation for a LIFE chamber, including (1) a consistent model of post-shot plasma conditions; (2) characterization of beam propagation, including gas ionization, debris, density gradients, and turbulence; (3) assessment of chamber gas dynamics, including aerosol formation;

(4) an optimized vent-and-fill protocol; and (5) demonstration of plasma cooling, clearing, and beam propagation in a scaled chamber. In addition, we will develop plans for a high-energy experimental campaign.

Mission Relevance

This project supports LLNL's mission of enhancing energy security for the nation and builds directly upon the Laboratory's world-class capabilities in inertial-confinement fusion and laser technologies. Our research is a key component of the Laboratory's strategic roadmap in energy security. Resolving key issues for practical, cost-effective laser inertial-fusion energy plants also supports the Laboratory mission in environmental security by enabling a source of abundant, clean power without nuclear waste disposal, safety, carbon sequestration, or proliferation issues. A demonstration of chamber clearing



Our theta-pinch experiment will enable us to create and study a xenon plasma under conditions similar to what we expect in the Laser Inertial Fusion Energy (LIFE) chamber.

and beam propagation at high repetition rates will address key technical issues about the feasibility of the LIFE concept while producing important scientific results.

FY10 Accomplishments and Results

In FY10 we (1) developed a radiation-hydrodynamic model of chamber gas cooling and used it to determine decoupling of electron and ion temperatures, so the gas stays hot (approximately 0.5 eV) between shots, placing a significant constraint on target injection; (2) confirmed these simulations with LLNL codes LASNEX and Cretin and conducted sensitivity tests with various models, including SCRAM, Hydra, Flychk, and Purgatorio, to understand the uncertainty in these predictions and identify experimental needs; (3) used Miranda, an LLNL large-eddy simulation code, to study the generation and damping of shocks and turbulence in the fusion chamber with different geometries, discovering that the dispersion of target debris in the chamber is highly sensitive to xenon opacity—specifically, the response of cold xenon layers to Marshak radiation—and that in some scenarios, target debris remains concentrated in a local cloud, leading to simpler clearing strategies; (4) submitted a record of invention for this idea for clearing strategies; (5) conducted integrated simulation of a laser-drive beam through the target chamber, finding negligible beam loss from inverse Bremsstrahlung absorption for xenon densities relevant to wall-protection schemes; (6) determined, through preliminary studies of aerosol formation, that aerosol precursors are unlikely to persist in the hot xenon gas near the chamber center, where significant laser interaction would be a problem; (7) conducted modeling suggesting that laser-based methods for the study of xenon cooling would fail to produce sufficient plasma for diagnostics to be effective at energies of interest, and determining that a theta-pinch method would be more effective; and (8) began assembly of the theta-pinch experimental setup.

Proposed Work for FY11

During FY11 we will (1) complete construction of the theta-pinch experiment, begin plasma operations, and test diagnostics; (2) continue radiation-hydrodynamic simulations to guide the theta-pinch coil design; (3) complete additional computational fluid dynamics simulations of several versions of the

debris cloud to study sensitivities in its performance, including simulations that investigate the use of cold gas jets to both provide thermal protection to the cryogenic target and boost debris-clearing mechanisms by introducing additional momentum into the gas flow; and (4) continue studies of the atomic physics of chamber fill gas to provide information on the regimes in which the theta pinch will operate.

Publications

Kane, J., et al., 2010. *Modeling of the LIFE mini-chamber theta-pinch experiment*. 40th Ann. Anomalous Absorption Conf., Snowmass Village, CO, June 13–18, 2010. LLNL-ABS-441575.

Design of Novel Catalysts to Capture Carbon Dioxide— Roger Aines (10-ERD-035)

Abstract

We propose to develop new, robust, small-molecule catalysts that mimic the behavior of the natural enzyme carbonic anhydrase. Such catalysts can dramatically increase the rate of carbon dioxide (CO₂) separation and thereby reduce the size and cost of industrial processes that seek to keep CO₂ from being emitted to the atmosphere. This separation cost is the primary barrier to worldwide carbon capture and storage necessary to control climate change. We will use quantum mechanical predictions of the catalytic behavior of small molecular systems that mimic the active centers in natural proteins that catalyze this reaction in animals and plants. The best-prospect molecules will be synthesized and tested for both catalysis and robustness to environmental interference.

Comparison to natural systems suggests that it may be possible to increase the chemical capture rate of CO₂ separation systems by up to a factor of 1000 using small, industrially robust catalysts that mimic the behavior of protein systems without their frailty. This would dramatically decrease the cost of carbon capture from point sources. More importantly, it could enable the direct capture of CO₂ from the atmosphere. This would allow us to manage diffuse sources of CO₂ emissions from airplanes and home heating, for example, via centralized air-capture facilities.

Mission Relevance

As part of the Laboratory's mission to enhance the environmental and energy security of the nation, LLNL is committed to developing innovative technologies to reduce atmospheric CO₂. To enable feasible application, the chemistry of the capture process must be more efficient than current methods to keep the capture device size manageable (which also controls capital expenditure). If successful, our project will provide the necessary increase in capture rate, which can make air capture a key new technology for the Laboratory.

FY10 Accomplishments and Results

In FY10 we (1) identified both unique and conserved features of carbonic anhydrases that are essential for the CO₂ reaction, (2) predicted the enzymatic efficiency of each newly designed catalyst using quantum mechanical calculations, (3) synthesized selected novel catalysts, (4) measured the kinetic behavior of these catalysts, (5) identified several new catalytic molecules that are based on natural protein structures but have a much smaller number of atoms focused on the active site, and (6) developed new computational approaches that are up to five times faster at evaluating the effectiveness of new catalysts.

Proposed Work for FY11

In FY11 we will (1) continue identifying and developing catalysts, with an emphasis on designs that mimic the hydrogen bonding of carbonic anhydrase; (2) conduct analysis to understand which designs resulted in the fastest catalysts; and (3) begin incorporating results from the environmental testing of catalysts to develop versions that are more robust in industrial applications.

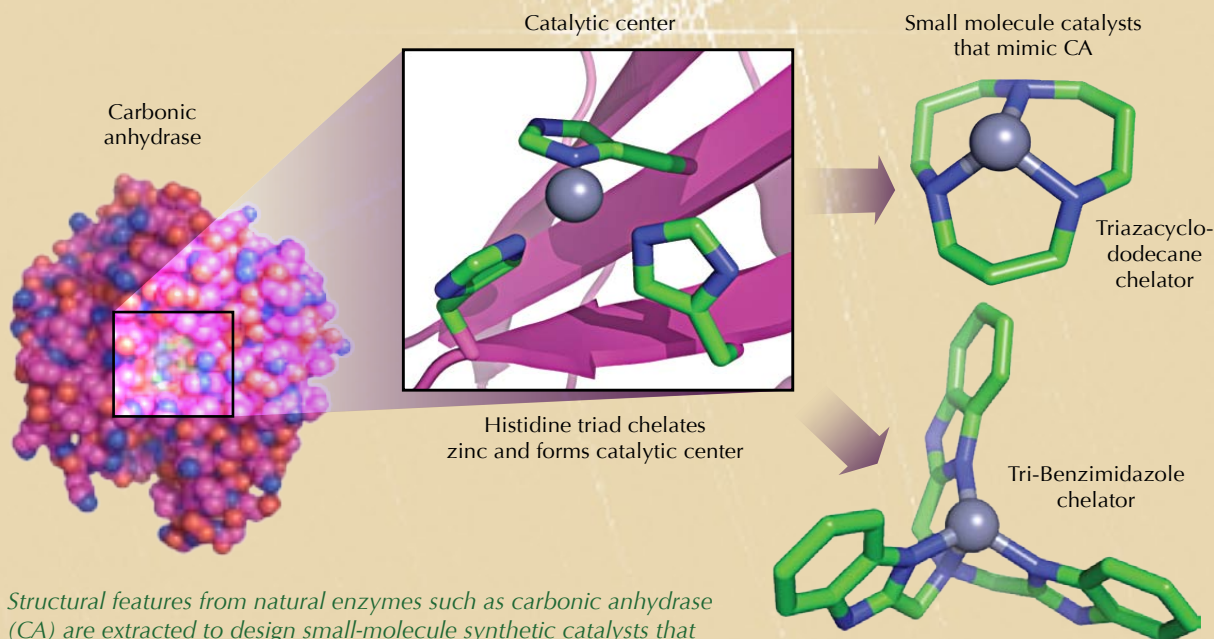
Publications

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

Aines, R., et al., in press. "Modeling, synthesis, and characterization of zinc-containing carbonic anhydrase active site mimics." *Energy Procedia*. LLNL-PROC-451972.

Kulik, H., 2010. *Computational design of carbonic anhydrase mimics for carbon dioxide capture*. LLNL-ABS-426922.

Wong, S. E., et al., in press. "Designing small-molecule catalysts for CO₂ capture." *Energy Procedia*. LLNL-PROC-451972.



Structural features from natural enzymes such as carbonic anhydrase (CA) are extracted to design small-molecule synthetic catalysts that are industrially robust and easy to create. Such catalysts can dramatically increase the rate of carbon dioxide separation and thereby reduce the size and cost of industrial processes for capturing carbon that would otherwise be released into the atmosphere.

Prediction of Underground Coal Gasification Cavity Growth, Coal Conversion, and Geophysical Signatures—David Camp (10-ERD-055)

Abstract

Underground coal gasification (UCG) is a critical emergent technology to boost U.S. energy security while dramatically decreasing greenhouse gas emissions. However, scientific questions and technical challenges impede sustainable production. Industry is seeking improved simulation and monitoring capabilities to predict performance and minimize environmental impact as a function of site, design, and operational characteristics. These challenges demand an accurate, coupled-process simulator. We propose to develop the world's most complete and accurate UCG simulator, resolve outstanding process questions, and identify field-observable signatures for monitoring operations. The work leverages prior LLNL investments in computational geosciences, modeling, and monitoring.

We expect our project will provide a strong understanding of and predictive capability for UCG operations. Our coupled simulation and geophysics monitoring approach will improve the siting, design, permitting, operation, monitoring, and environmental performance of pilot and commercial projects. In

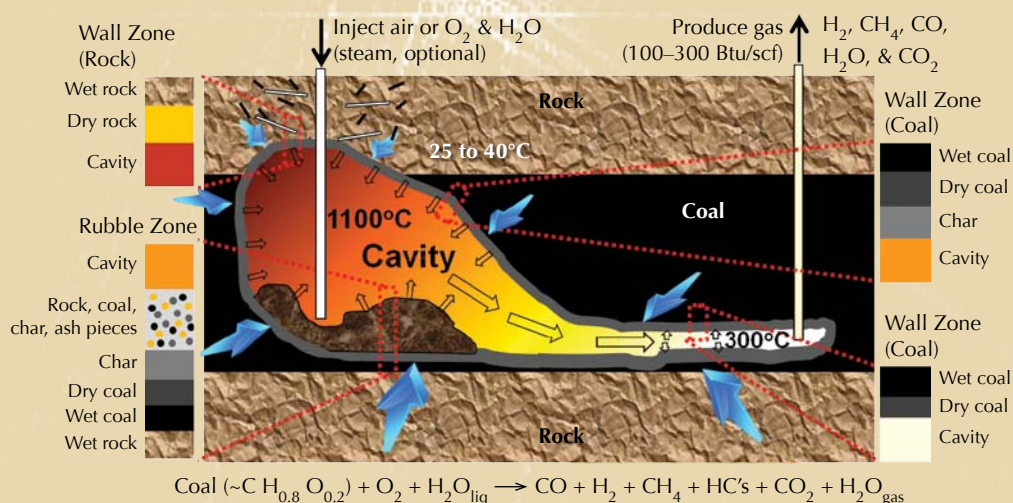
addition, our research will accelerate commercial deployment and facilitate technically sound regulations and permitting. Development of detailed submodels will require focused inquiry into complex transport, reaction, and fracturing phenomena, and the integrated model we deliver will enable a new level of scientific and technical interrogation of complex UCG behavior.

Mission Relevance

This project is highly aligned with the energy and environmental security mission of the Laboratory. It will help establish scientific underpinnings that will spur the deployment of underground coal gasification to reduce the cost and accelerate delivery of low-carbon, secure energy to the nation. In addition, this project capitalizes on previous investments in high-performance computing to provide leadership in unclassified computing applications.

FY10 Accomplishments and Results

In FY10 we (1) completed a wall zone model exceeding previous work in both technical scope and detail, (2) validated the wall zone model with existing laboratory data, (3) began coding a hub model that will act as an interface for the individual process models at the core of this effort, (4) produced the first version of a cavity boundary



In underground coal gasification, air is injected into an underground seam to convert coal into gas usable for fuel and chemical synthesis. We are building computer models to better understand this complex process.

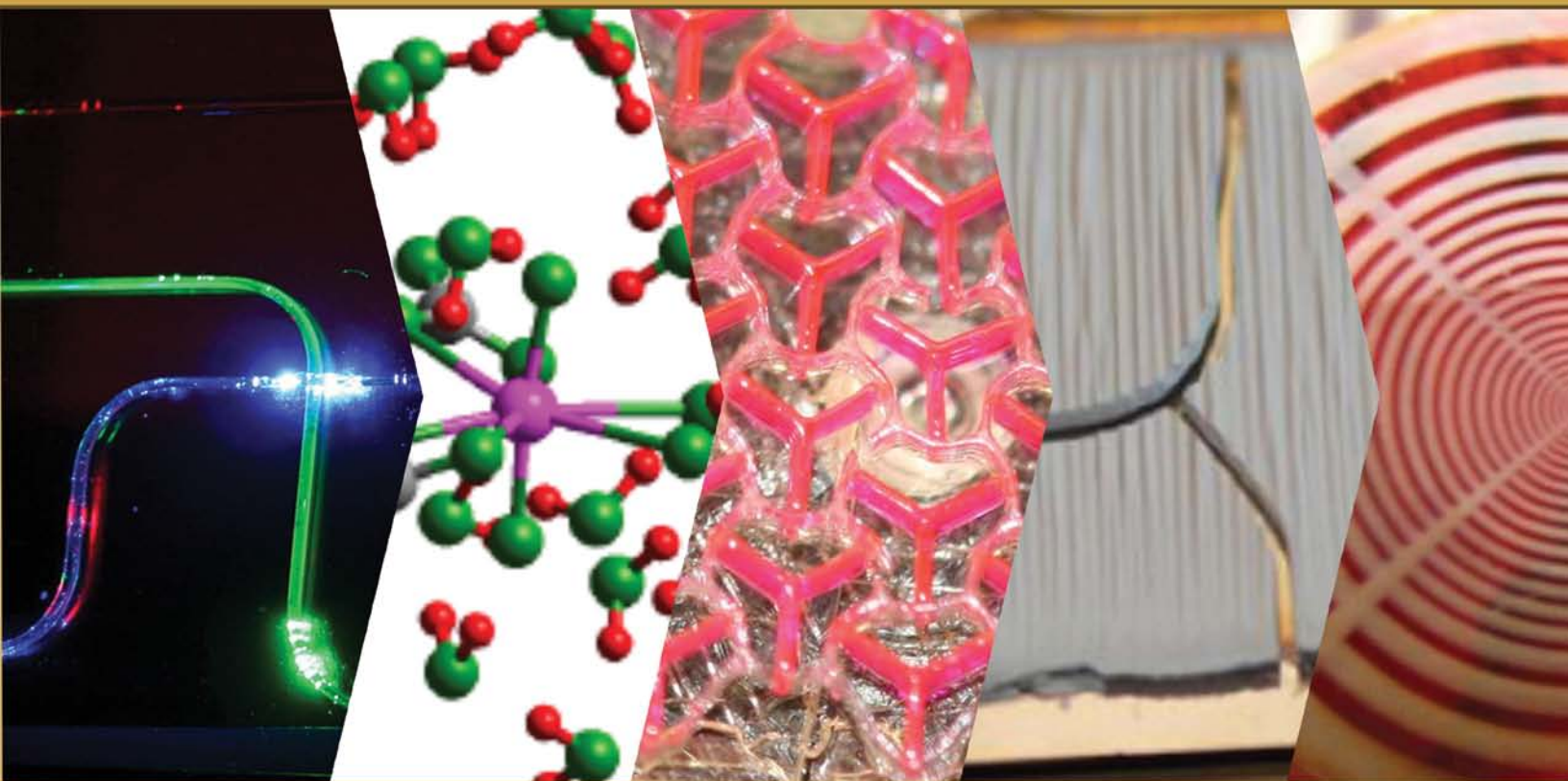
and submodel manager that tracks the boundaries between cavity and coal face and between cavity and rubble zone, (5) made enhancements to a new implicit geomechanics code, and (6) began developing a rigorous and flexible cavity gas model.

Proposed Work for FY11

In FY11 we will (1) create a rubble zone model; (2) complete our cavity gas and heat transfer model; (3) add a simplistic representation of spalling to the wall zone model; (4) complete the second spiral of integrated model development, including the cavity boundary and submodel manager that dynamically links the wall zone model, rubble zone model, cavity gas and heat transfer model, and hydrology model and statically links the implicit geomechanics model; (5) begin development of a three-dimensional local wall zone model that models—explicitly and in detail—spalling, fracture events, and fracture transport; and (6) begin to quantify geophysical signatures for monitoring, using results from our simulator.

Publications

Nitao, J. J., et al., 2010. *An integrated 3-D UCC model for predicting cavity growth, product gas, and interactions with the host environment*. 27th Ann. Intl. Pittsburg Coal Conf., Istanbul, Turkey, Oct. 11–14, 2010. LLNL-ABS-426990.



Engineering and Manufacturing Processes

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

Abstract

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

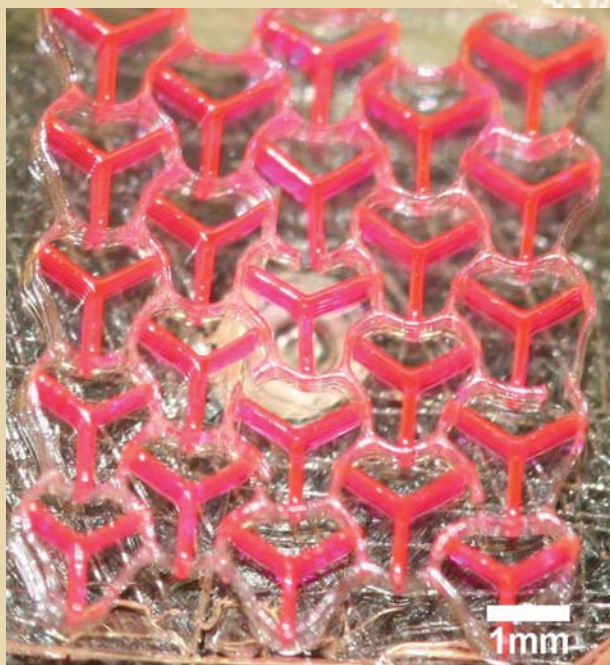
develop (1) feature resolution on the scale of tens of nanometers; (2) multilayered spherical structures with low surface roughness; (3) an ability to directly transcribe fine features on the internal surfaces of spherical shells; (4) graded-density materials ranging from full density to less than 5% in tens of microns; (5) an empirically validated, model-based design tool; and (6) new devices and structures.

Mission Relevance

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

FY10 Accomplishments and Results

We (1) fabricated many 3D components relevant to targets, including cylinders, lattice structures, and fully 3D structures with overhanging features, demonstrating the ability to craft features as small as 5 μm ; (2) fabricated and demonstrated a working plasmonic super lens and integrated it into our projection microstereolithography system, finding that light attenuation by the super lens precluded fabrication of nanoscale features and that generating sub-wavelength features would therefore require a stronger light source and a defect-free super lens; (3) validated an optical-chemical-fluidic model; (4) conceptually designed a holographic lithography system; and (5) generated a hybrid multimaterial lattice structure, demonstrating both the three-dimensionality and heterogeneous capability of the technique in a single structure and the ability to use microfluidic resin delivery and removal systems. In summary, this project has successfully established a projection microstereolithography capability for fabricating 3D mesostructures and microstructures and advanced the state of the art by improving resolution and materials flexibility and developing a corresponding process model. This new capability is expected to have significant impact on target



A lattice of heterogeneous unit cell structures. Each structure is made from two different polymer materials.

fabrication and other mission-relevant application areas, as evidenced by a recent award by the Defense Advanced Research Projects Agency that would not have been possible without this projection microstereolithography capability, which will be used to generate materials with controlled microstructural architectures.

Publications

Spadaccini, C. M., et al., 2010. *High-resolution projection microstereolithography*. LLNL-TR-468271.

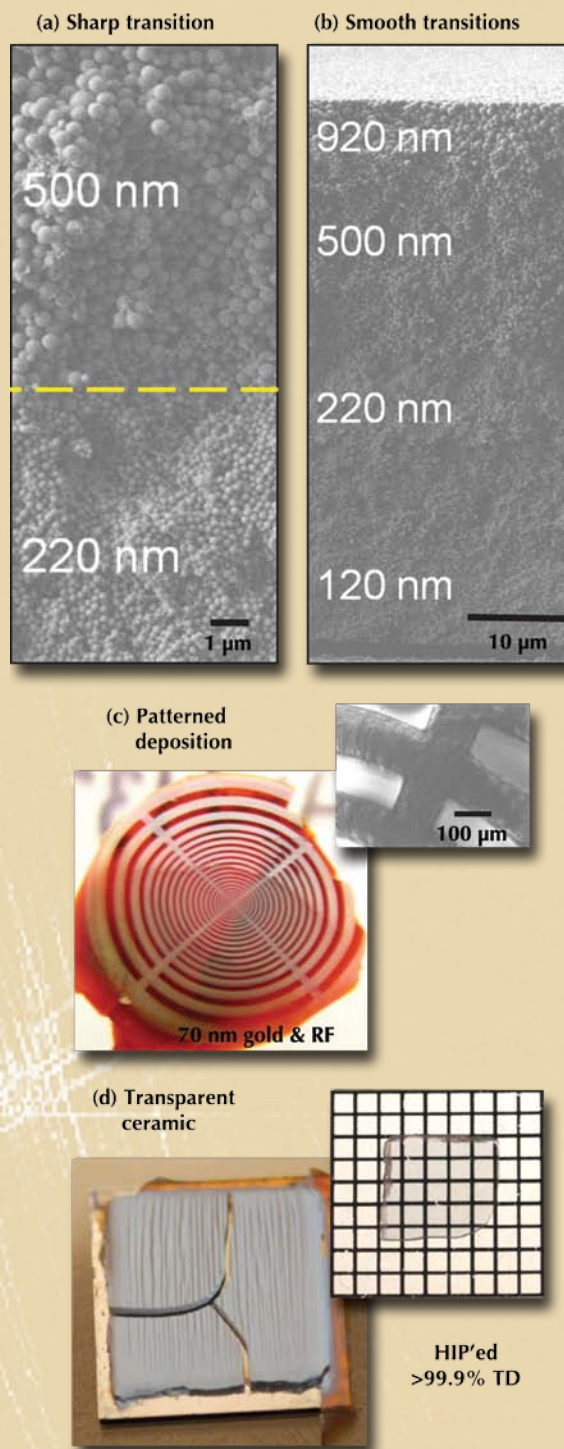
Spadaccini, C. M., et al., 2009. *High-resolution projection microstereolithography (PuSL) for 3-D fabrication*. National Nanomanufacturing Summit, Boston, MA, May 29, 2009. LLNL-PRES-413420.

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

Abstract

Our objective is to develop three new techniques using electrophoretic deposition to fabricate novel nanostructured materials. Functionally graded materials fabricated with gradients in composition, microstructure, or density produce enhanced bulk properties, but current techniques are limited to gradients of composition along a single axis. Using our new techniques, we plan to demonstrate new nanostructured materials, including transparent ceramic optics with three-dimensional tailored doping profiles and non-cubic transparent ceramics fabricated from aligned nanorods. To achieve this, we will develop the necessary particle chemistry, instrumentation, and protocols optimized through experiments and modeling.

Overall, we expect to develop a new nanofabrication system with three-dimensional composition control and controlled orientation of precursor material. Success in reaching these milestones will (1) dramatically expand the design of ceramic optics and immediately impact high-average-power laser design, (2) potentially create a paradigm shift in the field of optical materials by producing transparent ceramics from non-cubic materials, (3) provide an



Examples of multilayer films deposited with either (a) sharp or (b) smooth transitions between material layers. (c) Deposition of 70-nm gold particles onto a fixed electrode pattern that is gelled in situ using resorcinol formaldehyde (RF). The white areas are gold and the red areas are the gelled RF. Minimum feature size at the center of the pattern is approximately 10 μm. (d) Example of a transparent ceramic fabricated using electrophoretic deposition. The ceramic material was deposited with hot isostatic pressing (HIP) to a thickness of 1.4 mm at greater than 99.9% theoretical density (TD).

empirically validated deposition model for future designs and applications, and (4) result in high-impact publications on the fabrication technique, as well as the new materials and structures from each application.

Mission Relevance

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

FY10 Accomplishments and Results

In FY10 we (1) demonstrated the ability to change material composition and thickness of deposition layers, creating both sharp and gradual material transitions during deposition; (2) successfully deposited, onto a photolithographically patterned metal electrode, a two-dimensional extruded pattern with 10 μm resolution; (3) developed a new gelation process that enables deposition in an aqueous solution and then "locks in" the pattern by gelling the solution at elevated temperature; (4) synthesized near-monodisperse fluorapatite nanorods and demonstrated alignment of the rods in a 300-V/cm electric field; and (5) demonstrated transparent ceramic structures fabricated using the electrophoretic deposition process.

Proposed Work for FY11

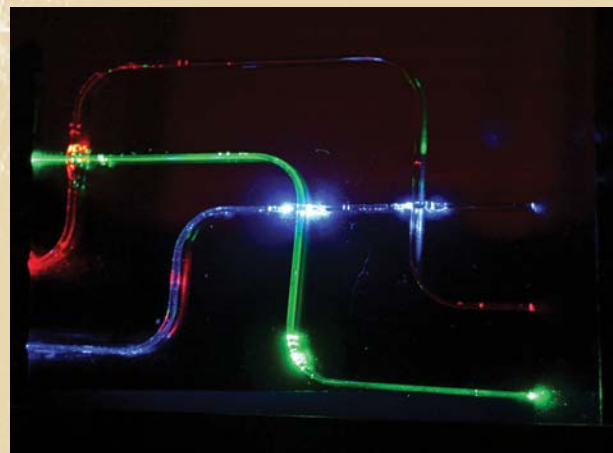
In FY11 we will demonstrate (1) transparent sintering of multilayer particle depositions, (2) transparent synthesis of nanorods of a non-cubic material such as fluorapatite, (3) a transparent sintered part patterned with two materials in the x-y plane, and (4) dynamic x-y control for depositing two materials on a transparent substrate.

Maskless, Low-Cost, High-Performance Polymer Waveguides—Eric Duoss (09-ERD-057)

Abstract

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

Throughout this study we will work with our collaborators to develop the necessary protocols to fabricate polymeric waveguides to achieve optical transmission losses below 0.1 dB/cm. These losses are strongly correlated with the material, surface roughness, and geometry of the waveguide. By optimizing direct ink writing fabrication for a selected set of polymers, we expect to achieve this low-loss



An optical image showing light confinement in three polymer waveguides fabricated with our direct ink writing technique.

level. We also expect to demonstrate this with multilayer waveguides patterned into compact three-dimensional structures. This optimization process will enable future applications requiring complex three-dimensional structures and materials not compatible with standard microfabrication techniques.

Mission Relevance

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

FY10 Accomplishments and Results

In FY10 we (1) developed methods for fabricating and testing polymer waveguides using the manufacturing technique developed in collaboration with the University of Illinois, (2) developed a new core- and sheath-extrusion technique that enables fabrication of optimal polymeric materials with low viscosity and decreased surface roughness, and (3) examined a range of variables such as write speeds, nozzle geometries, waveguide shapes, process temperatures, and environments to minimize transmission loss, surface roughness, and optical loss.

Proposed Work for FY11

We will (1) further explore the core- and sheath-extrusion technique to fabricate waveguides from a broader range of applicable polymer materials, including low-viscosity starting materials; (2) fabricate and test three-dimensional structures from these materials to demonstrate the ability to overlap waveguides without making optical contact; and

(3) demonstrate the ability to reduce loss to less than 0.1 dB/cm in these three-dimensional structures.

Novel Separation of Actinides— Raymond Mariella (10-FS-001)

Abstract

The separation of actinides and other elements of interest for nuclear forensics and threat reduction is currently performed using decades-old chemistries and ion-exchange columns. We propose to determine the technical feasibility of a novel method for separating actinide ions in solution. This method is based upon isotachopheresis (ITP), which has been applied in the purification of pharmaceuticals and other biochemical applications. This technique has the potential to separate inorganic ions more effectively than existing methods, which is key to analyzing very small samples. We will perform a quantitative assessment of the effectiveness of specific isotachophoretic approaches including predicting the physical and chemical properties, such as ion mobility, of inorganic ions under specific solvent conditions using a combination of ab initio calculations and semi-empirical methods.

We expect to obtain a thorough understanding of the analytical systems parameters under which ITP is most effective for the separation of inorganic samples, including the influence of the double layer surrounding actinide ions, the Debye length for different ions and ion complexes, and Debye–Hückel limits.

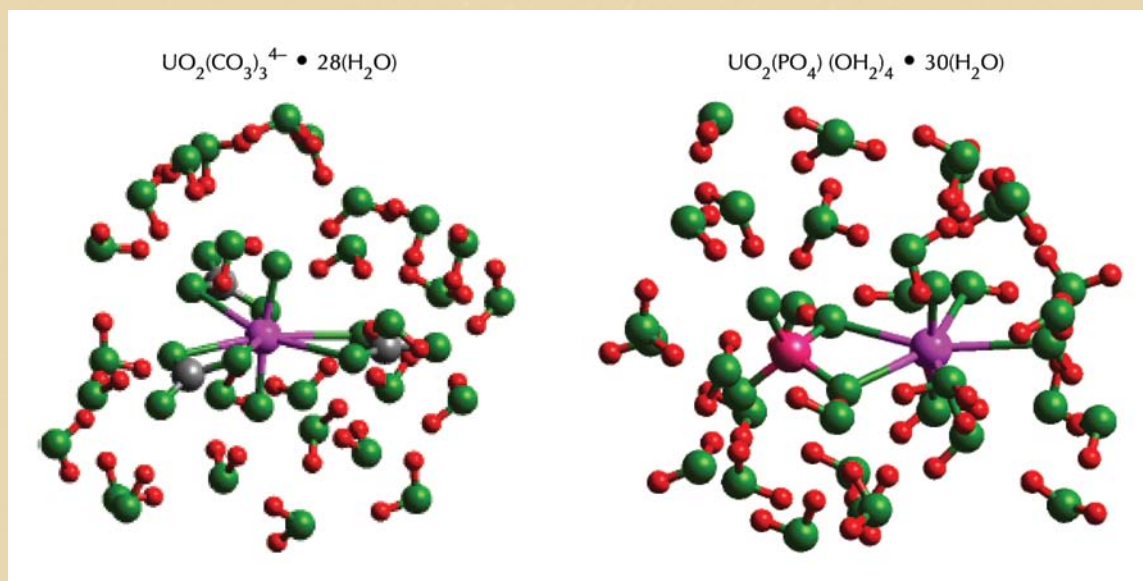
Mission Relevance

Inorganic separations are key to nuclear forensics for countering terrorism and nuclear proliferation. If found to be feasible and potentially superior to currently used separation approaches, ITP could provide the conceptual basis for an improved means to separate samples of nuclear explosion debris for nuclear forensic analysis, in support of the Laboratory's missions in homeland and national security.

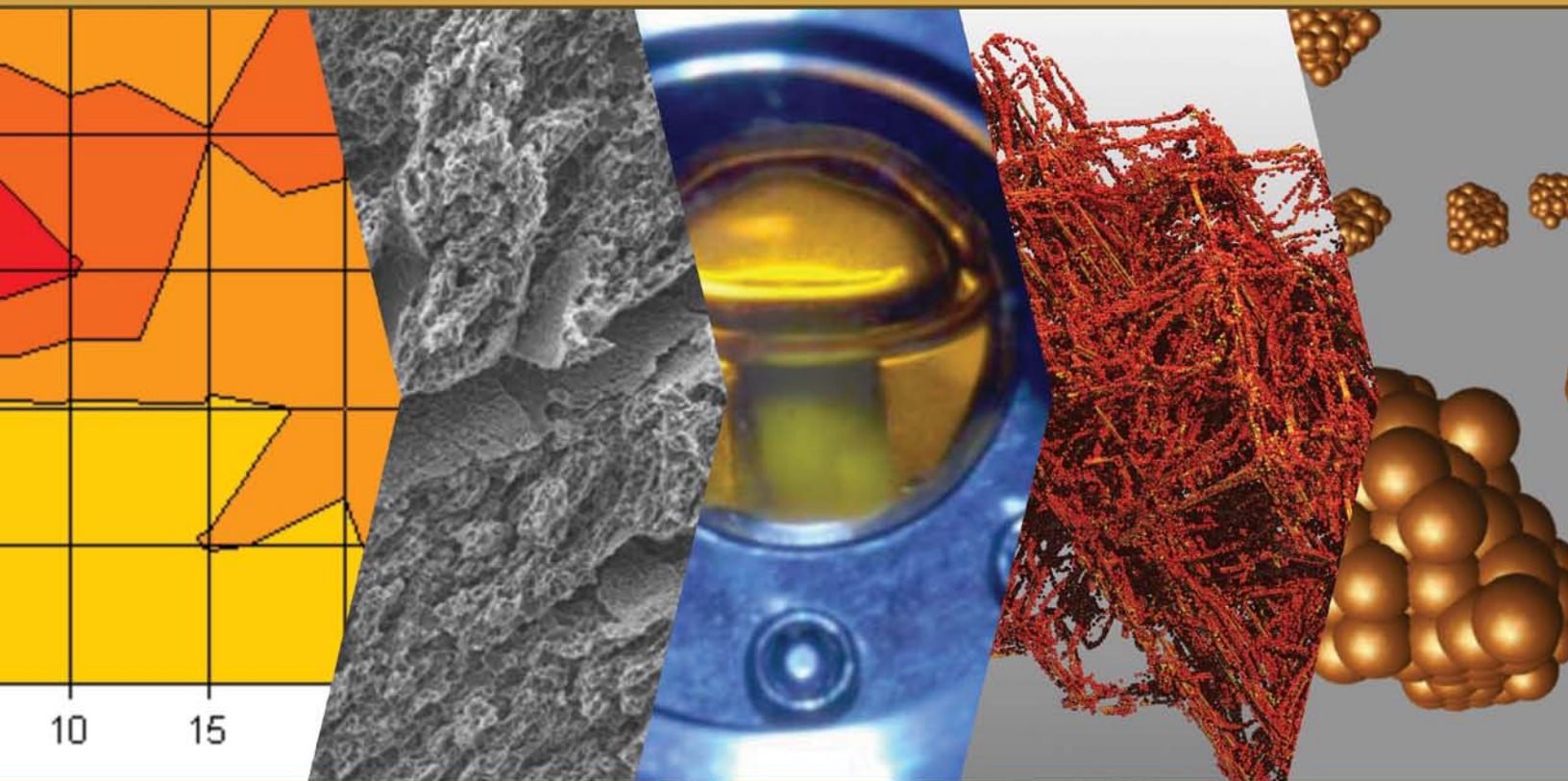
FY10 Accomplishments and Results

During FY10, we conducted an extensive search and study of the literature. As a result, we (1) determined that none of the publications, which date back to the conception of what is now called ITP, reported the relative or absolute mobilities of the actinide ions; (2) identified a theoretical approach that would enable us to calculate the relevant electrophoretic mobilities; (3) determined that the most important aspect of ITP is that it discards unwanted constituents, such as salts of calcium, magnesium, aluminum, sodium, potassium, and similar ions, while trapping and purifying desired ions, such as uranium dioxide (UO_2^{++}); (4) determined that a key aspect of ITP is that it concentrates minor or trace elements, matching the concentration of the leading electrolyte, which makes it highly appropriate for

the analysis of actinides, the starting concentrations of which can span a range of several decades; (5) determined that direct interfacing of separated actinide ions to inductively coupled plasma mass spectroscopy would be possible; and (6) determined that simple models, such as Debye–Hückel, are too limited to be of predictive value for ITP in applications in which final purified concentrations exceed 0.001 M, and that ab initio and Monte Carlo models, such as those published for UO_2^{++} , are therefore needed. In summary, this project's findings strongly support the use of ITP as a key step in the analysis of actinides, including pre- and post-detonation nuclear forensics; that it is the only alternative to time-tested but highly labor-intensive procedures involving ion-exchange columns; and that it performs separation more rapidly and is more conducive to automation.



Quantum mechanical modeling of uranium ion complexes, such as those shown above, could be used as input to model electrophoretic mobilities.



Materials Science and Technology

Nanomaterials for Fusion Application Targets—Alex Hamza (08-SI-004)

Abstract

The assembly of functional nanomaterials requires atomic-level control of the processes involved. Complex targets for the study of mix in burning hydrogen plasmas, nuclear physics in high-neutron-brightness environments, and fast-ignition inertial-confinement fusion require precisely placing nanoporous materials and small quantities of dopants inside a target capsule. In this project, innovative techniques will be developed for fabrication of these complex targets. Specifically, we will use a “chemistry-in-a-capsule” approach to grow nanoporous materials inside a spherical target. We will also 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 establishing a capability for design and assembly of tailored nanomaterials and nanostructures. More specifically, we will create the capability for assembly and manipulation of nanostructured materials in confined geometries with tailored composition and function. Because of the unique reactive, absorptive,

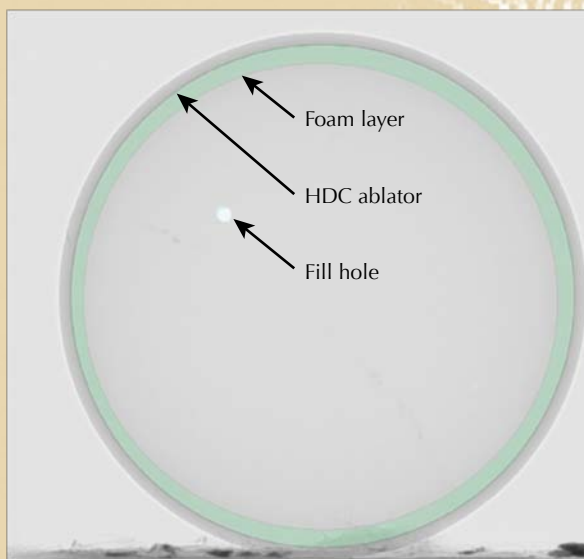
mechanical, and optical properties of nanostructured materials, this capability will be broadly applicable in catalysis, hydrogen storage, advanced nuclear materials, corrosion-resistant coatings, and photonics.

Mission Relevance

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

FY10 Accomplishments and Results

During FY10 we made significant progress towards fabrication of fusion application targets. Specifically, we (1) developed new aerogel chemistries to fabricate mechanically robust, low-density foams; (2) measured the viscosity change during gelation of several aerogel systems and learned how to modify their rheological properties by controlling polymerization kinetics; (3) studied distribution of fluids in a rotating horizontal circular cylinder both



An x-ray radiograph of a 2-mm diameter, 30- μm -thick diamond shell with an approximately 50- μm layer of dicyclopentadiene polymer gel is shown (left), and a 30-mg/cm³ dicyclopentadiene polymer foam that survived wetting with cryogenic hydrogen (right).

theoretically and experimentally; (4) designed and built a random position machine that provides a deterministic, continuous random change in orientation relative to the gravity vector to improve homogeneity of gel films produced inside a capsule; (5) imaged cryogenic hydrogen and its interaction with foam inside a target; and (6) completed our virtual sputter-chamber multiscale simulation tool and performed initial tests. In summary, this project demonstrated the processes necessary to fabricate ignition and fast ignition targets. Specifically, we demonstrated the viability of fabrication techniques for thin foam liners inside a spherical ablator shell, developed various methods to incorporate high-atomic-number dopants inside both the ablator shell and the foam liner, and made significant contributions towards an atomic-scale understanding of the processes involved in the magnetron sputter process used to fabricate beryllium ablator shells. The successful conclusion of this project has led to Laboratory programmatic support to integrate the demonstrated processes into fabrication of targets for specific experiments that support the Laboratory's stockpile stewardship mission.

Publications

Biener, J., et al., 2010. *Fusion application targets*. LLNL-TR-463691.

Detor, A. J., et al., 2009. "Stress and microstructure evolution in thick sputtered films." *Acta Mater.* **57**, 2055. LLNL-JRNL-405098.

Ghosal, S., et al., 2009. "Controlling atomic layer deposition of TiO_2 in aerogels through surface functionalization." *Chem. Mater.* **21**, 1989. LLNL-JRNL-412061.

Jeffrey, K., et al., 2009. "Ultra-low loading Pt nanocatalysts prepared by atomic layer deposition on carbon aerogels." *Nano Lett.* **8**, 2405. LLNL-JRNL-403291.

Kucheyev, S. O., A. V. Hamza, and M. A. Worsley, 2009. "Ion-beam-induced stiffening of

nanoporous silica." *J. Phys. Appl. Phys.* **42**, 182003. LLNL-JRNL-411937.

Kucheyev, S. O., et al., 2010. *Light-ion-irradiation-induced thermal spikes in nanoporous silica*. LLNL-JRNL-441611.

Rajulapati, K. V., et al., 2010. "Temperature dependence of the plastic flow behavior of tantalum." *Phil. Mag. Lett.* **90**(1), 35. LLNL-JRNL-414286.

Worsley, M. A., J. H. Satcher, and T. F. Baumann, 2009. "Enhanced thermal transport in carbon aerogel nanocomposites containing double-walled carbon nanotubes." *J. Appl. Phys.* **105**, 084316. LLNL-JRNL-406621.

Worsley, M. A., et al., 2009. "Mechanically robust and electrically conductive carbon nanotube foams." *Appl. Phys. Lett.* **94**, 073115. LLNL-JRNL-406546.

Worsley, M. A., et al., 2009. "Properties of single-walled carbon nanotube-based aerogels as a function of nanotube loading." *Acta Mater.* **57**, 5131. LLNL-JRNL-408159.

Worsley, M. A., et al., 2010. "Synthesis of graphene aerogel with high electrical conductivity." *J. Am. Chem. Soc.* **132**, 14067. LLNL-JRNL-447992.

Worsley, M. A., et al., 2009. "Stiff and electrically conductive composites of carbon nanotube aerogels and polymers." *J. Mater. Chem.* **19**, 3370. LLNL-JRNL-411350.

Zepeda-Ruiz, L. A., et al., 2010. "Surface morphology evolution during sputter deposition of thin films—lattice Monte Carlo simulations." *J. Cryst. Growth* **312**(8), 1183. LLNL-JRNL-417087.

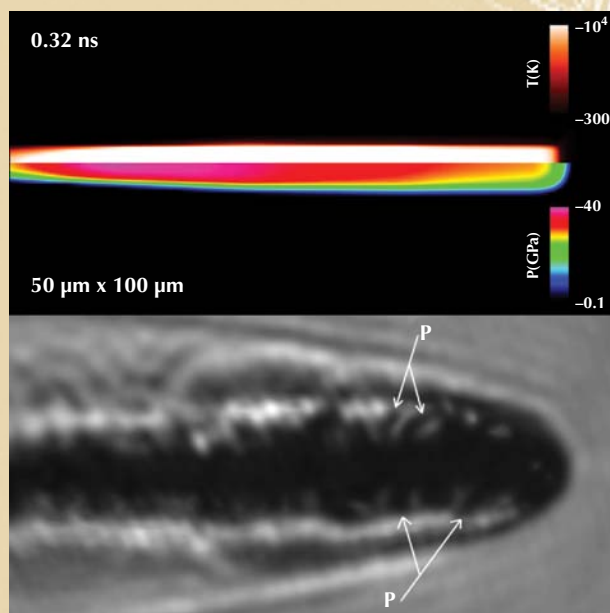
Zepeda-Ruiz, L. A., et al., 2009. "Understanding the relation between stress and surface morphology in sputtered films: Atomistic simulations and experiments." *Appl. Phys. Lett.* **95**(15), 151910. LLNL-JRNL-417093.

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

Abstract

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

Our research will significantly enhance fundamental understanding of the processes involved during laser-induced damage in optical materials under operational conditions similar to those found in inertial-confinement fusion lasers. Specifically,



Simulation (top) and experimental investigation (bottom) of the formation of a damage site in bulk fused silica. "P" denotes instabilities at the phase boundary.

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

FY10 Accomplishments and Results

We focused on understanding the energy-deposition phase of laser damage. We determined that (1) in fused silica, the process starts with the buildup of an electronic excitation that leads in 1 ns to the transformation of the host material to an absorber; (2) the modified region of exit surface damage starts expanding with a lateral speed of 1.5 km/s and an axial speed of 2.5 km/s; (3) the formation of axial cracks begins about 2 ns later and is accompanied by the termination of the axial expansion; (4) the modified region continues to expand laterally during the laser pulse, followed by the formation of lateral cracks until after roughly 25 ns, when the damage site reaches its final size; (5) surface swelling at this time leads to reduction of density by a factor of five, followed by the onset of material ejection at roughly the 25-ns point; and (6) in bulk damage, the shock initially propagates with a speed of about 12 km/s, while instabilities at the phase boundary propagate at about 4.6 km/s and morph after about 1 ns into cracks that continue to grow for about 20 ns, with a speed of about 1.7 km/s. In summary, this project achieved major advancements in understanding laser-induced damage in inertial-confinement

fusion optical materials by revealing some of the key fundamental damage processes and by providing novel experimental techniques to extend future studies in laser damage, which are also applicable to laser ablation and micromachining. These new experimental capabilities can be applied to the study of damage initiation and growth in a variety of materials, configurations, and geometries, towards better understanding of the limits of performance of current-generation materials and the development of next-generation materials with enhanced performance characteristics. The two records of inventions resulting from this project provide specific examples of such future directions and provide for protection of intellectual property. The capabilities developed in this project can also be used to validate hydrocodes that model laser damage and quantitatively predict material lifetime issues.

Publications

DeMange, P., et al., 2008. "Laser annealing characteristics of multiple bulk defect populations within DKDP crystals." *J. Appl. Phys.* **104**, 103103. UCRL-JRNL-236989.

Demos, S. G., and R. A. Negres, 2008. "Time-resolved imaging of material response during laser-induced bulk damage in SiO₂." *Proc. SPIE* **7132**, 71320Q. LLNL-ABS-403892.

Demos, S. G., R. A. Negres, and R. N. Raman, 2010. "Imaging the early material response associated with exit surface damage in fused silica." *Proc. SPIE* **7842**, 78420M. LLNL-PROC-462172.

Demos, S. G., et al., 2010. "Investigation of the electronic and physical properties of defect structures responsible for laser-induced damage in DKDP crystals." *Optic. Express* **18**, 13788. LLNL-JRNL-425231.

Negres, R. A., C. K. Saw, and S. G. Demos, 2008. "Interactions between x-ray induced transient defects and pre-existing damage precursors in DKDP crystals." *Proc. SPIE* **7132**, 713212. LLNL-ABS-403893.

Negres, R. A., et al., 2008. "Laser damage performance of KD_{2-x}H_xPO₄ crystals following

x-ray irradiation." *Optic. Express* **16**, 16326. LLNL-JRNL-400735.

Negres, R. A., M. D. Feit, and S. G. Demos, 2010. "Dynamics of material modifications following laser-breakdown in bulk fused silica." *Optic. Express* **18**, 10642. LLNL-JRNL-414381.

Raman, R. N., R. A. Negres, and S. G. Demos, 2009. "Imaging system to measure kinetics of material cluster ejection during exit-surface damage initiation and growth in fused silica." *Proc. SPIE* **7504**, 750418. LLNL-CONF-420042.

Raman, R. N., R. A. Negres, and S. G. Demos, in press. "Time-resolved microscope system to image material response following localized laser energy deposition: Exit surface damage in fused silica as a case example." *Optic. Eng.* LLNL-JRNL-436074.

Raman, R. N., et al., 2010. "Monitoring annealing via CO₂ laser heating of defect populations on fused silica surfaces using photoluminescence microscopy." *Optic. Express* **18**, 15207. LLNL-JRNL-423077.

Raman, R. N., et al., 2010. "Time-resolved imaging of material response following laser-induced breakdown in the bulk and surface of fused silica." *Proc. SPIE* **7581**, 75810D. LLNL-CONF-423286.

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

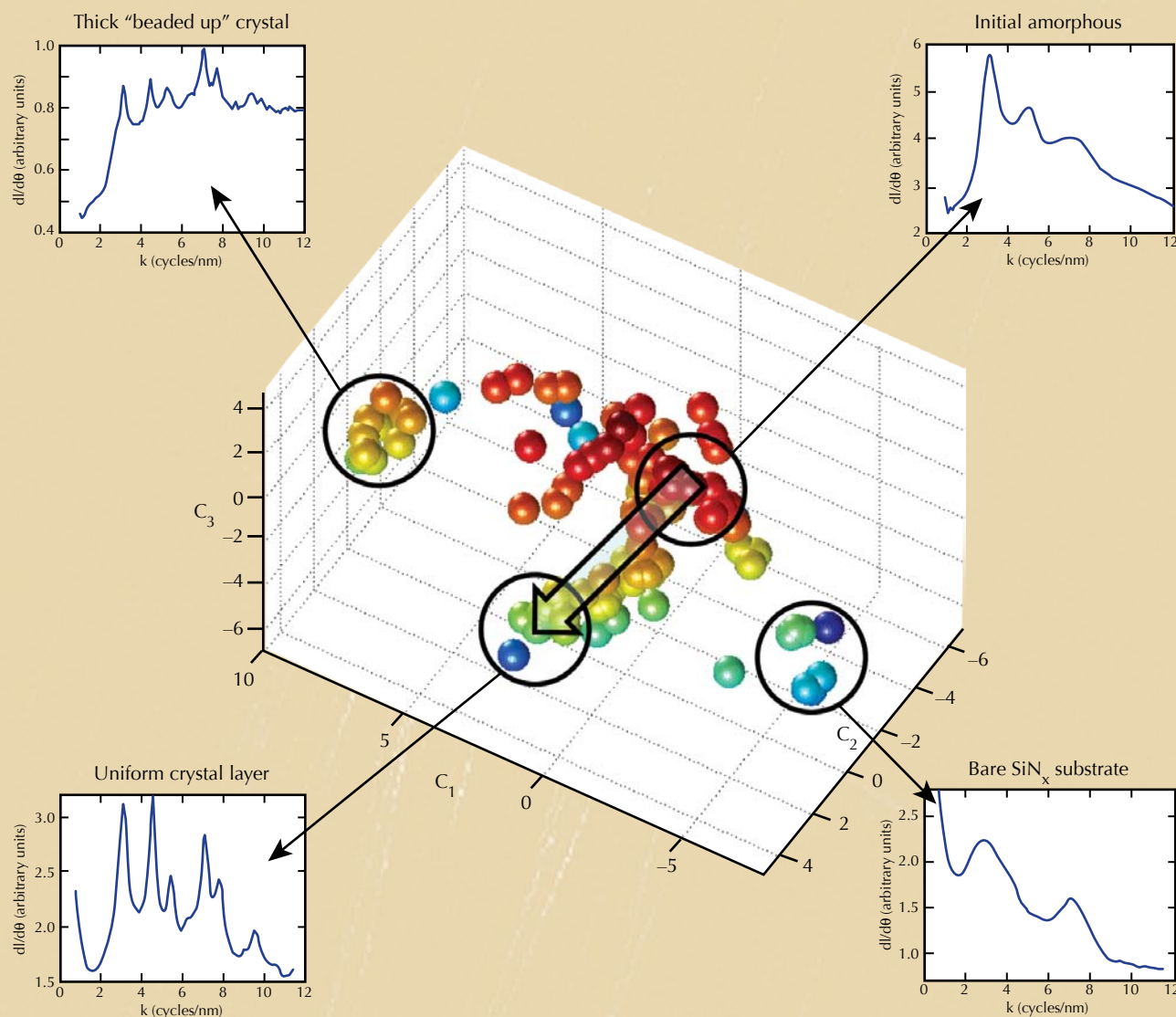
Abstract

Many fast phase transformations are currently known only through before-and-after experiments coupled to theoretical models of the assumed mechanism. However, by directly correlating experiments with theory on the same time and length scales, the mechanisms actually responsible for the resulting transformed structures can be uniquely evaluated. We propose to combine unique experimental capabilities—a dynamic transmission electron microscope (DTEM) and an aberration-corrected

transmission electron microscope—with large-scale atomistic simulations to develop a fundamental atomic-scale understanding of reversible amorphous-to-crystalline phase transformations in materials such as $\text{Ge}_2\text{Sb}_2\text{Te}_5$, Sb_2Te_3 , and GeSb . These alloys 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 computer 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 papers submitted to high-profile journals.



Principal component analysis (PCA) reduces complex variations in material diffraction patterns into a few significant components, suppressing noise and irrelevant details. Here we show how points in a series of experiments cluster in a six-dimensional PCA space (represented as three coefficients C_1 , C_2 , and C_3 and the red, green, and blue components of the color of each sphere), demonstrating how different dimensions of morphology and crystallinity can be extracted from a large and complex data set. This kind of analysis is pushing dynamic transmission electron microscope capabilities into new regimes of quantitative characterization of fast material processes.

Mission Relevance

This project supports Livermore's mission in stockpile stewardship because the experimental work will lead to new insights into the atomic-scale dynamics behind phase transformations while also expanding the use of DTEM for in situ diagnostics. The high degree of 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.

FY10 Accomplishments and Results

In FY10 we (1) implemented a new sample geometry with a very thin layer of $\text{Ge}_2\text{Sb}_2\text{Te}_5$ deposited on a metallic wedge of very high thermal conductivity and successfully demonstrated repeatable cycles of forward and reverse transformations, (2) performed detailed analysis of the transformation kinetics as measured with DTEM diffraction, and (3) successfully redirected our previously proposed computational effort from atomistic simulation to finite-element simulation because of an unexpected lack of available personnel time for atomistic simulation and surprising experimental results demanding finite-element continuum-level simulation for their explication. Specifically, nanostructured $\text{Ge}_2\text{Sb}_2\text{Te}_5$ was found to absorb laser intensity in a very nonuniform way because of its nanoscale geometry, leading to extreme inhomogeneity in laser-driven transformation in nanostructured films. Our project demonstrated the complex coupling of nanoscale geometry, laser absorption, and nucleation and growth of metastable phases on the nanometer and nanosecond scales directly relevant for envisioned memory applications of chalcogenide (i.e., sulfide, selenide, and telluride) phase-change materials, while expanding the range of established measurement, sample preparation, and data analysis techniques used in DTEM experiments. The developed techniques are ready for direct follow-on applications for existing DTEM projects, and the established collaboration with Stanford University researchers is expected to continue indefinitely.

Publications

Reed, B. W., et al., 2009. *Dynamic transmission electron microscopic investigation of telluride*

phase change materials. Banff Mtg. Structural Dynamics, Banff, Canada, Feb. 25–28, 2010. LLNL-ABS-420997.

Santala, M. K., et al., 2010. *Dynamic transmission electron microscope investigations and phase transformations in optical recording media*. Molecular Foundry and National Center for Electron Microscopy Users' Mtg. 2010—Nanoscience for Energy Technology, Berkeley, CA, Sept. 30–Oct. 1, 2010. LLNL-ABS-451193.

Santala, M. K., et al., 2010. *Dynamic transmission electron microscope investigations of dynamic processes in materials*. Microscopy and Microanalysis 2010, Portland, OR, Aug. 1–5, 2010. LLNL-ABS-423471.

Santala, M. K., et al., 2010. *Dynamic transmission electron microscope investigations of materials processes*. 17th Intl. Microscopy Congress, Rio de Janeiro, Brazil, Sept. 19–24, 2010. LLNL-ABS-427522.

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

Abstract

This project will couple simulation and experiment to examine the plastic response of dynamically compressed materials over a range of different strain rates. We aim to accomplish two scientific firsts: perform large-scale molecular dynamics simulations to investigate ramp compression using Livermore Computing Center facilities and measure in situ lattice response to ramp loading at high pressure using x-ray diffraction. 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 two main accomplishments: insight into the atomistic processes that govern the evolution of microstructure and lattice in face-centered-cubic materials as a function of strain rate and a lattice-level comparison

between simulation and experiment for ramp loading using in situ x-ray diffraction. All will be of large scientific impact because lattice behavior dependence on strain rate is a largely unexplored scientific field. Also, the coupling of large-scale molecular dynamics simulations and x-ray diffraction experiments will provide a benchmark for 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 the dynamic loading of materials to high pressures. This is central to Lawrence Livermore's core missions in stock-pile 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.

FY10 Accomplishments and Results

In FY10 we continued investigating the impact of strain rate on microstructure using large-scale molecular dynamics simulations and in situ x-ray

diffraction techniques developed for laser-based high-pressure compression. Specifically, we (1) performed large-scale simulations and laser-based ramp-compression experiments at similar strain rates; (2) analyzed the experimental data and conducted simulated diffraction studies, showing similar broadening of the x-ray diffraction peaks; and (3) followed a 300-ps ramp load through 4 μm of single-crystal copper, investigating the microstructural processes that occur while the pressure profile steepens into a single shock. This work revealed the mechanism by which the crystalline structure melted and demonstrated that unlike in single-shock simulation, a region of overheated solid existed before the liquid phase could nucleate and shock melting occurred. In summary, this project showed the impact of microstructure on loading history and demonstrated that large-scale molecular dynamics simulations and ramp-loaded laser experiments can be performed at similar strain rates and that in situ and simulated x-ray diffraction can be used to compare experiments with simulations. As a result of this project, ramp molecular dynamics simulations and in situ characterizations of microstructure are now being used in mission-relevant materials experiments at the National Ignition Facility.

Publications

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

Hawreliak, J., et al., 2010. *Molecular dynamics simulations of ramp-compressed copper*. LLNL-JRNL-464623.

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

Abstract

Shock- and ramp-wave sensors are key to high-pressure research, but existing sensor technologies



A snapshot of defects in a molecular dynamics simulation of the effects of strain rate on microstructure during dynamic compression. Letters indicate the axes of the three-dimensional simulation space.

for studying such waves have significant shortcomings. We will 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, optically active phase transitions, or other mechanisms. In addition to opening a fundamentally new basic-science frontier, this work may provide the scientific base for tools to address key issues in fusion-class lasers and stockpile stewardship. We will closely couple theory and experimentation to explore this relatively unexplored regime of ultrafast processes.

Our primary result will be elucidating strain-wave processes that can be discerned from terahertz radiation emitted by shocked materials, including the potentially unprecedented subpicosecond-time resolution of strain waves. 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 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.

FY10 Accomplishments and Results

In FY10 we performed laser shock experiments at Livermore's Jupiter Laser Facility that investigated terahertz radiation from gallium nitride shocked from 10 to 100 GPa. Although early experimental work detected radiation from shocked samples, this signal was difficult to consistently reproduce. This could possibly be a result of stronger nonlinearity in the material response of gallium nitride at high pressure or sensitivity of the detected signal to the shock-wave spatial profile. Given the more complex, lower-amplitude signal expected from cadmium selenide, the experiments with this material were deferred. Experiments on gallium nitride provided a baseline sensitivity that demonstrated a significantly smaller signal than expected based on extrapolation

from the acoustic regime. As part of our theoretical work, we predicted that terahertz radiation from a shock-induced phase transformation could substantially modulate the emitted radiation profile and strength, consistent with the possibility that emission may be reduced by material dynamics in gallium nitride at high shock stress. This project experimentally demonstrated the theoretical prediction of emission of coherently generated terahertz radiation by high-frequency acoustic waves—a new discovery that enables the characterization of acoustic or shock waves at unprecedented time resolution. This new phenomenon may be used in semiconductor manufacturing as a nanoscale imaging diagnostic, an application which has been patented as part of this project.

Publications

Armstrong, M. R., et al., 2009. "Coherent THz electromagnetic radiation emission as a shock wave diagnostic and probe of ultrafast phase transformations." *AIP Conf. Proc.* **1195**(1), 647. LLNL-CONF-414924.

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

Reed, E. J., 2010. "Atomic transformation pathways from terahertz radiation generated by shock-induced phase transformations." *Phys. Rev. B* **81**, 144123. LLNL-JRNL-414925.



A sub-picosecond laser pulse fired onto a piezoelectric sample produced a compressive shock wave that propagated through the material, generating terahertz radiation.

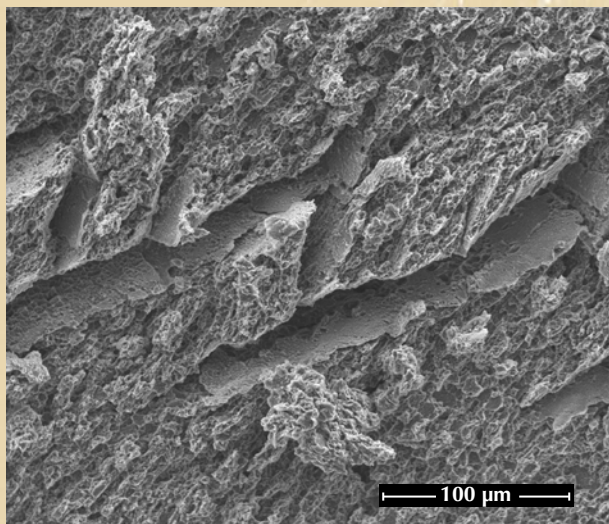
Reed, E. J., and M. R. Armstrong, 2010. *Method for generation of THz frequency radiation and sensing of large amplitude material strain waves in piezoelectric materials*. U.S. patent 7788980, Sept. 7, 2010.

Reed, E. J., et al., 2009. "A new mechanism for observation of THz acoustic waves: Coherent THz radiation emission." *Proc. SPIE* **7214**, 72140P. LLNL-CONF-409650-DRAFT.

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

Abstract

When solids deform at high pressures and strain rates, deformation mechanisms may change, modifying strength properties. Physics-based models for strength and tensile damage under extreme conditions, important for inertial-confinement fusion capsule design and defense applications, are still in their infancy. We will investigate the high-rate deformation of hexagonal and cubic metals through shock-and-release experiments involving in situ deformation measurements and sample recovery. Laser-ablation experiments will probe the 10- to 100-GPa regime on nanosecond timescales, where different flow behavior may occur. We will obtain imaging velocity and displacement histories, along



Scanning electron micrograph of the spall surface from a recovered magnesium crystal, showing ductile deformation at high strain rates.

with x-ray diffraction and scattering data, and perform simulations to complement experiments.

We will obtain systematic measurements of compressive and tensile strength from velocity histories on metal crystals of different orientations and on polycrystalline samples, and expect to measure defect densities from x-ray diffraction. Imaging records of velocity and displacement allow the response to be related to the microstructure, and comparison with molecular and continuum dynamics simulations provides insight into changes in plastic flow mechanisms. In all, this project will provide a detailed understanding of extreme deformation at the crystal-lattice level. This is important for predictive simulations, allowing materials to be selected and optimized in a systematic way for use in extreme environments such as inertial-confinement fusion.

Mission Relevance

This project supports LLNL's missions in national and energy security by greatly improving the quantitative science that underpins 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.

FY10 Accomplishments and Results

In FY10 we (1) performed shock-loading experiments on magnesium, including the important final orientation not previously studied; (2) found that the element, which is plastically extremely anisotropic at low deformation rates, becomes isotropic at very high rates—this discovery has implications for novel methods of forming magnesium components; (3) performed metallography on recovered specimens of magnesium and observed significant variations in the signatures of deformation as a function of strain rate and pressure; (4) performed metallography on beryllium samples recovered from previous experiments, and found systematic variations in microstructural twinning as a function of shock pressure and duration, which are motivating programmatic studies of twinning in shock-recovered tantalum; and (5) obtained diffraction data where the line widths include a contribution from the defect density. This

project succeeded in linking the plastic response of hexagonal-structured metals to microstructural deformation modes at extreme strain rates, increasing our ability to understand, predict, and control materials in advanced engineering applications such as inertial-confinement fusion. We also observed for the first time the solid–solid phase transition in magnesium under dynamic loading.

Publications

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

Milathianaki, D., et al., 2010. *In situ lattice measurement of the shock-induced hcp to bcc phase transition in polycrystalline Mg*. LLNL-JRNL-464437.

Milathianaki, D., et al., 2010. *Plastic deformation mechanisms in shock loaded Mg deduced by elastic precursor amplitude and stress relaxation*. Intl. Symp. Plasticity 2010 and its Current Applications, St. Kitts Marriott Resort, Jan. 3–8, 2010. LLNL-ABS-423466.

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

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

Swift, D. C., et al., 2010. *Orientation dependence of flow stress and spall strength*. LLNL-JRNL-464453.

Swift, D. C., et al., 2010. *Peralta effect of ductility in dynamic loading at extreme strain rates*. Intl. Symp. Plasticity 2010 and its Current Applications, St. Kitts Marriott Resort, Jan. 3–8, 2010. LLNL-ABS-415197.

Swift, D. C., 2009. “Sensitivity of rocky planet structures to the equation of state.” arXIV:0908.3294v1 [astro-ph.EP]. LLNL-TR-414058.

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

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

Abstract

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

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

This research will advance 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 important 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 in stockpile stewardship.

FY10 Accomplishments and Results

In FY10 we (1) completed pad experiments focused on removing the contributions of moment force and lap shape, (2) quantified and combined the phenomena affecting pressure distribution—moment force, viscoelastic, and optic–lap mismatch—and incorporated them into our SurF code, (3) optimized the chemical etching process for mitigating fracture precursors, (4) developed a detailed two-dimensional mass-transport model to predict performance of the etching process, and (5) completed experiments and analyzed the impact of thermal mitigation on fracture precursors. This project has developed a scientific and quantitative understanding of material removal during optical polishing (an important step toward developing deterministic finishing methods), identified the precursors of fused silica surface

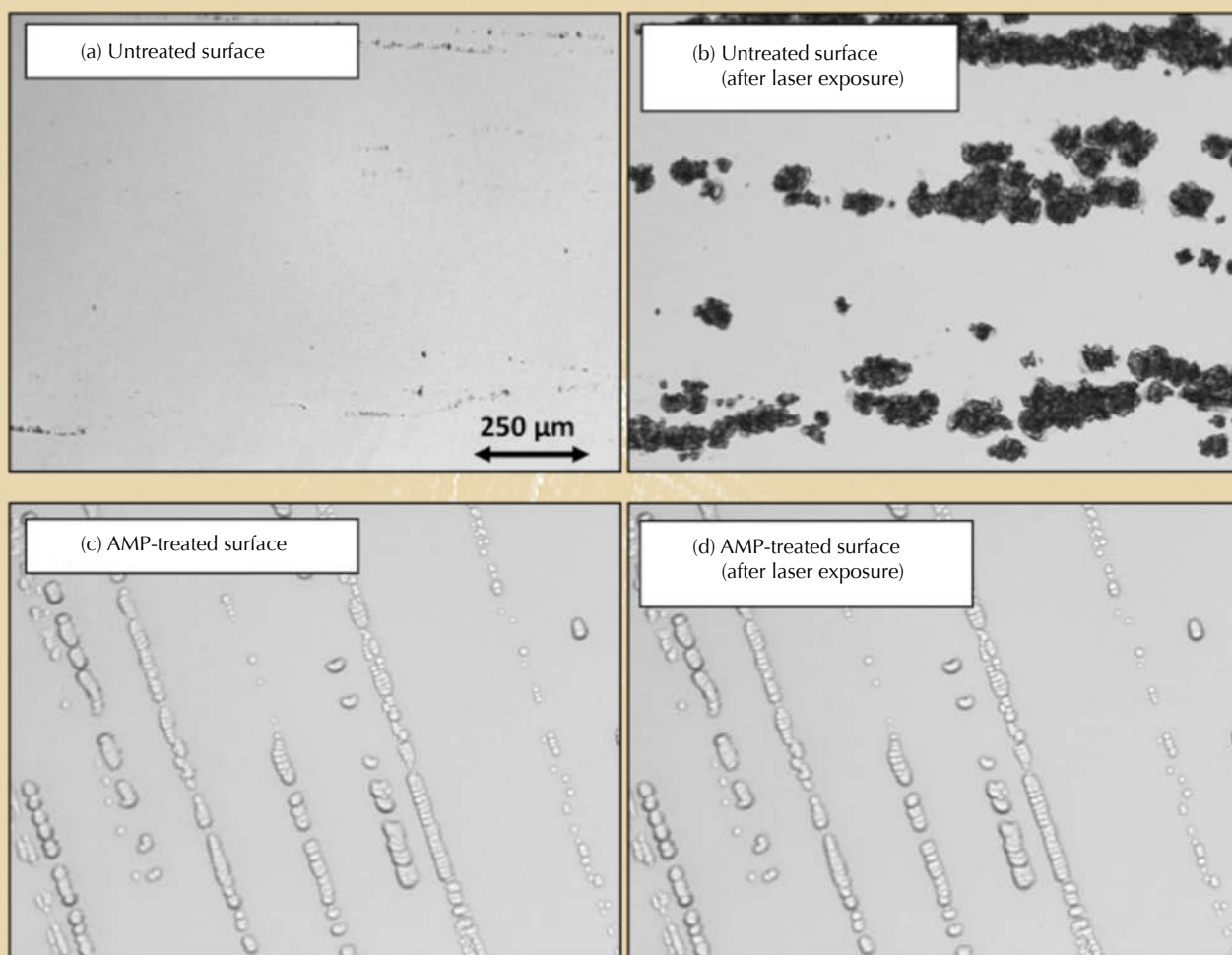
laser-damage initiation, and developed chemical etching mitigation methods now being used to treat fused silica optics for laser fusion and other efforts.

Publications

Feit, M., et al., 2009. "Modeling wet chemical etching of surface flaws on fused silica." *Proc. SPIE* **7504**, L1. LLNL-CONF-420320.

Laurence, T., et al., 2009. "Metallic-like photoluminescence and absorption in fused silica surface flaws." *Appl. Phys. Lett.* **94**, 151114. LLNL-JRNL-407531.

Laurence, T., et al., 2010. "Ultrafast photoluminescence as a diagnostic for laser damage initiation." *Proc. SPIE* **7504**, 16-1. LLNL-PROC-420432.



Optical micrographs of untreated fused silica surfaces and surfaces treated with the advanced mitigation process (AMP) before (a and c) and after (b and d) laser exposure at 8, 10, and 12 J/cm² (3 ns, 351 nm). The damage prevention afforded by the AMP technique is apparent.

Miller, P., et al., 2010. "Fracture-induced sub-band-gap absorption as a precursor to optical damage on fused silica surfaces." *Opt. Lett.* **35**(16), 2702. LLNL-JRNL-426084.

Miller, P., et al., 2009. "Laser damage precursors in fused silica." *Proc. SPIE* **7504**, X1. LLNL-PROC-420439.

Suratwala, T., et al., in press. "HF-based etching processes for improving laser damage resistance of fused silica optical surfaces." *J. Am. Chem. Soc.* LLNL-JRNL-425118.

Suratwala, T., M. Feit, and W. Steele, 2010. "Toward deterministic material removal and surface figure during fused silica pad polishing." *J. Am. Ceramic Soc.* **93**(5), 1326. LLNL-JRNL-412964.

Wong, L., et al., 2010. "The effect of HF/NH₄F etching on the morphology of surface fractures on fused silica." *J. Non-Crystalline Solid* **355**, 797. LLNL-JRNL-404973.

Physics of Local Reinitiation and Morphological Evolution of Mitigated Sites for Ultraviolet Optics—Manyalibo Matthews (08-ERD-057)

Abstract

Our objective is to develop a fundamental understanding of the physics of the reinitiation and morphology of mitigated laser-induced damage on ultraviolet optics. Although effective mitigation strategies are known, reinitiation, optical intensification, and residual stress are still serious issues because the materials science that governs reinitiation and damage evolution is not understood. We will integrate advanced diagnostics, materials characterization, and fundamental computation to clarify the origins of reinitiation and the processes that govern the final shape of mitigated damage sites. Optimized techniques that suppress reinitiation and optical intensification will be explored.

The optics damage mitigation process employs laser-induced heating, melting, and evaporation to remove damaged material, heal subsurface cracks, smooth the surface, and anneal residual stress in the affected region. Development to date has been driven primarily by experimental work supported by empirical models that provide only rough guidance for control of temperature and material transport. Present technology has limited ability to control the size, morphology, and damage threshold of a mitigated site, which fundamentally impacts yield and performance. We expect to develop a stronger scientific basis and advanced diagnostics to guide development of mitigation techniques and extend the understanding of laser interaction with optical materials.

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.

FY10 Accomplishments and Results

In FY10 we (1) used ALE3D and analytic models to simulate high-temperature, laser-driven processes associated with damage mitigation on fused silica surfaces in which the downstream modulation of light was directly correlated to laser-induced thermocapillary flow on silica surfaces; (2) compared Hertz–Knudsen and Anisimov-based evaporation models against experiment, leading to new understanding of the laser-driven vapor-phase transport of silicon oxide and silicon dioxide; (3) tested three-dimensional multigroup diffusion radiation transport models in ALE3D; (4) modeled and developed novel 4.6-micrometer-laser damage mitigation techniques (featured on the cover of *Applied Optics*);

(5) determined the efficacy of adding glass fictive temperature calculations to existing ALE3D codes and compared the results with experiment, while molecular dynamics force fields were compared to estimate high-temperature silica properties, and published the results of our studies in the peer-reviewed literature; and (6) developed laser-based diagnostics capable of accurate, high-resolution thermal conductivity measurements and applied the diagnostics to several materials. The methods and concepts developed in this project for 10.6-micrometer-laser damage mitigation were adopted for use by the Optical Mitigation Facility at the National Ignition Facility.

Publications

Adams, J. J., et al., 2010. "Results of applying a non-evaporative mitigation technique to laser-initiated surface damage on fused silica." *SPIE* **7842**, 784281. LLNL-PRES-456823.

Elhadj, S., et al., 2010. "Determination of the intrinsic temperature-dependent thermal conductivity from analysis of surface temperature of laser-irradiated materials." *Appl. Phys. Lett.* **96**, 0171101. LLNL-JRNL-420233.



Comparing thermal and microstructural differences caused by mid- and far-infrared lasers (top and bottom rows, respectively) used for repairing laser-induced microfractures on silica surfaces (cover of May 10, 2010 issue of Applied Optics).

Elhadj, S., et al., 2008. *High-temperature thermographic measurements of laser-heated silica*. 2008 Materials Research Society Fall Mtg., Boston, MA, Dec. 1–5, 2008. LLNL-ABS-404904.

Elhadj, S., et al., 2009. "High-temperature thermographic measurements of laser-heated silica." *SPIE* **7504**, 750419. LLNL-PROC-421306.

Feit, M. D., et al., 2010. "Morphological changes induced by CO₂ laser-based damage mitigation of SiO₂ surfaces." *SPIE* **7842**, 784230. LLNL-PROC-461512.

Guss, G. M., et al., 2009. "In situ monitoring of surface postprocessing in large aperture fused silica optics with optical coherence tomography." *Appl. Optics* **47**(8), 4569. LLNL-JRNL-401368.

Matthews, M. J., et al., 2010. "Analysis of microstructural relaxation phenomena in laser-modified fused silica using confocal Raman microscopy." *Opt. Lett.* **35**, 1311. LLNL-JRNL-421570.

Matthews, M. J., et al., 2009. "Residual stress and damage-induced critical fracture on CO₂ laser-treated fused silica." *SPIE* **7504**, 750410. LLNL-PROC-419968.

Raman, R. N., et al., 2010. "Monitoring annealing via CO₂ laser heating of defect populations on fused silica surfaces using photoluminescence microscopy." *Optic. Express* **18**, 15207. LLNL-JRNL-423077.

Shen, N., et al., 2010. "Laser smoothing of sub-micron grooves in hydroxyl-rich fused silica." *Appl. Surf. Sci.* **256**, 4031. LLNL-JRNL-381080.

Shen, N., et al., 2010. "Study of CO₂ laser smoothing of surface roughness in fused silica." *SPIE* **7504**, 750411. LLNL-PRES-416935.

Shestakov, A. I., R. M. Vignes, and J. S. Stölken, in press. "Derivation and solution of multifrequency radiation diffusion equations for homogeneous refractive lossy media." *J. Comp. Phys.* LLNL-JRNL-422310.

Soules, T. F., et al., 2010. "Molecular dynamics as a tool to study silica laser damage mitigation." *SPIE* **7842**, 784231. LLNL-PRES-456803.

Soules, T. F., et al., 2010. "Silica molecular dynamic potentials—a practical assessment." *J. Non-Cryst. Solids* **356**. LLNL-CONF-452912.

Yang, S. T., et al., 2010. "Comparing the use of 4.6-mm lasers versus 10.6-mm lasers for mitigating damage growths on fused silica." *SPIE* **7842**, 784263. LLNL-PROC-461691.

Yang, S. T., et al., 2010. "Comparing the use of mid-infrared versus far-infrared lasers for mitigating damage growth on fused silica." *Appl. Optic.* **49**, 2606. LLNL-JRNL-423683.

Yang, S. T., et al., 2009. "Thermal transport in CO₂ laser-irradiated fused silica: In situ measurements and analysis." *J. Appl. Phys.* **106**, 1031061. LLNL-JRNL-414595.

Radiation-Tolerant Materials— Michael Fluss (09-SI-003)

Abstract

One challenge specific to sustainable nuclear energy is developing radiation-tolerant materials for encapsulating reactor fuel as well as structural components of nuclear energy systems that can maintain required properties despite neutron-induced changes. Materials with nanometer-scale dispersed particles appear to be good candidates for radiation tolerance, but there are significant gaps in our understanding of the properties of these metals. Our goal is to understand the scientific principles that govern behavior of this class of materials, to explore the limits of their radiation tolerance, and to discover means by which this tolerance can be extended through materials refinement or development of new material systems.

We hope to discover the fundamental materials science necessary to realize radiation-tolerant materials that can maintain required operational specifications despite neutron-induced changes. The behavior of nanometer-scale structured materials through

modeling validated by sequential and simultaneous ion-beam experiments with heavy ions, helium, and hydrogen will bridge length scales from microscopic to macroscopic and timescales from days to decades in describing advanced radiation tolerance. Key deliverables are both experimental radiation tools for the discovery of advanced radiation-resistant materials and simulation and modeling tools for the design, development, and deployment of advanced nuclear energy systems for fission or fusion.

Mission Relevance

Our proposed research supports Laboratory missions in both energy and national security. Elimination of reprocessing in the fuel cycle would reduce cost and increase energy security. Materials for ultradeep burn-up of fission fuel are key to using all the potential energy in uranium. This simple idea is the path to a sustainable nuclear fuel cycle that lowers the barriers of waste disposition, decreases the threat of proliferation, incorporates safeguards by design, and establishes economic competitiveness through sustainability and energy independence.

FY10 Accomplishments and Results

In FY10 we experimentally characterized the microstructure that develops in oxide-dispersion-strengthened (ODS) materials with helium; helium and iron; and hydrogen, helium, and iron under various ion-beam radiation scenarios. Specifically, we (1) used the triple ion beams at the Jannus facility in Saclay, France, to irradiate specimens of iron, ferrochrome, MA957 ODS steel, and K3 ODS steel, determining the formation mechanism of the resulting nano-particle dispersoid microstructure—which is described in a paper in *Physical Review B*—and identifying the importance of sub-nanometer particles as sequestering agents for helium management; (2) examined the irradiated specimens with transmission electron microscopy and micromechanical characterization; (3) continued investigating the mechanical properties of micrometer-sized specimens, making progress in understanding size effects for micro-tensile specimens and performing depth-dependent nano-indentation on specimens irradiated with a dual helium and iron beam; (4) made progress in developing an advanced rate-theory simulation approach to model the interaction of

helium with dispersed oxide particles; (5) performed advanced theory, simulation, and modeling with the new approach, with an emphasis on time-transcending methods; (6) planned a systematic experimental study of ferrochrome as a function of chromium concentration in collaboration with the Jannus Saclay facility; and (7) continued modeling of helium and oxide particle interactions and solubility.

Proposed Work for FY11

In our final year we will (1) complete the analysis on 16 dual- and triple-beam ion-irradiated iron, ferrochrome, and ODS materials using electron microscopy; (2) carry out a series of irradiations to measure the change in mechanical properties of ODS steels under high-dose ion-beam irradiations; (3) conduct a preliminary study of the deterioration of refractory coated steels under helium or heavy-ion irradiation; and (4) document the results of our research in high-impact peer-reviewed journals, as well as for the International Atomic Energy Agency's Coordinated Research Program on Simulation and Modeling.

Publications

Donev, V., et al., 2010. "A first-passage Monte Carlo algorithm for complex diffusion-reaction systems." *J. Comp. Phys.* **229**, 3214. LLNL-JRNL-413160.

Fluss, M. J., 2009. *Ultra-high burn-up: Is it possible?* 8th Intl. Workshop on Fundamental Plutonium Properties, Chelyabinsk, Russia, Sept. 12–16, 2009. LLNL-ABS-405639.

Fluss, M. J., and G. Bench, 2009. *Accelerated nuclear energy materials development with multiple ion beams*. DOE Workshop on Fusion-Fission Research, Gaithersburg, MD, Sept. 30–Oct. 2, 2009. LLNL-CONF-415877.

Fluss, M. J., and L. Hsiung, 2009. *TEM characterization of oxide particles in ODS steels in preparation for ion-beam experiments*. Joint EC-IAEA Topical Mtg. Development of New Structural Materials for Advanced Fission and Fusion Reactor Systems, Barcelona, Spain, Oct. 5–9, 2009. LLNL-ABS-414204.

Fluss, M. J., G. Bench, and S. Tumey, 2011. *Single and multi-ion-beam facilities and their application to nuclear energy*. 15th Intl. Conf. Emerging Nuclear Energy Systems, San Francisco, CA, May 15–19, 2011. LLNL-CONF-464259.

Fluss, M. J., et al., 2010. *ODS steel for high-burn-up fission fuels and first-wall fusion systems*. U.S.–Russian Workshop on the Fundamentals of Plutonium Science, Moscow, Russia, July 19, 2010. LLNL-CONF-428106.

Hsiung, L., M. J. Fluss, and A. Kimura. "Structure of oxide nanoparticles in Fe-16Cr MA/ODS ferritic steel." *Mater. Lett.* **64**, 1782. LLNL-JRNL-427350.

Hsiung, L., et al., 2010. *Cavity formation in multi-ion-beam-irradiated ODS steel*. 25th ASTM Symp. Effects of Radiation on Nuclear Materials, Anaheim, CA, June 15–17, 2011. LLNL-PROC-455652.

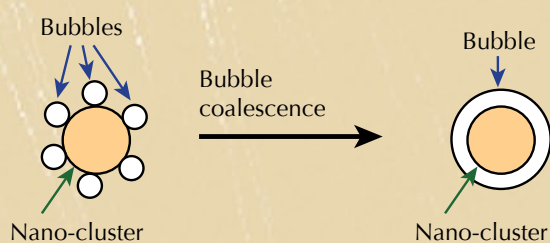
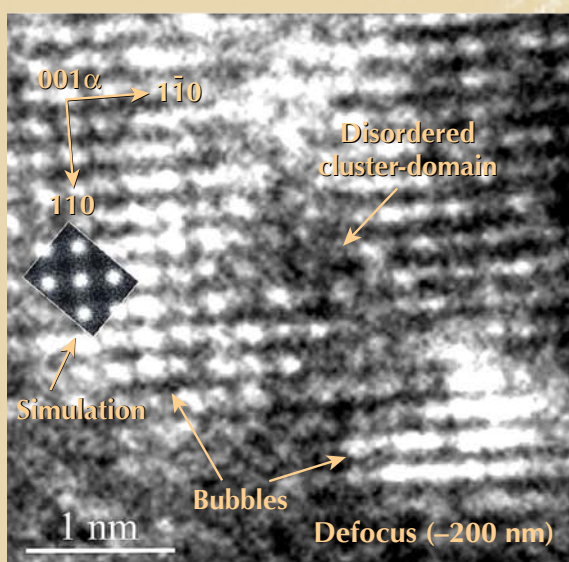
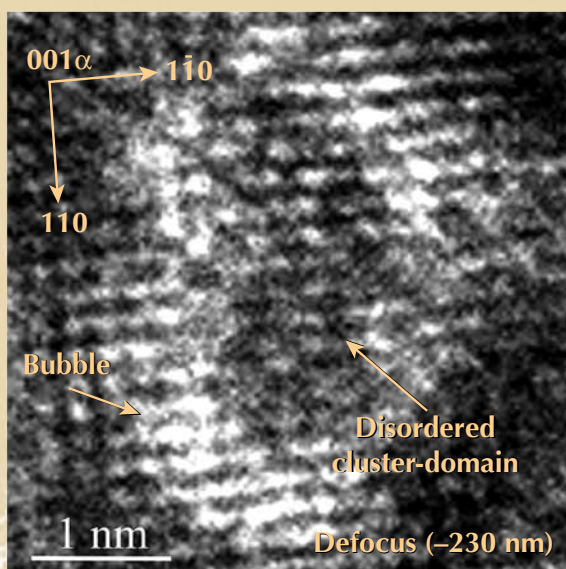
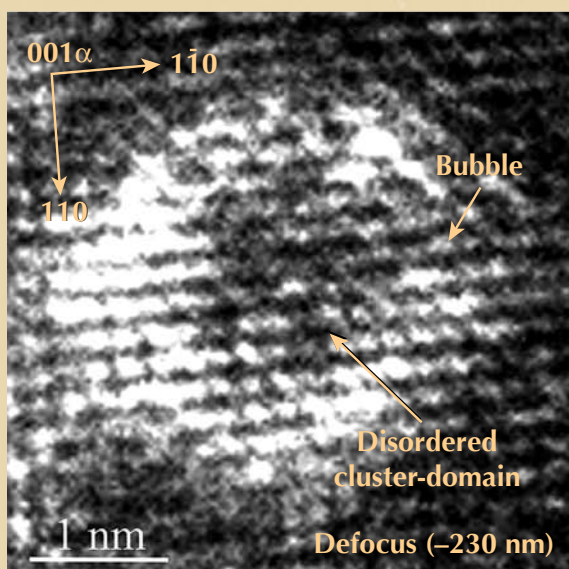
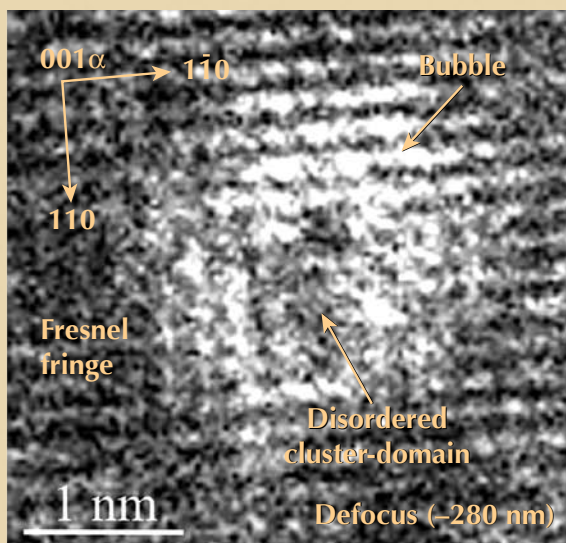
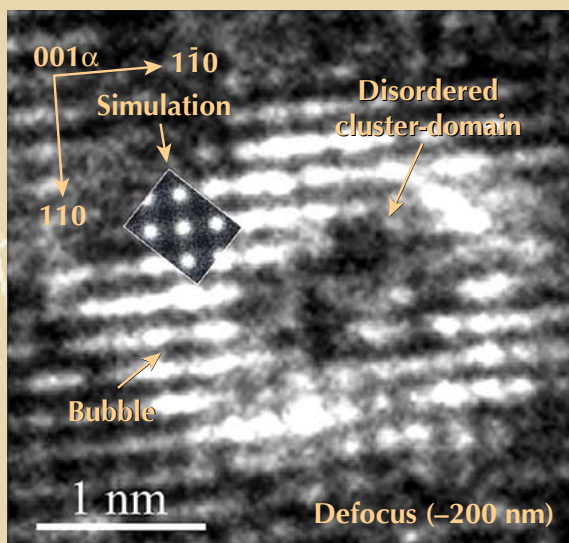
Hsiung, L., et al., 2010. "Formation mechanism and the role of nanoparticles in Fe–Cr ODS steels." *Phys. Rev. B* **82**, 184103. LLNL-JRNL-456731.

Hsiung, L., et al., in press. "HRTEM study of oxide nanoparticles in 16Cr-4Al-2W-0.3Ti-0.3Y₂O₃ ODS steel." *Proc. MRS Fall Mtg. 2009*. LLNL-PROC-420389.

Hsiung, L., et al., in press. "HRTEM study of oxide nanoparticles in K3 ODS ferritic steel developed for radiation tolerance." *J. Nucl. Mater.* LLNL-JRNL-419534.

Hsiung, L., et al., 2009. *ODS dual beam (Fe + He) experiment*. Intl. Atomic Energy Agency Technical Mtg. Physics of Materials Under Neutron and Charged Particle Irradiations, Vienna, Austria, Nov. 23–29, 2009. LLNL-PROC-418166.

Hsiung, L., et al., 2010. *TEM study of oxide nanoparticles in ODS steels developed for radiation tolerance*. 139th Ann. Mtg. Materials, Metals, and Materials Soc., Seattle, WA, Feb. 14–18, 2010. LLNL-PROC-418163.



The four upper micrographs show the trapping of helium bubbles by amorphous particles in ferrochrome. The bottom micrograph shows the coalescence of helium at such a particle, suggesting a new mechanism, which is depicted in the bottom right figure.

Nanosecond Characterization of Dynamic Void Evolution in Porous Materials— Anthony Van Buuren (09-ERD-002)

Abstract

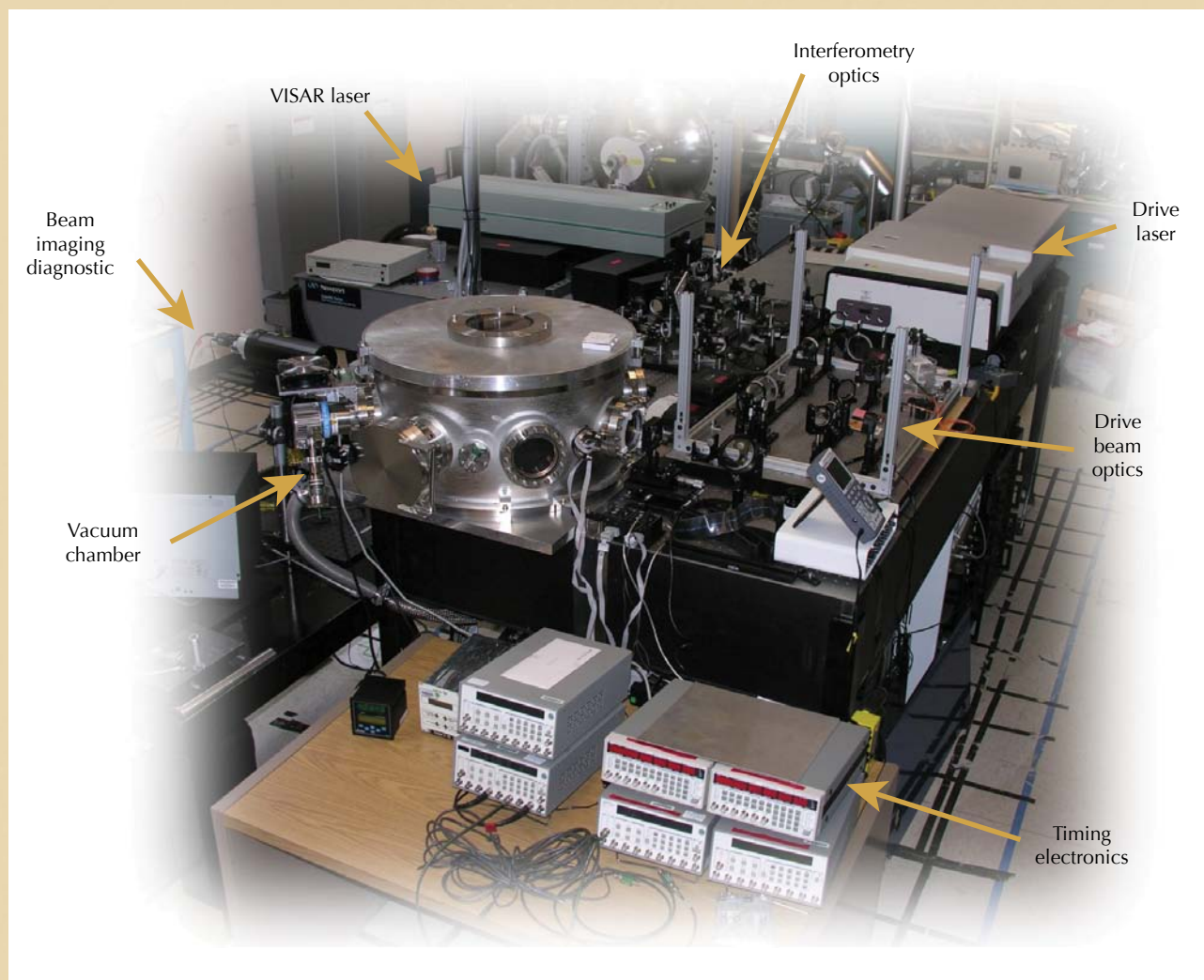
Very little is currently understood about how the morphology of nanostructured foams responds to shock conditions. Existing models of porous materials are believed to be well grounded experimentally at very low and very high levels of porosity. However, the models make inconsistent assumptions and none have been verified in situ. We propose to characterize the morphology of nanofoams under shocked conditions and use these results to validate models of void evolution in materials. We will quantify dynamic structural changes with a state-of-the-art, ultrafast, small-angle x-ray scattering system.

Ultimately, we hope to obtain a predictive capability for these materials under extreme conditions as a function of initial structure and compression dynamics.

We will leverage LLNL's recent successful capability of measuring small-angle x-ray scattering using a single x-ray pulse, which enables the use of pump-probe experiments to measure structural changes in situ during a shock. We will apply these methods to nanofoams for the first time and expect to answer a major question: How reliable are existing theoretical models used to describe the compression of foams?

Mission Relevance

Key deliverables of this project include the ability to characterize the evolution of foam microstructures under shock conditions and the validation



Experimental apparatus at the Laboratory is being used to study shocked foams to validate models of void evolution in materials.

of theoretical models, both of which are critical for future laser targets for stockpile stewardship and inertial-confinement fusion experiments, which support LLNL's national and energy security missions.

FY10 Accomplishments and Results

In FY10 we measured the dynamic small-angle x-ray scattering from resorcinol-formaldehyde carbon aerogels having a density of approximately 350 mg/cm^3 and a thickness of 350 to 450 μm in ablatively loaded shock experiments at the Advanced Photon Source at Argonne National Laboratory. Last year, we determined that voids measured in shock-recovered foams were anisotropic in nature, which was a problem because the gated small-angle x-ray scattering detector used in the ultrafast pump-probe experiments integrates the angular dependence of x-ray scattering, masking this anisotropy. If anisotropy is not taken into account, the time-dependent void volume and size distribution calculations are flawed. To mitigate this problem, we repeated experiments at the Advanced Photon Source using beam line 14ID, which employs a chopper system to produce gated x-ray pulses that enables a normal two-dimensional small-angle x-ray scattering detector to be used for the pump-probe experiments. The results were significantly different from previous measurements in that we were able to determine void distribution to be a combination of spherical and cylindrical shapes.

Proposed Work for FY11

In FY11 we will (1) measure the dynamic small-angle x-ray scattering of carbon aerogel as a function of density, (2) expand the work to examine nanoporous copper, and (3) use the Advanced Photon Source to conduct ultrafast, dynamic small-angle x-ray scattering experiments with a conventional charge-coupled device detector and an ultrafast x-ray chopper, for a time resolution of 100 ps, as well as a pink beam, which is required for obtaining a sufficient signal-to-noise ratio for the dynamic experiments.

Understanding the Surface Properties That Lead to Optical Degradation in High-Fluence, High-Average-Power Optical Materials—Jeffrey Bude (09-ERD-003)

Abstract

Laser-induced surface damage to optical materials limits the maximum operating fluence of fusion-class laser systems. Moreover, surface properties that limit optical performance are not well understood. We will develop a fundamental understanding of these properties in high-fluence, high-average-power optical materials. A suite of sensitive high-resolution optical techniques and advanced computational modeling will be employed to study the electronic and optical properties of dielectric surfaces at the nanometer scale. We intend to clarify the links between surface properties, laser-induced surface damage, and the effects of long-term, high-fluence optical fluxes on damage resistance in optical materials.

We expect to (1) determine the physical origin of ultrafast photoluminescence from defects associated with damage in silica and determine whether fast photoluminescence is a predictor of damage in other optical materials using confocal time-resolved photoluminescence imaging; (2) determine the effects of long-term, high-fluence optical exposure on surface properties and damage resistance of optical materials; and (3) clarify the links between material properties, surface nanostructure, electronic structure, optical absorption, and high-fluence optical damage in optical materials. This work will guide development of damage-resistant optics and will help to understand the limits of optical materials operated under high fluence, as well as understand high-fluence, high-average-power conditions.

Mission Relevance

This research directly addresses stockpile stewardship and fusion energy challenges by optimizing large advanced laser systems. It will serve to establish science-based rules for optics reliability prediction, improve damage diagnostics, and suggest

pathways to increase damage resistance in optical materials. More broadly, understanding defect-assisted absorption and material modification is a frontier problem in condensed-matter physics.

FY10 Accomplishments and Results

In FY10 we (1) developed a fluorescent resonant energy transfer-based model and a phonon blockade model for quasi-continuum photoluminescence and tested them on computational and experimental model systems, finding that photoluminescence correlated to damage in potassium dihydrogen phosphate, calcium fluoride, and silica etch precipitates but not in antireflection coatings; (2) determined that low-stress-intensity silica fractures did not generate increased photoluminescence or damage; (3) performed optical stress experiments in several materials in various atmospheric environments and found increases in quasi-continuum photoluminescence and surface roughness, as well as evidence of surface etching; (4) calibrated and performed molecular dynamics simulations for silica fracture; and (5) advanced our understanding of laser-supported absorption fronts of energy transport, ran hydrodynamic and ab initio Urbach absorption simulations, and performed shaped-pulse-damage experiments.

Proposed Work for FY11

In FY11 we will (1) complete analysis of optical stress effects on the surface properties of optical materials and determine stress effects on damage thresholds for surfaces, flaws, and damage sites; (2) perform experiments and simulations to isolate the precursors of high-fluence surface damage; (3) perform experiments to understand the role of surface preparation on optical absorption and damage for coating-induced damage degradation on etched silica flaws, fractures, and reactive-ion-etched and gas-phase-etched surfaces; (4) complete experiments and simulations to understand the origin of quasi-continuum photoluminescence and to improve our understanding of the physical links among photoluminescence, defect absorption, and damage; and (5) refine our models for laser-supported absorption fronts.

Publications

Carr, W., J. Bude, and P. DeMange, 2010. "Laser-supported solid-state absorption fronts in silica." *Phys. Rev. B* **82**, 184304. LLNL-JRNL-42387.

Laurence, T. A., et al., 2009. "Metallic-like photoluminescence and absorptivity in fused silica surface flaws." *Appl. Phys. Lett.* **94**, 151114. LLNL-JRNL-407531.

Laurence, T. A., et al., 2009. *Ultra-fast photoluminescence as a diagnostic for laser damage initiation*. 2009 SPIE Laser Damage Symp., Boulder, CO, Sept. 21–23, 2009. LLNL-PRES-416938.

Laurence, T. A., et al., 2010. "Ultrafast photoluminescence as a diagnostic for laser damage initiation." *Proc. SPIE* **7504**, 750416. LLNL-PROC-420432.

Miller, P. E., et al., 2010. "Fracture-induced sub-band gap absorption as a precursor to optical damage on fused silica surfaces." *Optic. Lett.* **35**, 2702. LLNL-PROC-426084.

Miller, P. E., et al., 2009. *Identification of laser damage precursors in fused silica optics*. 2009 SPIE Laser Damage Symp., Boulder, CO, Sept. 21–23, 2009. LLNL-ABS-413560.

Miller, P. E., et al., 2010. "Laser damage precursors in fused silica." *Proc. SPIE* **7504**, 75040X. LLNL-PROC-420439.

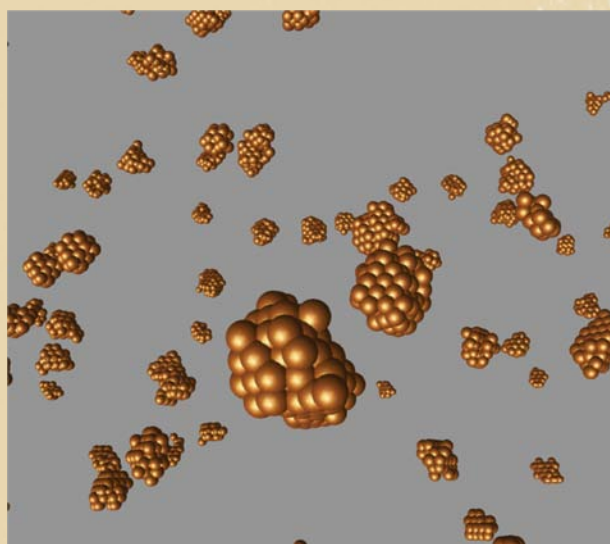
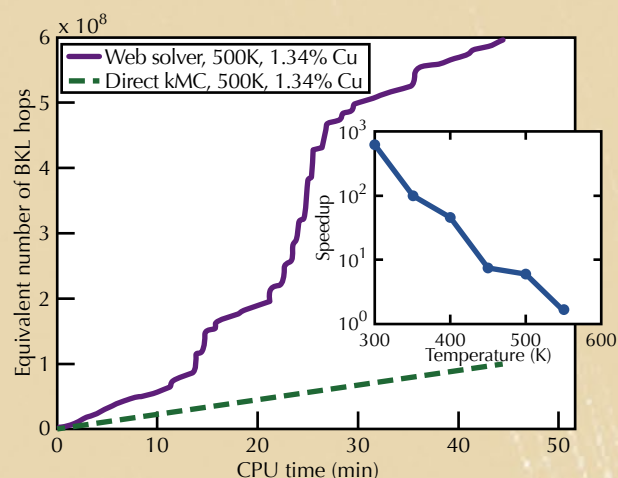
Shen, N., et al., 2009. *Isothermal anneal of damage precursors on fused silica surfaces*. 2009 SPIE Laser Damage Symp., Boulder, CO, Sept. 21–23, 2009. LLNL-POST-416936.

Suratwala, T. I., et al., 2011. "HF-based etching processes for improving laser damage resistance of fused silica optical surfaces." *J. Am. Ceram. Soc.* **94**(2), 416. LLNL-JRNL-425118.

Multi-Resolution Adaptive Monte Carlo for Microstructure Simulations— Vasily Bulatov (09-ERD-005)

Abstract

The objective of our project is to extend the time and length scales of material microstructure simulations to those relevant for engineering applications. Our development will focus on atomistic (lattice) Monte Carlo as a general and accurate framework and will rely on iron–copper and iron–chromium binary alloys as test-bed material systems. Of principal interest is the kinetics of diffusive phase



In our test-bed problem, phase-separation kinetics in the binary alloy iron–copper, our new algorithm accelerated kinetic Monte Carlo simulations of the phase kinetics by three orders of magnitude (top). Lattice Monte Carlo is one of the two levels of resolution (bottom).

transformations, including nucleation and growth of precipitates, ordering, segregation, and the effects of continuous and pulsed irradiation drive on these phenomena. Several novel methods will be developed that, in combination, will significantly enhance the computational efficiency of microstructure simulations while maintaining or improving their accuracy.

We expect to develop a novel computational approach of multi-resolution adaptive Monte Carlo that will extend the time and length scales for accurate simulations of the kinetics of microstructure evolution in binary alloys. Eventually, we will extend this approach to more complex materials such as those used in nuclear reactors. Unlike existing phenomenological methods, our multi-resolution approach is entirely self-consistent—on its fully refined level, it reduces to a detailed atomistic representation. At the same time, our simulation approach links the fundamental mechanisms of atomic diffusion directly and seamlessly to alloy microstructure evolution on scales relevant for current and future engineering applications.

Mission Relevance

Our new simulation capability can find multiple applications in several existing and emerging mission areas in which the behavior of materials away from equilibrium is important, including national and energy security. For example, our new efficient methods and computer codes can be employed for computational extrapolation of material damage observed in an accelerated radiation test to the expected radiation resistance of the same material over its work life in nuclear reactors.

FY10 Accomplishments and Results

In FY10 we (1) developed, implemented, and exercised two exact algorithms for accelerated kinetic Monte Carlo simulations of continuum-time Markov chain models; (2) selected and developed a coarse-grained object Monte Carlo representation for binary alloys with vacancies; and (3) ran extensive atomistic simulations to reveal the effects of local (atomic-level) stress on vacancy migration energy.

Proposed Work for FY11

In FY11 we will (1) finish implementing the accelerated kinetic Monte Carlo methods and use them for model systems, in addition to those models for binary alloys with vacancies—for example, protein folding and domain-wall motion in ferro-electrics; (2) parameterize a coarse-grained Monte Carlo model of the binary alloy system iron–copper by matching to exact Monte Carlo simulations; (3) simulate the kinetics of phase transformations in binary alloy systems for a variety of conditions using both exact and coarse-grained simulation methods; and (4) examine alternative coarse-graining methods for continuum-time Markov chain systems—for example, those based on algebraic, multigrid ideas.

Publications

Baumer, R. E., et al., 2010. *Atomistic simulations of radiation damage in amorphous metals*. LLNL-POST-447641.

Bulatov, V., 2010. *Multiresolution adaptive Monte Carlo for microstructure simulations*. LLNL-PRES-439972.

Collection of Refractory Debris from the National Ignition Facility for Stewardship-Relevant Measurements— Dawn Shaughnessy (09-ERD-026)

Abstract

Solid debris collected from National Ignition Facility (NIF) shots will be used to measure cross sections of radiochemical detectors for nuclear testing. Such measurements will significantly reduce uncertainties in interpreting radiochemical data. This project will develop a system for collecting solid debris samples at fusion-class lasers for radiochemical analysis and measurement of stockpile stewardship cross sections. Distribution of the debris will first be determined through simulation and experiment. Next, several designs will be tested, and a priority list of stewardship-relevant measurements will be determined. The methodology will be benchmarked through measurement of yttrium cross sections, but ultimately a variety of radiochemical detectors will be evaluated.

If successful, this project will yield a prototype solid collector that can be fielded during early NIF shots for testing. If, as we expect, this new device significantly improves the acquisition and understanding of radiochemical data, it would then be a candidate for future program support and deployed in the NIF chamber for routine radiochemical measurements. Initially, we will consider several collector designs, then select the most promising ones and conduct testing at NIF to evaluate collection efficiency and ease of insertion and extraction from this particular chamber. Once a prototype has been fully developed, measurements of the yttrium cross section will begin as ride-along experiments on other NIF shots.

Mission Relevance

This project supports LLNL's national security mission by reducing thermonuclear device uncertainties—a major goal of stockpile stewardship—by enabling solid collection to reliably measure cross sections, validate code calculations, and lower uncertainties in the interpretation of radiochemical data. In addition, the measurements on NIF that this project enables will help recruit staff in the core competency area of radiochemistry.

FY10 Accomplishments and Results

In FY10 we (1) analyzed aluminum and glass plates exposed to NIF shots to determine ablation as a function of laser energy (up to 1 MJ) and distance from the target chamber center and to quantify the amount of debris collected, determining that a direct collection scheme is feasible for NIF; (2) began developing sample holders for the diagnostic insertion modules; (3) initiated planning for our direct collection scheme based on results from analyzed NIF samples; (4) began designing field material ablation tests at NIF under actual shot conditions to determine which material should comprise the collector, and constructing parts and holders for these tests; and (5) analyzed salt films used at the Titan laser, Los Alamos National Laboratory's Trident laser, and the Zebra Z-pinch generator at the Nevada Terawatt Facility at the University of Nevada, Reno.

Proposed Work for FY11

In FY11 we plan to (1) construct and field our final collector mount, (2) design solid collection

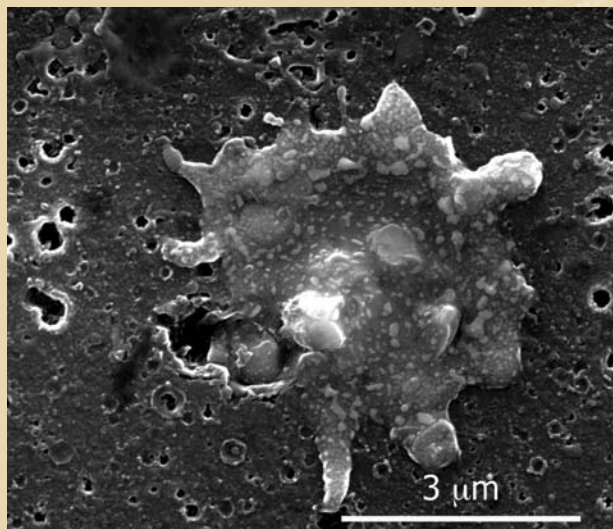
experiments to be conducted at NIF both before and after the ignition campaign, (3) investigate collector insertion and extraction options, (4) complete analysis of material-compatibility test samples and ablation test samples using thin salt films and metal foams for possible use at NIF, (5) complete sensitivity analysis of using solid collection at NIF for measurement of the stockpile stewardship-relevant yttrium cross section, and (6) design and construct a sample tritium-removal system for the subsequent analysis of collector samples.

Publications

Gostic, J. M., et al., 2010. *Status of solid debris collection for radiochemical diagnostics and measurements on NIF*. 42nd Interlaboratory Working Group Mtg., Los Alamos, NM, May 24–27, 2010. LLNL-PROC-432952.

Nelson, S. L., et al., 2010. *Aerosol-assisted solid debris collection for the National Ignition Facility*. 42nd Interlaboratory Working Group Mtg., Los Alamos, NM, May 24–27, 2010. LLNL-PRES-432795.

Nelson, S. L., et al., 2009. *Collection of solid debris for the National Ignition Facility*. 36th Intl. Conf. Plasma Science and 23rd Symp. Fusion Engineering, San Diego, CA, May 31–June 5, 2009. LLNL-ABS-409698.



An electron microscope image of an aluminum blast shield fielded during a laser shot at the National Ignition Facility. The mass in the center is a gold particle that was emitted from the hohlraum target case from a distance of 50 cm away.

Nelson, S. L., et al., 2009. *Collection of solid debris for the National Ignition Facility*. Fall American Chemical Society National Mtg. and Exposition, Washington, DC, Aug. 16–20, 2009. LLNL-ABS-413590.

Nelson, S. L., et al., 2010. *RAGS: The gaseous sample collection diagnostic at the National Ignition Facility*. 37th IEEE Intl. Conf. Plasma Science, Norfolk, VA, June 20–24, 2010. LLNL-PROC-462002.

Nelson, S. L., et al., 2009. *Sample collection and radiochemistry for the National Ignition Facility*. IFSA 2009, 6th Intl. Conf. Inertial Fusion Sciences and Applications, San Francisco, CA, Sept. 6–11, 2009. LLNL-POST-413383.

Shaughnessy, D. A., S. L. Nelson, and K. J. Moody, 2010. *Development of solid collection diagnostics through blast shield analysis*. 37th IEEE Intl. Conf. Plasma Science, Norfolk, VA, June 20–24, 2010. LLNL-ABS-424229.

Shaughnessy, D. A., et al., 2010. *Analysis of NIF debris collection samples toward an experimental understanding of NIF debris*. 5th Ann. Intl. Workshop on Computational Challenges in Fusion Facility Modeling, Bordeaux, France, June 26–28, 2010. LLNL-PRES-433480.

Shaughnessy, D. A., et al., 2009. *Collection of solid debris for the National Ignition Facility*. 237th American Chemical Society National Mtg. and Exposition, Salt Lake City, UT, Mar. 22–26, 2009. LLNL-ABS-408402.

Shaughnessy, D. A., et al., 2009. *Gaseous sample collection at the National Ignition Facility*. Fall American Chemical Society National Mtg. and Exposition, Washington, DC, Aug. 16–20, 2009. LLNL-ABS-409696.

Shaughnessy, D. A., et al., 2010. *Status of solid debris collection for radiochemical diagnostics and measurements*. Workshop on Neutron Capture in ICF Plasmas, Berkeley, CA, Mar. 24, 2010. LLNL-PRES-426025.

Shaughnessy, D. A., et al., 2009. *Stockpile stewardship measurements using solid collection at the National Ignition Facility*. Nuclear Explosives Design Physics Conf., Livermore, CA, Oct. 26–30, 2009. LLNL-ABS-461988.

Magnetorheological Finishing for Large-Aperture High-Fluence Optical Applications—Joseph Menapace (09-ERD-049)

Abstract

Our goal is to understand the magnetorheological finishing (MRF) processes governing the deterministic removal of material from, and achieving figure control on, optical surfaces. In addition, we will investigate how these processes affect the manufacture of precise, high-fluence optics for inertial-confinement fusion and other high-power laser systems. Specifically, we will (1) develop an understanding of the details of MRF material removal on free-form optics so that state-of-the-art protocols can be developed for meter-size optics, (2) develop new polishing slurries and protocols to polish novel crystalline optical materials that are important for inertial-confinement fusion laser systems, and (3) investigate MRF to precisely polish out or mitigate flaws and damage on high-fluence optical materials.

This study will greatly enhance the scientific knowledge of MRF polishing, which has applications in precision optics, space science, and semiconductors. Specifically, the ability to deterministically finish an optical surface using a sub-aperture tool will allow optical glass fabricators to improve the figure of an optic in a less iterative and more repeatable, economical, and deterministic manner. We will also enhance the understanding of advanced sub-aperture polishing that can be used to remove damage and compensate for short-range internal flaws in optics artifacts that limit the suitability of small- and large-aperture optical materials in high-fluence, high-repetition-rate laser applications.

Mission Relevance

This project supports the Laboratory's missions in national and energy security by expanding the knowledge base for fabricating optical components critical to the high-energy, high-power, fusion-class laser systems used to validate complex coupled-physics computer simulations, including codes used in lieu of nuclear stockpile testing.

FY10 Accomplishments and Results

In FY10 we (1) designed protocols for and installed interferometric hardware and used it to measure the surface figure on ground and polished curved, subscale fused-silica specimens to determine sagittal departure and back focal length; (2) conducted damage removal and final polishing with small MRF wheels; (3) developed baseline MRF polishing processes for curved optics, including damage removal, mid-spatial frequency artifact smoothing, and final figuring; (4) tested and refined MRF fluids and delivery system stability for new nonaqueous fluids; (5) performed damage testing of optics made with a new fluid formulation; (6) transitioned damage-removal and final figuring protocols for fused silica to our large-aperture MRF tool; (7) demonstrated damage removal and final figuring protocols on a 430-by-430-cm off-axis aspheric fused-silica lens; and (8) submitted a record of invention and full patent application for a nonaqueous MRF fluid capable of polishing water-soluble crystals and a patent application for an MRF technique for polishing sapphire and titanium-sapphire.

Proposed Work for FY11

In FY11 we will (1) transition protocols and activities to the large-aperture MRF tool for surface-figure correction and polishing on ground and polished curved, large-aperture fused-silica specimens; (2) conduct damage removal and final polishing using large MRF wheels and sub-aperture pad-polishing heads; (3) refine polishing processes for large-aperture curved optics; (4) fabricate large-aperture fused-silica demonstration optics; (5) perform

damage testing of optics made using refined protocols; and (6) explore process scale-up that would be needed for polishing larger-aperture potassium dihydrogen phosphate optics.

Publications

Menapace, J. A., 2010. "Developing magnetorheological finishing (MRF) technology for the manufacture of large-aperture optics in megajoule-class laser systems." *Proc. SPIE* **7842**, 78421W. LLNL-ABS-428008.

Menapace, J. A., P. R. Ehrmann, and R. C. Bickel, 2009. *Magnetorheological finishing (MRF) of potassium dihydrogen phosphate (KDP) crystals: Nonaqueous fluids development, optical finish, and laser damage performance at 1064 nm and 532 nm*. SPIE Laser Damage Symp., Boulder, CO, Sept. 21–23, 2009. LLNL-PRES-414344.

Miller, P. E., et al., 2009. "Laser damage precursors in fused silica." *Proc. SPIE* **7504**, 75040X. LLNL-PROC-420439.

Characterization of Tritium Uptake and Release by Inertial-Confinement Fusion Reactor Materials—James Fair (09-ERD-050)

Abstract

We will quantify the uptake and release of tritium by laser inertial-confinement fusion reactor materials for a range of surface preparation, exposure, and decontamination conditions. Data from this project will form the basis for designing and implementing tritium decontamination processes by systematically exploring its uptake and release in laboratory-scale packed-bed reactors and full-scale fusion-class laser optic enclosures. Key outputs will be mass transfer coefficients, other rate constants, and adsorption isotherms. The study will also characterize local electronic sensing as a method for directly measuring

surface tritium activity and seek measures to maximize the availability of fusion facilities, significantly decreasing operating costs.

We expect to create the ability to (1) predict tritium release rates under controlled decontamination conditions, (2) predict tritium uptake rates under known exposure conditions, and (3) accurately and precisely measure surface tritium concentration for inertial-confinement fusion reactor components using direct electronic sensing devices. These results will form the technical basis upon which reliable and safe tritium decontamination subsystems and processes for laser inertial-confinement fusion reactors can be efficiently developed, implemented, and controlled.

Mission Relevance

This project supports LLNL's national security mission by providing experimental data from fusion-class laser systems to validate complex coupled-physics computer simulations for stockpile stewardship. In addition, our research will substantially increase our understanding of the behavior of tritium and tritiated compounds as they interact with optical components associated with large inertial-confinement fusion laser systems.

FY10 Accomplishments and Results

In FY10 we (1) characterized the uptake and release behavior of stainless steel, copper, and silica over a range of initial exposure and subsequent purge conditions; (2) used the data to validate the general theoretical transport model for tritium developed in FY09 for aluminum; (3) expanded the number of convection models to include a wide range of enclosures, from small lab-scale up to the scale of the National Ignition Facility chamber; and (4) evaluated the effects of very-high-concentration tritium exposure on steel and copper and found good descriptions using the numerical transport model.

Proposed Work for FY11

In FY11 we will (1) study the effect of initial surface hydration on tritium uptake and determine activation energies for some of the dominant observed surface reactions between tritium and water; (2) more accurately identify some of the dominant surface reaction-rate mechanisms, with particular focus on the surface gas phase for water equilibrium relations and their role in determining net tritium removal during wet-air surface treatment; and (3) develop new and revised system-level numerical models for gas-handling systems.

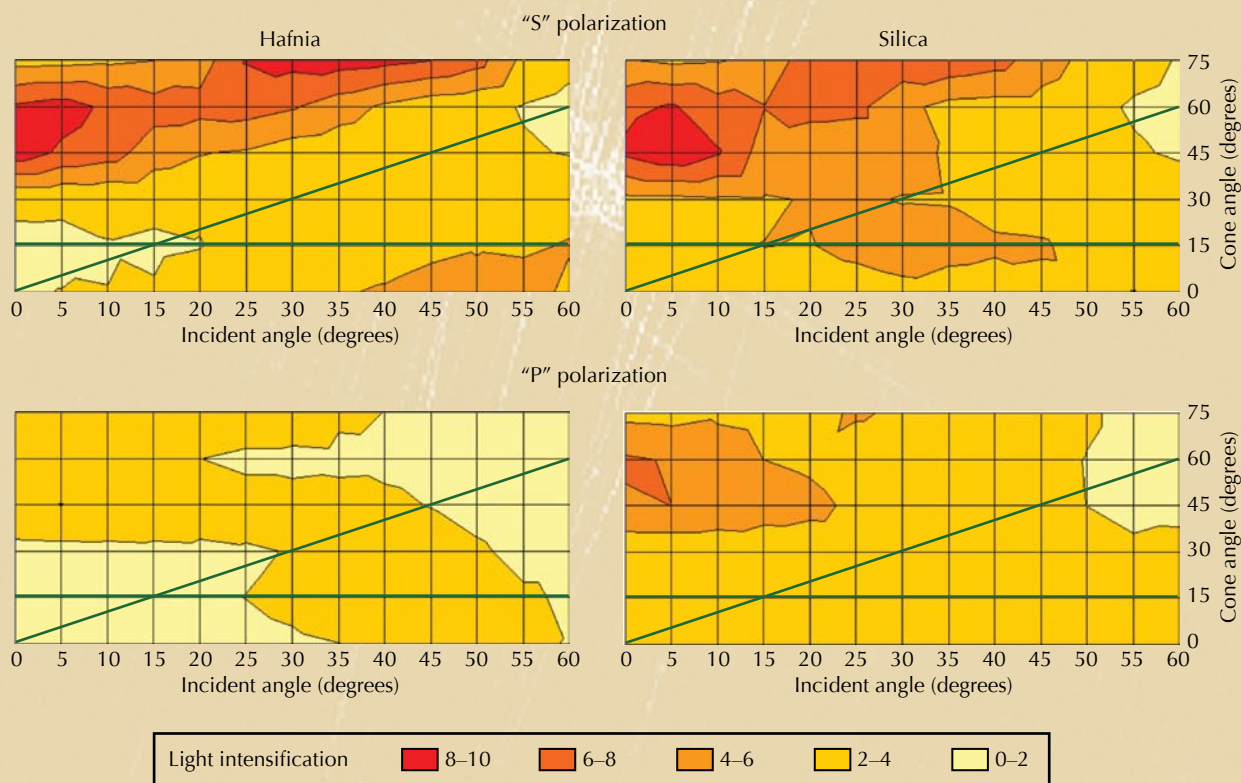
Methods for Mitigation of Damage to Multilayer Mirrors—Christopher Stolz (09-ERD-051)

Abstract

The objective of our proposed study is to develop methods to arrest damage growth in optical interference coatings. This damage is caused by laser-induced fracture and absorption from

sub-stoichiometric coating materials. Advancements to increase mirror fluence survivability have focused on material selection, absorption and defect reduction, and laser conditioning. Currently, state-of-the-art mirror coatings are limited by damage at a few growth sites, suggesting the possibility of a localized mitigation solution. We will explore laser- and mechanical-based mitigation methods coupled with an effort to understand thin-film properties, advanced electric-field modeling, and downstream-modulation modeling. We will validate site stability with laser damage testing and microscopy.

We expect to determine a thin-film mitigation process that will increase the resistance of laser transport mirrors to beam damage. Electric-field modeling will determine the proper film boundary to minimize electric-field effects. Beam-modulation modeling will determine the proper mitigation geometry for a reflective component. Once this process is established, it will be validated on mirrors suitable for use on fusion-class lasers. A second phase of this proposal will be devoted to reducing defects during coating deposition and an increased



Results of the computer simulation of light intensification within conical damage-mitigation features.

understanding of the role of substrate quality (scratches and digs) and subsurface damage on the resistance of mirrors to laser damage.

Mission Relevance

Transport mirrors are the fluence-limiting component in the fundamental wavelength section of advanced fusion-class lasers. Interest in reconfiguring these lasers to the second harmonic to realize even higher fusion gains elevates transport mirrors to the fluence-limiting optical component of the entire laser system. Fusion-class lasers are an essential tool for the Stockpile Stewardship Program and other national security applications, as well as for inertial-confinement fusion as an advanced concept for energy security and independence.

FY10 Accomplishments and Results

In FY10 we (1) designed a rotary vane filter to be installed in a coating deposition chamber to minimize coating defects, (2) procured hardware to build a microscope and laser ablation system to create particulates for study of their temperature and velocities, (3) demonstrated femtosecond laser-machining coating-mitigation sites at a laser intensity of 40 J/cm², (4) developed an electric-field model to optimize mitigation site geometry, and (5) discovered a correlation between scratch dimensions on coated mirrors and laser resistance, which can help develop scratch and dig specifications for substrates before coating.

Proposed Work for FY11

In FY11 we propose to (1) optimize the operational parameters of the newly constructed rotary vane particulate filter for minimizing coating defects, (2) optimize the laser plume-heating process to minimize coating defects, and (3) develop a femtosecond laser-machining damage-mitigation process, install it on a laser-conditioning station, and demonstrate the ability of a damage-mitigated large-aperture (40-cm) mirror to survive a laser intensity of at least 30 J/cm².

Publications

Qiu, S. R., et al., 2010. "Modeling of light intensification by conical pits within multilayer

high-reflector coatings." *Proc. SPIE* **7504**, 75040M. LLNL-CONF-420302.

Qiu, S. R., et al., 2010. "Searching for optimal mitigation geometry for multilayer high-reflector coatings." *Proc. Optical Interference Coatings 2010*. LLNL-ABS-423280.

Wolfe, J. E., S. R. Qiu, and C. J. Stolz, 2010. "Multilayer coating laser damage stabilization by femtosecond laser machining." *Proc. Optical Interference Coatings 2010*. LLNL-ABS-423126.

Wolfe, J. E., et al., 2010. "Laser damage resistant pits in dielectric coatings created by femtosecond laser machining." *Proc. SPIE* **7504**, 750405. LLNL-PROC-420294.

Biomolecule-Directed Synthesis of Highly Ordered, Nanostructured Porous Zinc Oxide—Thomas Han (09-LW-024)

Abstract

Zinc oxide (ZnO) is an n-type semiconductor with potentially important optical and piezoelectric properties. Despite these promising properties, progress in developing new applications for this material is limited by the current inability to control surface area and architecture. We propose to develop a new methodology to synthesize highly ordered, nanostructured ZnO with a high surface area. To this end, we will use a phage-display technique employing the M13 bacteriophage to identify unique sets of small peptides that can readily bind and nucleate ZnO nanocrystals. The identified peptides will be covalently bonded to structure-directing surfactants and polymers. The newly synthesized biopolymer will be used to template ZnO nanocrystals, which will adopt the three-dimensional structure of the self-assembling biopolymer.

If successful, this project will lead to highly ordered, high-surface-area, mesoporous ZnO, which could have many significant applications including ultraviolet-light-emitting diodes, lasers, photovoltaic solar cells, gas sensors, and biosensors. Furthermore,

this new synthetic technique can be extended to the generation of novel three-dimensional materials such as high-surface-area explosive and chemical-warfare sorbents, biocompatible porous solids for bone replacement, materials for fuel cells and photovoltaic solar cells, laser targets, and fracture-resistance shields and armor-plate materials. We also expect this work to generate high-profile publications.

Mission Relevance

This project supports LLNL's national security mission by creating a capability to generate new materials for fusion targets, explosive detectors, and sorbents, and it supports the energy security mission by helping synthesize novel materials for photovoltaic solar cells and fuel cells.

FY10 Accomplishments and Results

In FY10 we (1) successfully synthesized three-dimensional mesoporous ZnO nanostructures using amino-acid-based surfactants that we also synthesized; (2) systematically studied the effects of different amino acids during the synthesis of nanostructured ZnO and learned that depending on the amino acids employed, the newly synthesized surfactants were able to synthesize ZnO particles that were either spherical, filaments, or platelets; (3) identified peptide sequences that bind to ZnO nanoparticles, which will aid in controlling the nucleation and growth of one-dimensional ZnO; and (4) successfully synthesized high-surface-area ZnO using activated carbon aerogel as a hard template. This composite material has a surface area that ranges from 400 to 1500 m²/g, depending on the loading percent of ZnO. In addition, we fully removed carbon by heating at elevated temperatures to obtain pure ZnO. The successful conclusion of this project provided novel routes to synthesize various semiconductors with three-dimensional nanostructures, which can significantly impact various research efforts in solar energy, batteries, and catalysts. This project will be continued in collaboration with researchers at the University of California at Santa Barbara to further understand the roles of ZnO-binding peptides during

nucleation and growth of one-dimensional ZnO nanostructures.

Publications

Han, T. Y.-J., 2010. *Epitaxial growth mechanism of zinc oxide nanowires from solution on polycrystalline substrates*. 22nd Conf. Crystal Growth and Epitaxy—West, Fallen Leaf Lake, CA, June 6–9, 2010. LLNL-PRES-434135.

Han, T. Y.-J., et al., 2011. "Synthesis of ZnO coated activated carbon aerogel by simple sol–gel route." *J. Mater. Chem.* **21**, 330. LLNL-JRNL-457054.

Direct Observation of Phase Transformations and Twinning under Extreme Conditions: In Situ Measurements at the Crystal Scale—Joel Bernier (10-ERD-053)

Abstract

We will develop an experimental technique for the direct three-dimensional observation of mechanical twinning and crystal-lattice-distortion phase transformations—both of which affect equation of state, strength, and stiffness—in polycrystalline materials under high pressure and temperature in situ. Such in situ observations at the crystal scale are essential for motivating, validating, and verifying advanced constitutive models. We will study body-centered-cubic, hexagonal closely packed (HCP) phase transformations in iron by leveraging recent advances in synchrotron x-ray diffraction, and characterize the high-pressure HCP phase through direct observations. Experiments will take place at Argonne National Laboratory's Advanced Photon Source. Direct observations of these phenomena in situ at the crystal scale represent first-of-kind, discovery-class science.

We expect to develop a three-dimensional in situ characterization technique that determines (1) the orientations and centers of mass of parent and transformed regions in individual embedded grains, (2) full strain and stress tensors averaged over

these regions with a resolution of at least 10^{-4} , and (3) quasi-static thermo-mechanical loading in situ using a diamond anvil cell. This will provide direct variant selection, stress state, and growth measurements for the body-centered-cubic HCP phase transformation in individual grains embedded in an iron polycrystal; observations of mechanical twinning in HCP iron (if any); as well as material properties for the high-pressure HCP iron phase. These first-of-kind measurements will help determine the validity of constitutive models at high pressures.

Mission Relevance

High-fidelity materials models comprise a critical piece of the multiphysics simulation codes employed at LLNL in support of stockpile stewardship, particularly with respect to surety evaluation. This project will enable rigorous verification and validation of cutting-edge models at the crystal scale.

FY10 Accomplishments and Results

In FY10 we (1) conducted an in situ diamond anvil cell experiment in which the body-centered-cubic HCP phase transformation in iron was observed and characterized at ambient temperature; (2) carried out, in collaboration with researchers at Los Alamos National Laboratory, an in situ compression experiment in which hundreds of individual twinning events were detected in a sample of magnesium alloy; (3) created and released

data-reduction software for the fundamental compression experiment; and (4) published the results from both experiments in peer-reviewed journal articles.

Proposed Work for FY11

Our main objectives in FY11 are to (1) conduct additional diamond-anvil cell experiments on iron to assess the effects of initial dislocation content and temperature, (2) perform diamond-anvil cell experiments on cerium, and (3) extend the data-analysis methodology to include the effects of explicitly represented dislocation content, which is key for extracting critical strength measurements—specifically, we aim to extract enough information from the anisotropic spreading of an ensemble of diffraction spots to inform the evolution of densities of particular Burgers vectors, which quantify differences between the distorted lattice around the dislocation and the perfect lattice. Success in this task will enable forward-modeling efforts in the next phase.

Publications

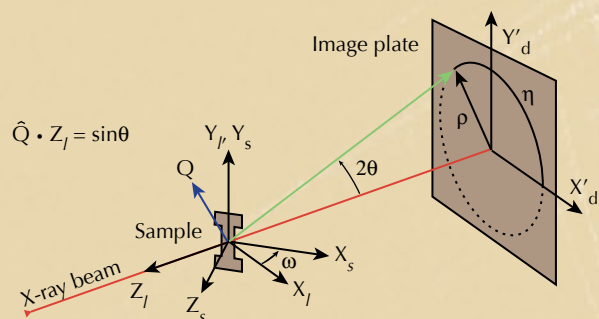
Bernier, J., et al., in press. "Far-field high-energy diffraction microscopy: A tool for intergranular orientation and strain analysis." *J. Strain Anal. Eng. LLNL-JRNL-466499*.

Edmiston, J., et al., 2011. "Precision of lattice strain and orientation measurements using high-energy monochromatic x-ray diffraction." *J. Appl. Crystallogr.* **44**(2). LLNL-JRNL-457412.

Material–Coolant Interactions in Fusion Reactors—Joseph Farmer (10-ERD-056)

Abstract

Inertial confinement and magnetic fusion technologies require high-performance coolant systems for removal of heat from the chamber wall. In some cases, the coolants are multifunctional, enabling heat transport away from the fusion reactor wall and providing a medium for breeding tritium.



Recent advances in three-dimensional x-ray diffraction, which allows for the identification and tracking of individual grains embedded in a polycrystal, are being leveraged to study hexagonal closely packed phase transformations in iron.

Liquid-phase coolants suitable for use at the extreme temperatures and irradiations expected in these reactors pose a serious threat to reactor materials, which include advanced steels, refractory metal alloys, and ceramic composites. Determining coolant–materials compatibility is critical for enabling fusion energy systems. We propose to evaluate materials damage and determine degradation mechanisms to provide an understanding of compatibility issues and how to resolve them. Our research will provide a comprehensive database to enable various coolant–material combinations to be assessed.

We expect to (1) assess the threat of corrosion, stress corrosion cracking, and hydrogen embrittlement in candidate reactor materials; (2) elucidate the mechanisms involved in degradation of these materials; (3) develop predictive models to explain observed phenomena, thereby demonstrating scientific understanding of compatibility issues; and (4) identify viable strategies for mitigating such attacks. Structural materials of interest include materials most likely to be used for construction of fusion reactor systems such as oxide dispersion-strengthened ferritic steels, refractory metal alloys, and silicon- and zirconium-carbide and composites of

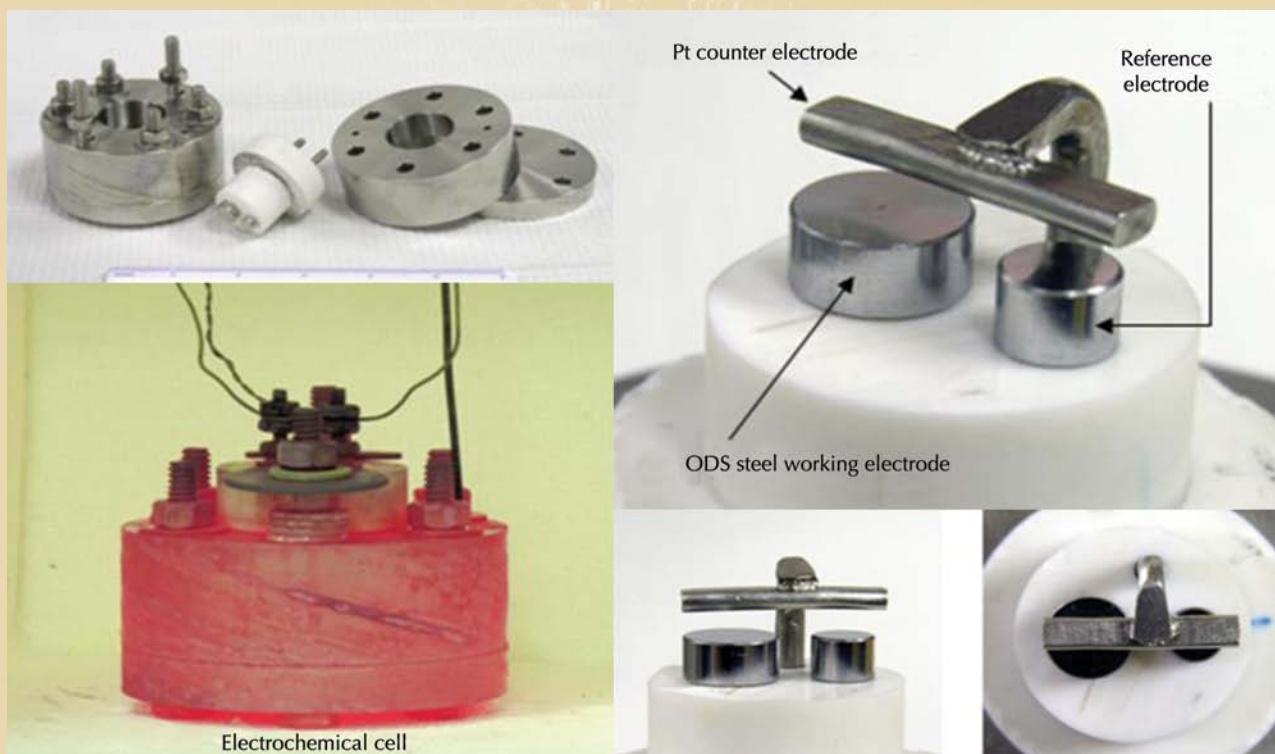
these materials. We will examine coolants of interest such as molten fluoride salts and liquid metals, including solutions of lead, bismuth, and lithium.

Mission Relevance

This project supports LLNL's mission of enhancing energy security for the nation and builds directly upon the Laboratory's world-class capabilities in fusion energy technologies. The proposed research is a key component of the Laboratory's strategic roadmap in energy security. Resolving key issues for practical, cost-effective fusion energy plants also supports the Laboratory mission in environmental security by enabling a source of abundant, clean power without nuclear waste disposal, safety, carbon sequestration, or proliferation issues.

FY10 Accomplishments and Results

In FY10 we (1) developed an in situ corrosion-characterization apparatus and technique to determine material behavior in molten salts at temperatures of up to 1,000°C; (2) applied this technique to oxide dispersion-strengthened steel and tantalum samples; (3) used Argonne National Laboratory's Advanced Photon Source synchrotron to gain



We developed the first high-temperature electrochemical cell designed for work with high-temperature molten fluoride salts. This cell enabled several in situ measurement techniques and devices including linear polarization, a zero-resistance ammeter, and electrochemical impedance spectroscopy.

insight into a previously undiscovered helium and nano-oxide interface; and (4) made preparations for lithium–lead interaction experiments, including obtaining the required raw materials.

Proposed Work for FY11

Our two main thrusts in FY11 will be corrosion-control experiments focused on oxide dispersion-strengthened steels and the tantalum–tungsten alloy, as well as simulating tritium—focusing on the effect of hydrogen on the metals. Specifically, we will build on our FY10 work to (1) study the effect of the reduction–oxidation reaction approach of adding selected metals to molten salt; (2) test strengthened material coated with tantalum, both with and without damage to the coating; (3) examine the interaction of the strengthened material and tantalum with lithium–lead coolant; (4) conduct hydrogen-charging experiments; (5) study the effect of temperature on hydrogen retention; and (6) determine the mechanical properties correlation with hydrogen content.

Publications

Farmer, J. C., 2009. *Structural materials and fission fuels for LIFE*. UCRL-TR-377784.

Farmer, J., et al., 2010. *Coolant compatibility studies for fusion and fusion–fission hybrid reactor concepts: Corrosion of oxide dispersion strengthened iron-chromium steels and tantalum in high temperature molten fluoride salts*. LLNL-TR-432011.

El-Dasher, B., et al., 2010. *Corrosion of oxide dispersion strengthened iron-chromium steels and tantalum in fluoride salt coolant: An in-situ compatibility study for fusion and fusion–fission hybrid reactor concepts*. LLNL-JRNL-432673.

Thermodynamic and Kinetic Modeling of Advanced Nuclear Fuels—

Patrice Erne Turchi (10-ERD-059)

Abstract

A key issue on the path to nuclear energy becoming an essential component of the U.S. clean energy strategy is complete burn of the nuclear fuel. We propose research that will enable high-burn-up fuels

by establishing the basic science for development and qualification of advanced nuclear fuel that will couple modern computational materials modeling, fabrication, and characterization capabilities with targeted performance-testing experiments using ion-beam facilities. This work will establish the scientific foundation and guide selection of the optimum fuel type for advanced reactor concepts.

We expect to experimentally quantify the phase stability and kinetics of phase transformations, interdiffusion, microstructural evolution, micro-mechanical properties, and the influence of severe radiation environments on fuel performance and, by the end of the project, develop a validated model for advanced nuclear energy materials under extreme conditions of radiation, temperature, and evolving chemistry. We will provide a science-based path forward to an optimized inert matrix fuel, while contributing to the development of a validated nuclear-fuel database. We expect this project will further establish LLNL's credibility in the nuclear energy community.

Mission Relevance

Our approach to advancing the science of advanced nuclear energy fuels aligns well with the Laboratory's energy and national security missions. Development of both advanced fuel cycles and hybrid fusion–fission concepts is inexorably intertwined with the same scientific challenges. This research will extend LLNL capabilities and further enable actinide and high-energy-density science, high-performance computing and simulation, energy manipulation, and capabilities to develop materials on demand.

FY10 Accomplishments and Results

In FY10 we (1) extended LLNL's phase-field code to make it fully compatible with the thermodynamic and kinetic databases used with the Thermo-Calc and DICTRA codes to predict microstructure evolution; (2) integrated a search algorithm into the thermodynamic software for predicting optimum composition of a multicomponent alloy with specific properties, such as melting temperature and phase fraction in the solid phase; (3) conducted ab initio studies of americium–plutonium, uranium–molybdenum, and neptunium–zirconium to predict phase

diagrams; (4) collaborated with scientists at Texas A&M University to study actinide-based alloys and conduct experiments on nuclear fuels in outer years; and (5) wrote two papers for publication in peer-reviewed journals and gave multiple invited presentations, including a plenary and a keynote address.

Proposed Work for FY11

Using metallic inert matrix fuels as our prototypical system, in FY11 we will (1) synthesize and characterize a series of actinide alloys including uranium–zirconium, uranium–plutonium–zirconium, plutonium–americium, and uranium–americium, as well as inert metallic matrix materials based on zirconium–iron–copper; (2) quantify phase stability, interdiffusion, and microstructural evolution when driven far from equilibrium with ion-beam facilities using both experiment and integrated first-principles thermodynamic and kinetic modeling; and (3) quantify the nonequilibrium inert matrix fuel behavior in the presence of fission products representative of ultrahigh burn-up.

Publications

Bajaj, S., et al., 2010. *Thermodynamic assessment of the Np–Zr and U–Ti phase diagrams*. Nuclear Materials 2010, Karlsruhe, Germany, Oct. 4–7, 2010. LLNL-ABS-439095.

Landa, A., P. Söderlind, and P. E. A. Turchi, 2010. *Density-functional study of the U–Zr and U–Mo alloys*. Nuclear Materials 2010, Karlsruhe, Germany, Oct. 4–7, 2010. LLNL-ABS-430211.

Landa, A., P. Söderlind, and P. E. A. Turchi, in press. “Density-functional study of U–Mo and U–Zr alloys.” *J. Nucl. Mater.* LLNL-JRNL-461538.

Landa, A., et al., 2011. “Density-functional study of bcc Pu–U, Pu–Np, Pu–Am, and Pu–Cm alloys.” *J. Nucl. Mater.* **408**(1), 61. LLNL-JRNL-441353.

Turchi, P. E. A., et al., 2010. *Thermodynamic assessment of advanced nuclear forms*. 10th

Intl. Workshop on Fundamentals of Plutonium Science, Moscow, Russia, July 12–16, 2010. LLNL-ABS-428973.

Development of High-Performance Lead-Free Solders for Microelectronics and Semiconductor Applications—John Elmer (10-LW-002)

Abstract

The international effort to replace lead-containing solders has resulted in the development of a wide variety of solders based on low-melting-point alloys of tin. Intermetallic phase formation in these alloys and difficult nucleation of beta-tin during solidification result in large and undesirable anisotropic grains with poor mechanical properties. Long-term reliability of these joints is a serious concern for military and high-performance applications. We propose to develop synchrotron methods for in situ investigations of microstructure evolution in tin and lead-free solders. This work will be carried out at the Advanced Photon Source at Argonne National Laboratory, leveraging existing equipment from a previous program funded by the Office of Basic Energy Science.

We expect to develop a new characterization tool using in situ x-ray diffraction to directly observe solidification, phase transformation, and intermetallic compound growth between lead-free solders and substrates of copper and copper metallized with nickel and gold. We will investigate different commercial lead-free solders of tin alloys with silver and copper and compare to pure tin to determine effects of alloying content on the resulting microstructure. We anticipate that these tin-based solders will display large under-cooling (the difference between the melting temperature and temperature at solidification) that will be related to large grain sizes and nonequilibrium formation of undesired microconstituents. Results will guide future work directed at developing high-performance lead-free solders.

Mission Relevance

Our project supports the Laboratory mission of ensuring the safety, security, and reliability of the U.S. nuclear deterrent. Mission-critical solder joints used in weapons systems must be extremely reliable over a much longer period of time than is required for conventional consumer electronics. Solder compositions, techniques, pad metallization, and inter-metallic compound formation are all of concern. In addition, conventional solder packaging of diode arrays is insufficient for reliable operation of future fusion energy sources, and advanced laser targets and holders have important thermal and mechanical solder joints.

FY10 Accomplishments and Results

In FY10 we developed an experimental method using in situ x-ray diffraction to directly observe phase transformations in solder alloys. This experimental technique was verified at the Advanced Photon Source synchrotron, where we ran in-situ x-ray diffraction experiments on tin and indium, which are base elements for lead-free solders, to directly observe under-cooling and microstructure formation in this important alloy system. Results were collected for tin and indium on graphite (non-wetting), copper, and gold-coated copper substrates. Under-coolings up to 50°C were observed for tin, but much less for indium. During this run of experiments, we also performed tests to directly observe the sintering kinetics of silver nano-ink with in-situ x-ray diffraction methods and successfully accomplished the first in-situ observations.

Proposed Work for FY11

We will conduct a second synchrotron run at the Advanced Photon Source with the experimental setup developed in FY10 to gather more statistics on pure tin and tin-rich alloys. We will also use and assess micro-alloying methods to evaluate the effects of nanometer-scale particulates and other nucleants at reducing under-cooling in tin and tin-rich alloys for microstructural refinement.

Publications

Elmer, J. W., and E. D. Specht, 2010. "Direct observations of silver nanoink sintering and eutectic remelt reaction with copper." *Scripta Mater.* **63**(12), 1224. LLNL-JRNL-446113.

Elmer, J. W., and E. D. Specht, 2010. "Measurement of Sn and In solidification undercooling and lattice expansion using in-situ x-ray diffraction." *J. Electron. Mater.* **40**(2), 201. LLNL-JRNL-435591.

In Situ Spectroscopy and Microscopy for the Study of Advanced Materials for Energy Storage—Jonathan R. Lee (10-LW-045)

Abstract

This project is designed to apply a suite of in situ x-ray spectroscopy and electron microscopy techniques to investigate the performance of advanced materials for energy storage, specifically electrodes based on group IV element nanocrystals and capacitors based on nanoporous carbon. The development of new materials for energy storage is essential for securing the nation's energy future, and characterization of the chemical and physical phenomena that occur during charge transfer processes is a key component of this endeavor. Our studies will yield insight into the evolution in electronic and geometrical structures of the nanostructured materials during cycling, which is key to identifying the mechanisms of energy storage and electrode degradation, as well as improving the design of next-generation materials.

If successful, we expect that the project will yield information regarding the mechanisms of energy storage in nanostructured electrodes and their degradation with repeated charge and discharge cycling. Complementary specific-charge measurements will allow determination of the effects of surface chemistry, structure, and interfacial properties on electrode performance. All of this information will have significant impact in the field of electrical energy storage and on the design of next-generation electrode

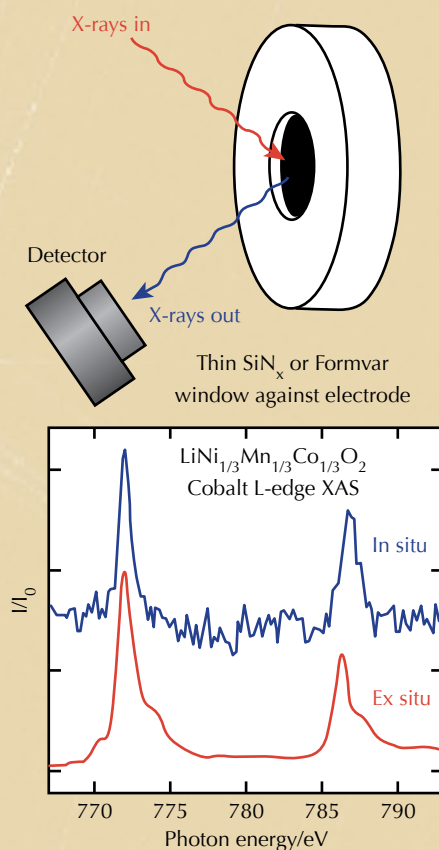
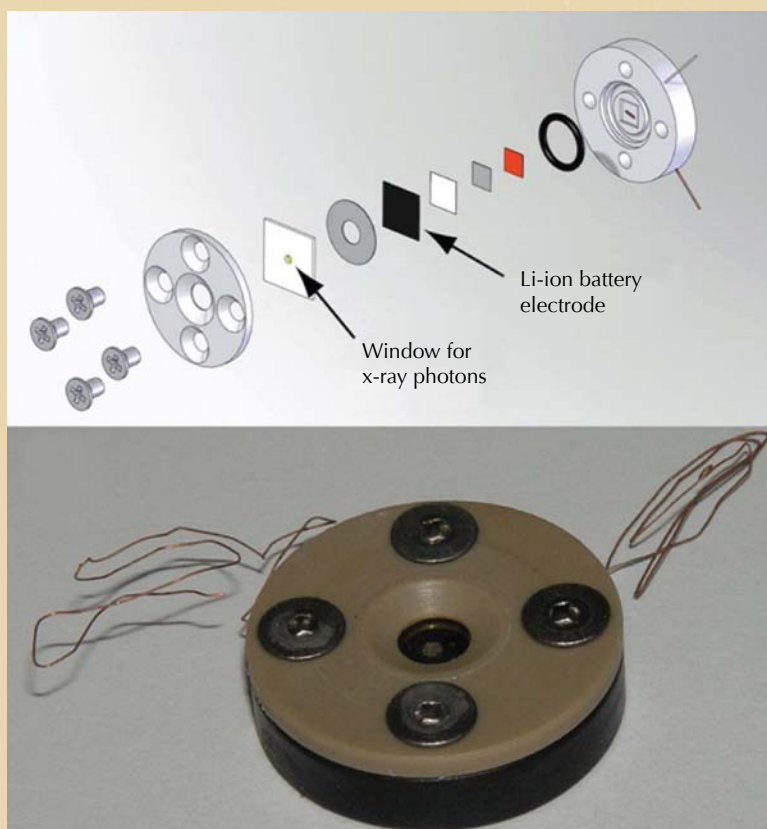
materials. We will also gain insight into the modes and mechanisms of energy storage by nanoporous materials, which show great promise in capacitive energy storage applications. Finally, we will demonstrate the enormous potential of a suite of unique in situ analysis tools.

Mission Relevance

This project supports a core Laboratory mission to enhance the energy and environmental security of the nation. Moreover, it is aligned with future research needs that were defined by a recent DOE Office of Basic Energy Sciences study on electrical energy storage—specifically, the need to implement new in situ techniques to investigate chemical, electrochemical, and physical processes at solid–liquid and solid–gas interfaces.

FY10 Accomplishments and Results

In FY10 we successfully (1) designed and implemented a new experimental cell for in situ, high-resolution x-ray spectroscopy; (2) used in situ and ex situ x-ray spectroscopy to characterize the electronic and geometrical structures of a series of lithium battery anodes and cathodes—including group IV nanocrystalline anodes and transition-metal oxide cathodes—as a function of charge and discharge cycling, thus achieving the first-ever measurements of lithium soft x-ray emission and the first-ever in situ soft x-ray studies of battery materials in a liquid environment; (3) conducted concurrent in situ and ex situ transmission electron microscopy imaging of some of the electrode materials; and (4) carried out x-ray spectroscopy studies of nanoporous carbon—including samples functionalized with surface coatings deposited by atomic layer deposition—for capacitive energy storage.



The experimental cell (left) developed in this project is used to gain new insight into the behavior of energy-storage materials under operating conditions using soft x-ray spectroscopic measurements (right).

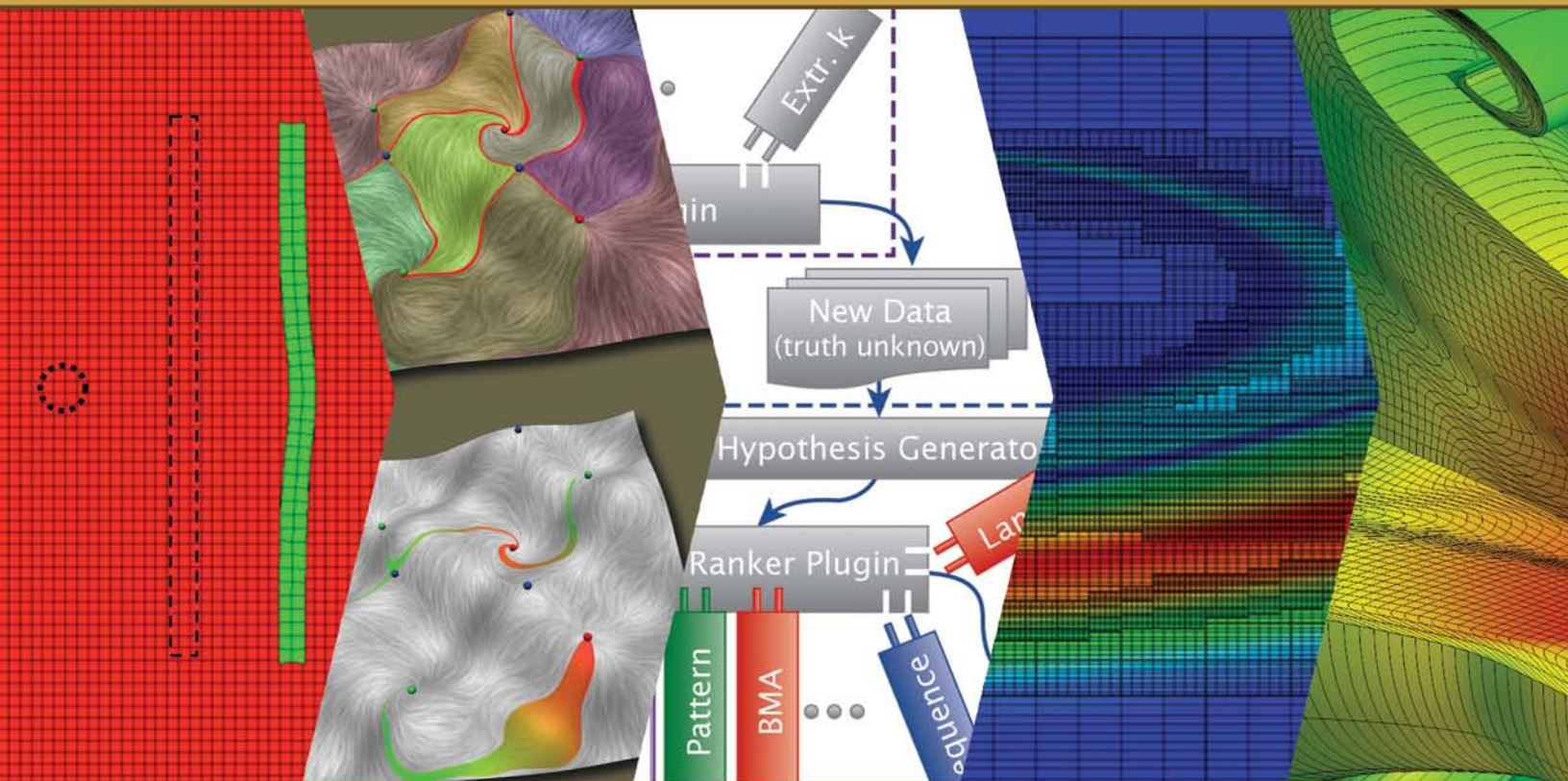
Proposed Work for FY11

In FY11 we propose to (1) continue in situ x-ray spectroscopy and transmission electron microscopy studies of the novel electrode materials for rechargeable lithium-ion batteries, building upon experiments conducted in FY10; (2) apply the lithium x-ray spectroscopy capability to these studies, including the first measurements of x-ray absorption and in situ soft x-ray spectroscopy of lithium; and (3) conduct in situ x-ray spectroscopy and electron microscopy studies of nanoporous carbon electrodes for capacitive energy storage.

Publications

Lee, J. R. I., et al., 2010. *X-ray spectroscopy for the investigation of advanced materials for electrical energy storage*. 37th Intl. Conf. Vacuum Ultraviolet and X-ray Physics, Vancouver, Canada, July 11–16, 2010. LLNL-PRES-462146.

Lee, J. R. I., et al., 2010. *X-ray spectroscopy for the investigation of advanced materials for electrical energy storage*. Advanced Light Source Users Meeting, Berkeley, CA, Oct. 13–15, 2010. LLNL-PRES-462146.



Mathematics and Computing Sciences

Storage-Intensive Supercomputing— Maya Gokhale (07-ERD-063)

Abstract

This project addresses the efficient computation of data-intensive problems in national security and basic science by advancing storage-intensive supercomputing capabilities. We propose to (1) develop new algorithms and applications to solve large-scale data analytics problems on this emerging class of architectures; (2) explore new programming models, tools, and libraries to address the difficulty in developing software applications for storage-intensive architectures; (3) develop new system architectures for storage-intensive supercomputing in partnership with industry collaborators; and (4) enable an order-of-magnitude improvement in price and performance over today's architectures for a broad range of data-intensive problems.

Across the Laboratory, and in the scientific and national security communities at large, scientists and analysts are searching for techniques, tools, and computing architectures to manage and analyze large 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. 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

Efficient computation of data-intensive problems is relevant to the Laboratory mission in cyber and space security and intelligence, as well as the large-scale analysis of data generated by simulation or experiments for myriad additional Laboratory efforts. 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.

FY10 Accomplishments and Results

We (1) assembled a hardware test bed—a small set of nodes containing node-local nonvolatile memory and coprocessors; (2) used the test bed to evaluate a new asynchronous, highly concurrent programming model for graph search problems, and showed that it is possible to process graphs more quickly on a node with 16 GB of memory and flash storage than on a node with 256 GB of memory; (3) presented our experiments on the test bed in two conference publications; (4) demonstrated applications in cybersecurity using field-programmable gate arrays to accelerate network packet classification, including an application that can classify multimedia packets at 80 GB per second; and (5) optimized the metadata-rich, query-oriented file system and evaluated it in intelligence analysis and scientific data management. In summary, this project demonstrated the benefits of incorporating node-local, nonvolatile storage, with implications for exascale systems, and further demonstrated extreme performance acceleration with coprocessors of network packet classification for cybersecurity. New efforts that will continue this research include Office of Science projects in node-local storage for exascale architectures, fault-oblivious operating environments for exascale architectures, and data management in exascale environments.

Publications

Ames, S., M. Gokhale, and C. Maltzahn, 2010. *Design and implementation of a metadata-rich file system*. LLNL-TR-422677.

Jiang, W., and M. Gokhale, 2010. *Real-time classification of multimedia traffic using FPGA*. 20th Intl. Conf. Field Programmable Logic and Application, Milano, Italy, Aug. 31–Sept. 2, 2010. LLNL-CONF-426266.

Khan, F., M. Gokhale, and C.-N. Chuah, 2010. *FPGA-based real-time network traffic analysis using traffic dispersion patterns*. 20th Intl. Conf. Field Programmable Logic and Application, Milano, Italy, Aug. 31–Sept. 2, 2010. LLNL-CONF-426380.

May, J., 2009. *Pianola: A script-based I/O benchmark*. 3rd Petascale Data Storage Workshop, Austin, TX, Nov. 17, 2008. LLNL-CONF-407121.

Molina-Estolano, E., et al., 2009. *Mixing Hadoop and HPC workloads on parallel file systems*. 4th Petascale Data Storage Workshop, Portland, OR, Nov. 14–20, 2009. LLNL-CONF-416890.

Molina-Estolano, E., et al., 2010. *Performance analysis of mixed distributed filesystem workloads*. 2010 ACM/IEEE Conf. Supercomputing, New Orleans, LA, Nov. 13–19, 2010. LLNL-CONF-416890.

Pearce, R., M. Gokhale, and N. Amato, 2010. *Multithreaded asynchronous graph traversal for in-memory and semi-external memory*. 2010 ACM/IEEE Conf. Supercomputing, New Orleans, LA, Nov. 13–19, 2010. LLNL-CONF-427572.

Top, P., and M. Gokhale, 2009. *Application experiments: MPPA and FPGA*. Intl. Conf. Engineering of Reconfigurable Systems and Algorithms, Las Vegas, NV, July 13–16, 2009. LLNL-CONF-409662.

Ulmer, C., and M. Gokhale, 2010. *A configurable hardware document-similarity classifier to detect Web attacks*. 25th IEEE Intl. Parallel and Distributed Processing Symp., Anchorage, AK, May 16–20, 2010. LLNL-CONF-420263.

Ulmer, C., et al., 2010. "Massively parallel acceleration of a document-similarity classifier to detect Web attacks." *J. Parallel Distr. Comput.* **71**(2), 225. LLNL-JRNL-422668.

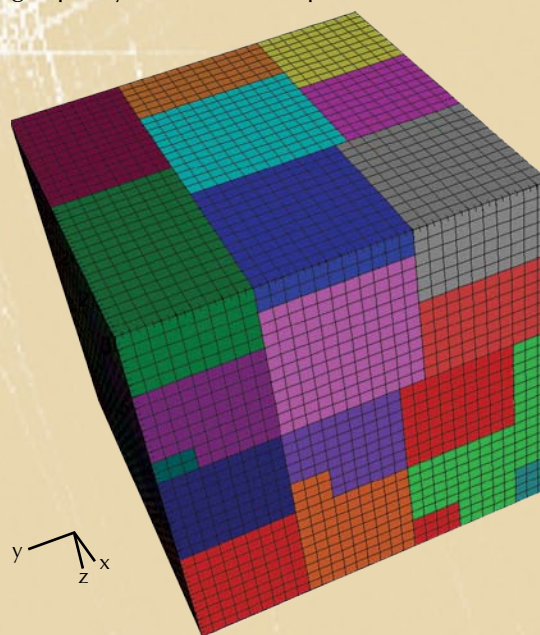
New Algorithms to Scale Domain Decomposition Up to BlueGene Architectures—David Hysom (08-ERD-014)

Abstract

We propose to develop novel mesh-partitioning algorithms and software for supercomputer simulations that are scalable for more than 100,000 processors and deliver higher-quality results than the current state of the art. In a typical numerical

simulation, a physical object being studied, often comprised of one or more computational domains, is first discretized to a model that computers can understand. The physical domain is often represented in a form of grid called a mesh. As the size of the mesh increases and requires more memory than a single-processor possesses, the computational mesh must be partitioned and these partitions must then be distributed across the available processors. 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. The amount of parallelism and inter-processor 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, which is only an eighth of the available processors, simulations are slowed by a factor of two or more simply from load imbalance and communication.

We expect to deliver production-quality code that produces higher-quality domain decompositions for applications of Laboratory relevance and that are scalable to the full BlueGene/L and Dawn machines. High-quality domain decompositions will translate



Novel brick-coarsening mesh partitioning reduces communication costs for supercomputer simulations.

directly into better load balance and more efficient use of the machine. Multi-block 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 LLNL's sustained preeminence in the field of stockpile stewardship simulations.

FY10 Accomplishments and Results

We have measured the performance and scalability of our proposed method using a set of large complex data sets, where we have scaled to a mesh with 110 million zones using our method. To the best of our knowledge, this is the largest complex mesh to which a partitioning method has been successfully applied. Specific accomplishments in FY10 include (1) obtaining results for up to 32,000 processors on BlueGene/L, (2) completing our partitioning library, and (3) developing an application programming interface for interfacing our partitioning library with programmatic codes. The successful conclusion of this project resulted in a novel "brick coarsening" mesh-partitioning method that is scalable to (at least) 32,000 processors, and produces higher-quality partitions, with fewer edge cuts, than other widely used methods. Our mesh-partitioning method achieves good load balancing by clustering neighboring zones into equal-sized blocks called bricks. More importantly, the algorithm reduces the inter-processor communications by laying out the bricks in an offset manner, similar to conventional brick laying in masonry. Our library is being used

and refined in conjunction with the mesh quality improvement toolkit MESQUITE, developed with support of the Office of Science Scientific Discovery through Advanced Computing.

Publications

Yoo, A., D. Hysom, and B. Gunney, 2010. *A novel coarsening method for scalable and efficient mesh generation*. LLNL-TR-463495.

Robust Ensemble Classifier Methods for Detection Problems with Unequal and Evolving Error Costs—Barry Chen (08-ERD-022)

Abstract

Computer and electronic detection applications involving counterterrorism or nonproliferation are often characterized by unequal and evolving costs (i.e., consequences) for false alarms and missed detections. Conventional statistical classifiers do not adequately address these issues. To solve these problems, 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 to deliver a 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 unequal or evolving misclassification costs and unbalanced training data. The resulting methodology will significantly advance the state of the art in classification technology, in terms of both detection performance and insight into the effects and interactions of design factors. The capability to solve detection problems of this type has broad applicability to many mission-relevant applications.

Mission Relevance

The ensemble classifiers developed in this project can be broadly applied to a wide range of objectives in LLNL's counterterrorism and nonproliferation missions, including the detection of (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.

FY10 Accomplishments and Results

In FY10 we (1) developed new ensemble classifiers that can incrementally adapt to changing costs as well as data distributions to maintain high classification performance—our system is based on adaptive probability density estimation provided by an ensemble of tree-based histograms; (2) demonstrated, by combining multiple base classifier types with varied splitting criteria, modest improvements in classification performance; (3) applied these classifiers to address cyber security applications where data are imbalanced and misclassification costs are asymmetric; and (4) developed a software toolbox of our classifiers, which includes a user's manual, for use by customers within the Laboratory as well as DOE. The successful conclusion of this project resulted in the development of a family of new classification systems delivering robust, high-performance, easy-to-use solutions for detection problems involving unequal misclassification costs and evolving data. These systems represent the state of the art in classification technology and are now being successfully applied to many programmatic applications of importance to the Laboratory including detection of cyber threats, hidden signals, radiation threats, and high explosives.

Publications

Chen, B. Y., T. D. Lemmond, and W. G. Hanley, 2009. "Building ultra-low false alarm rate support vector classifier ensembles using random

subspaces." *Proc. IEEE Symp. Computational Intelligence and Data Mining*. LLNL-CONF-407542.

Prenger, R. J., et al. 2010. "Class-specific error bounds for ensemble classifiers." *Proc. 16th ACM SIGKDD Intl. Conf. Knowledge Discovery and Data Mining*, p. 843. LLNL-CONF-417778.

Enhanced Event Extraction from Text Via Error-Driven Aggregation Methodologies—Tracy Lemmond (08-ERD-023)

Abstract

Knowledge discovery systems construct massive information repositories via the extraction of events from unstructured text and are highly vulnerable to extraction errors. We propose to enhance performance of the data-ingestion process via an aggregate meta-extraction capability, leading to reliable downstream inference in support of counterterrorism and nonproliferation efforts and, more generally, to a fundamental breakthrough in natural language processing and knowledge discovery. Our approach builds probabilistic models of errors made by a suite of existing base extractors and quantifies the impact of these errors on downstream inference. This will be used to optimally combine the extractors, reinforcing individual strengths and mitigating weaknesses.

Our research will yield a methodology for probabilistically characterizing error processes underlying knowledge discovery, providing vital insight into the expected reliability of knowledge discovery systems. This will serve as a foundation for developing the aggregate meta-extraction system, which we expect to substantially improve the accuracy rate of current state-of-the-art methods. The significant resources invested by LLNL and its customers over the last decade in knowledge discovery systems demand higher-quality data ingestion, along with a more thorough understanding of their performance and reliability. Moreover, because our approach incorporates existing tools, we can leverage the considerable

investments made in the academic and commercial sectors over the prior decades.

Mission Relevance

Lawrence Livermore is developing systems to assemble information from multiple information and intelligence sources in support of its national 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.

FY10 Accomplishments and Results

In FY10 we completed the development of a flexible aggregation framework for combining named entity extractors. The framework integrates a collection of novel aggregation algorithms, each of which incorporates a variety of machine-learning and probabilistic methods that utilize different underlying models, including one that leverages temporal textual information to improve aggregation under conditions of sparse data. The developed system, named Extraction Manager, optimizes the deployment of these algorithms in an operational setting and is highly extensible to permit

relationship extractor aggregation to be integrated when the technology becomes available in the future. Extraction Manager is also designed to serve as a plug-in architecture so that new extractors, aggregation algorithms, and language modules can be readily incorporated into the system to enhance performance. We have filed a provisional patent on this work and published our results. The next step is identifying potential industrial partners while also pursuing existing opportunities for follow-on funding for additional research on this technology.

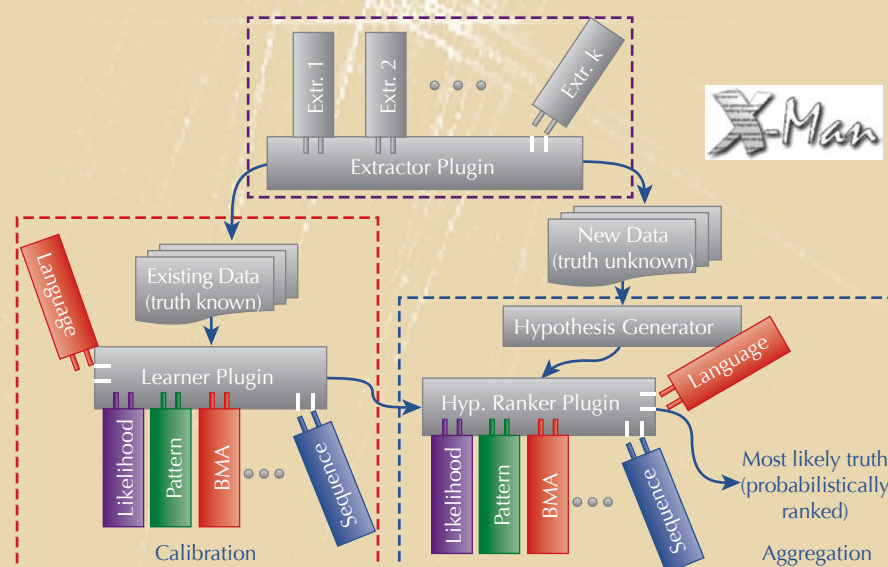
Publications

Glaser, R., et al., 2010. *Pattern-based aggregation of named entity extractors*. 2011 SIAM Intl. Conf. Data Mining, Mesa, AZ, April 28–30, 2010. LLNL-CONF-455911.

Hanley, W., et al., 2010. *Staged aggregation of named entity extractors*. LLNL-TR-463352.

Kidwell, P., et al., 2010. *Bayesian model averaging of named entity extraction algorithms*. LLNL-TR-456693.

Lemmond, T., et al., 2010. "Enhanced named entity extraction via error-driven aggregation." *Proc. 2010 Intl. Conf. Data Mining*, p. 31. LLNL-CONF-424662.



Conceptual diagram of the Extraction Manager aggregation framework develop with this project.

Scalable Methods for Discrete-Ordinate Transport Algorithms on Massively Parallel Architectures—Robert Falgout (08-ERD-026)

Abstract

We propose to develop parallel multilevel solutions for the mono-energetic Boltzmann transport equations on inner neutron iteration and lambda iteration for x rays. Our algorithms 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 that will be developed in this project have the potential to greatly improve the robustness and efficiency of these codes.

FY10 Accomplishments and Results

In FY10 we (1) recast our space-angle semi-coarsening multigrid method in terms of the full discrete-ordinate linear system to enable the possibility of algebraic approaches for solving Boltzmann equations, which will be useful in unstructured grid

settings where geometrically coarsening the spatial grid may not be feasible; (2) related our geometric method to a Galerkin coarsening approach for the (dense) scalar flux equations and showed that fairly simple interpolation operators can be used, which enables an alternative for developing algebraic approaches; and (3) developed parallel sweep algorithms and corresponding parallel performance models for long characteristics discretizations of the Boltzmann equations and showed that the asymptotic performance of this algorithm is similar to the kernel-boundary alignment algorithm, but there are no stages with idle processors. Using this algorithm as a pre-conditioner for standard discrete-ordinate discretizations may serve as a scalable approach for inverting the streaming operators on unstructured grids. The successful conclusion of this project enabled scalable and robust multigrid methods for solving the mono-energetic Boltzmann equations and established the scaling properties of sweep algorithms on hundreds of thousands of processors. Livermore's Advanced Simulation and Computing Program is supporting the deployment of our sweep algorithms to improve the scaling behavior of some of their codes, and there is interest in further development of an algebraic variant of our multigrid solver.

Publications

Bailey, T. S., and R. D. Falgout, 2009. "Analysis of massively parallel discrete-ordinates transport sweep algorithms with collisions." *Proc. Intl. Conf. Mathematics, Computational Methods, and Reactor Physics*. American Nuclear Society, LaGrange Park, IL. LLNL-CONF-407968.

Lee, B., 2010. "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." *SIAM J. Sci. Comput.* **31**, 4744. LLNL-JRNL-409949.

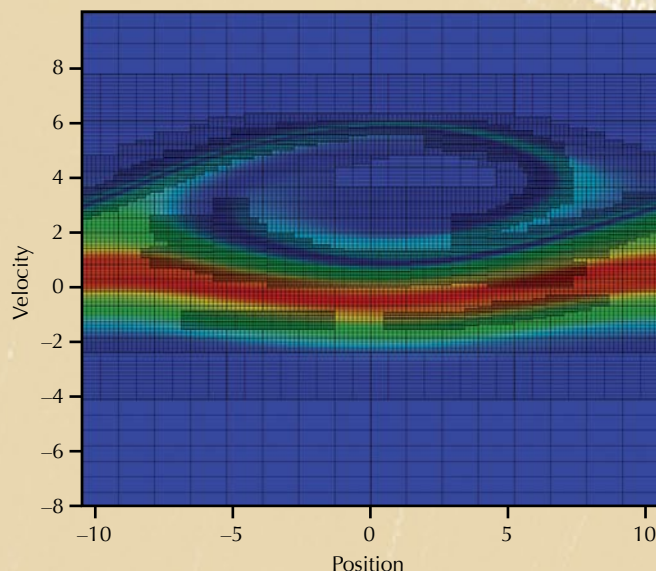
Lee, B., 2010. "Improved multiple-coarsening methods for Sn discretizations of the Boltzmann equation." *SIAM J. Sci. Comput.* **32**, 2497. LLNL-TR-409109.

Efficient Numerical Algorithms for Vlasov Simulation of Laser–Plasma Interactions—Jeffrey Hittinger (08-ERD-031)

Abstract

The objective of this project is to develop efficient, high-fidelity continuum algorithms for the Vlasov–Maxwell system that will facilitate routine laser–plasma interaction simulations. For more efficient designs of laser-driven high-energy-density experiments, noiseless simulations based on continuum models are required to predict the nonlinear onset and behavior of stimulated plasma instabilities. Continuum Vlasov simulations are very expensive computationally because they require discretization in a high-dimensional phase space. We will investigate the use of adaptive mesh refinement in phase space as well as the use of nonlinear, high-order algorithms to reduce the cost and improve the 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- to 48-hour runs on 128 processors) and groundbreaking 6D Vlasov simulations on Livermore’s massively parallel



Adaptive mesh Vlasov–Poisson results for a strongly driven bump-on-tail instability problem. With the new technique, the simulation uses 69% fewer cells (approximately 40,000) than are used with the equivalent uniform fine grid.

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.

FY10 Accomplishments and Results

In FY10 we (1) extended a 2D single-level and single-species, fourth-order, finite-volume Vlasov–Poisson simulation capability to 4D; (2) generalized the Poisson model to a full Maxwell electromagnetic model; (3) devised a new low-dissipation, oscillation-suppressing finite-volume algorithm; (4) developed diagnostics; (5) applied the single-level code to a study of linear and nonlinear electron plasma wave bowing; (6) implemented a 2D multispecies, adaptive mesh refinement Vlasov–Poisson model based on these algorithms; (7) initiated performance studies of both the single-level and adaptive mesh codes; and (8) published a peer-reviewed journal article on our new discretization and gave conference presentations on our algorithms and electron plasma wave simulations.

Proposed Work for FY11

In FY11 we will (1) complete the 5D and 6D implementations, (2) apply the codes to more physically motivated verification problems, (3) continue performance and scalability studies in several dimensions, and (4) prepare publications on algorithmic performance and new physics results.

Publications

Banks, J. W., and J. A. F. Hittinger, 2009. *Adaptive and high-order methods for laser–plasma interaction problems*. IMACS World Conference on

Computational and Applied Mathematics in Science and Engineering, Athens, GA, Aug. 3–5, 2009. LLNL-ABS-413421.

Banks, J. W., and J. A. F. Hittinger, 2010. "A new class of nonlinear finite-volume methods for Vlasov simulation." *IEEE Trans. Plasma Sci.* **38**, 2198. LLNL-JRNL-420843.

Banks, J. W., et al., 2009. *VALHALLA: An adaptive, continuum Vlasov code for laser-plasma interaction*. 39th Ann. Anomalous Absorption Conf., Bodega Bay, CA, June 14–19, 2009. LLNL-POST-413664.

Cohen, B. I., 2009. "Stimulated Brillouin backscattering and ion acoustic wave secondary instability." *Phys. Plasmas* **16**, 032701. LLNL-JRNL-407238.

Cohen, B. I., et al., 2009. "Erratum: Stimulated Brillouin backscattering and ion acoustic wave secondary instability." *Phys. Plasmas* **16**, 089902. LLNL-JRNL-412473.

Cohen, B. I., et al., 2009. "Stimulated Brillouin backscattering and ion acoustic wave secondary instability." *Phys. Plasma.* **16**, 032701. LLNL-JRNL-407238.

Hittinger, J. A. F., et al., 2010. *Beyond 1D: algorithmic advances for more tractable Vlasov simulation*. 40th Ann. Anomalous Absorption Conf., Snowmass Village, CO, June 13–18, 2010. LLNL-ABS-429862.

Hittinger, J. A. F., et al., 2010. *Two-dimensional Vlasov simulation of driven, nonlinear electron plasma waves*. 40th Ann. Anomalous Absorption Conf., Snowmass Village, CO, June 13–18, 2010. LLNL-ABS-429863.

Understanding Viral Quasi-Species Evolution through Computation and Experiment—Carol Zhou (08-ERD-036)

Abstract

Our objective is to produce a computational model of genetic-state change that will provide insight into the RNA virus genomic shift and enable a testable hypothesis of viral evolution. Because of

their extreme rate of evolution, RNA viruses rapidly adapt to medical countermeasures. Our work will have applications in vaccine and therapeutic development. We are designing and implementing a novel computational methodology for stochastic simulation of genetic-state migration during cellular replication of RNA viruses, where point mutations and homologous recombination events drive genetic shift under various selection pressures. Our collaboration with a virologist will provide empirical data for model validation and hypothesis testing.

We expect to develop a novel research tool that will enable us to understand how RNA viruses evolve and adapt and become resistant to vaccines and antiviral drugs. Using this tool, we will be able to conduct experiments to understand the basis of rapid mutation, recombination, and viral quasi-species memory—which enable reversion of vaccine strains to infectious wild types—and to understand mechanisms of the emergence of new agents of human and animal disease. The results from our modeling and simulations will enable development of new biodefense technologies by providing key insight into how viruses adapt and evolve under different selective pressures and help us determine the limits of genome variability constrained by host factors, such as the heat shock protein Hsp90 protein-folding machinery.

Mission Relevance

This project supports the Laboratory's missions in national and homeland security by applying advanced computing to the identification, characterization, and simulation of virulence mechanisms to increase our understanding of virulence and the evolution of pathogenicity for efforts in countering bioterrorism.

FY10 Accomplishments and Results

In FY10 we designed and developed (1) a novel algorithm for sensitive detection of sequence-structure motifs and key residues by robust filtering of structures (StralSV), (2) an algorithm for detecting and characterizing unusual mutations in the structure-sphere context (Spherical-StralSV), (3) an algorithm for identifying residues in a protein structure that are in close contact (Acheck), and (4) a stochastic model for picornavirus genetic state-change

applied to the Sabin (vaccine strain) to Mahoney (wild type) transition. Because our collaborator at the University of California at San Francisco shifted direction to pursue technologies for deep sequencing of viral quasi-species, we shifted our emphasis from the Hsp90 protein to the poliovirus polymerase, which became our primary subject for algorithm validation. A record of invention covering our algorithms is in preparation. In addition, the Transformational Medical Technologies program of the Department of Defense Threat Reduction Agency will sponsor the three-year Protein Function Prediction Platform project to support continued research and development of computational methods for protein structure characterization and function prediction that will employ and further extend bioinformatics methods we developed in this project.

Publications

Anisimov, A., et al., 2010. "Amino acid and structural variability of *Yersinia pestis* LcrV protein." *Infect. Genet. Evol.* **10**, 137. UCRL-JRNL-420969.

Kostova T., C. Zhou, and A. Zemla, in press. "On the role of degradation rates for the dominance of the fittest in Eigen's quasispecies model." *J. Biological Dynam.* UCRL-JRNL-439096.

Zemla, A., et al., 2010. *StralSV: assessment of sequence variability within similar 3D structures and application to polio RNA-dependent RNA polymerase*. UCRL-JRNL-463671.

Supercomputing-Enabled Transformational Analytics Capability (SETAC)—Celeste Matarazzo (09-SI-013)

Abstract

We propose to develop fundamentally new analytical approaches for cyber security situational awareness for protecting and defending our nation's computing networks. Our Supercomputing-Enabled Transformational Analytics Capability (SETAC) will focus on transforming the analysis process to provide

real-time situational understanding by enhancing our current signature-based analysis with distributed machine-learning behavioral analytics that can be applied as data travels through a network. SETAC requires research in hardware that is powerful enough to apply analytic algorithms to multiple gigabit-per-second data streams, and also requires new analytic algorithms that can provide a high-fidelity, real-time behavioral view of the network through distributed "intelligent agents."

If successful, SETAC will provide real-time behavioral analytics for cyber security data. Our proposed system capabilities will include (1) identification and classification of high-volume streaming network traffic, (2) high-performance sensor nodes to increase processing capabilities and provide distributed detection across the network, (3) a distributed computing test bed to develop advanced global collection and analysis approaches, (4) new analysis algorithms to analyze data across the distributed system, and (5) system- and component-level metrics for performance assessment.

Mission Relevance

This proposal supports LLNL missions in nonproliferation and homeland security as well as supporting efforts in advanced defense capabilities. Our research will enhance Laboratory threat prevention and response technologies by addressing thrust areas in knowledge discovery, advanced analytics and architectures for national security and actionable situational awareness, and information dominance.

FY10 Accomplishments and Results

In FY10 we significantly upgraded the agent infrastructure to improve reliability and robustness, and tested the results. Specifically, we (1) scaled up the agent framework and deployed hundreds of agents throughout LLNL; (2) evaluated the security of the agent framework; (3) evaluated hardware architectures and the embedded processing application extension platform within the routers; (4) extended our behavior-based machine-learning algorithms and deployed them within the distributed agent framework; (5) developed a probabilistic activity model of hosts in our agent framework for anomaly detection;

(6) evaluated the usefulness of host data for cyber security indicators; (7) upgraded the system's software to automatically restart after a computer reboot so that the agents run continuously; (8) programmed the agents to collect and report host performance information so that we can know memory, central processing unit usage, and other parameters and determine whether anything is amiss; and (9) published and presented our work extensively, including winning the "best paper" award at the 14th Pacific–Asia Conference on Knowledge Discovery and Data Mining.

Proposed Work for FY11

In FY11 we propose to (1) increase the number of data-collection agents deployed at LLNL, (2) conduct online experiments within the Deterlab test bed, (3) deploy behavior-based machine-learning algorithms on the embedded hardware architectures and conduct online tests, (4) extend the behavior-based machine-learning algorithms to detect attacks in the distributed-agent framework, (5) evaluate the efficacy of the activity model of hosts for anomaly detection, and (6) add a new capability for battle-damage assessment to include comparing activity models developed before an attack to ongoing

behavior during an attack, as well as investigating active learning methods in which response can be measured by the SETAC sensor and analytic capabilities to actively assess the level of network damage.

Publications

Abello, J., T. Eliassi-Rad, and N. Devanur, 2010.

"Detecting novel discrepancies in communication networks." *Proc. 10th IEEE Intl. Conf. Data Mining*. LLNL-CONF-46444.

Akoglu, L., M. McGlohon, and C. Faloutsos, 2010.

"OddBall: Spotting anomalies in weighted graphs." *Proc. 14th Pacific-Asia Conference on Knowledge Discovery and Data Mining*. LLNL-CONF-44444.

Gallagher, B., and T. Eliassi-Rad, 2009. *Classification of HTTP attacks: A study on the ECML/PKDD 2007 discovery challenge*. LLNL-TR-414570.

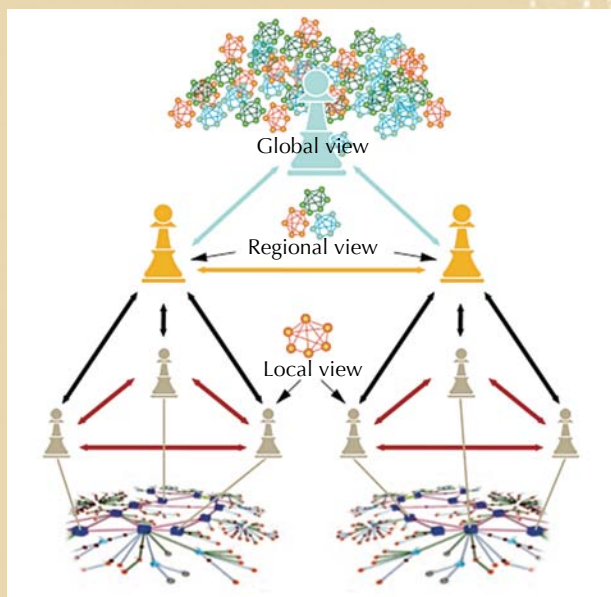
Gallagher, B., et al., 2009. *Guilt by association: Exploiting implicit relationships in network data for traffic classification*. LLNL-TR-414362.

Gallagher, B., et al., 2010. "Homophily in application layer and its usage in traffic classification." *Proc. 29th IEEE Conf. Computer Communications*. LLNL-CONF-421451.

Henderson, K., and T. Eliassi-Rad, 2009. *Solving the top-K problem with fixed-memory heuristic search*. LLNL-TR-410187.

Henderson, K., et al., 2010. "MetricForensics: A multi-level approach for mining volatile graphs." *Proc. 16th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*. LLNL-CONF-43279.

Iliofotou, B., et al., 2010. "Profiling-by-association: A resilient traffic profiling solution for the Internet backbone." *Proc. 6th ACM Intl. Conf. Emerging Networking Experiments and Technologies*. LLNL-CONF-46104.



The Supercomputing-Enabled Transformational Analytics Capability (SETAC) will deploy thousands of software sensor agents that collect, analyze, and share data to provide real-time behavioral analytics for cyber security.

Jiang, W., and M. Gokhale, 2010. *Real-Time classification of multimedia traffic using FPGA*. 20th Intl. Conf. Field Programmable Logic and Applications, Milano, Italy, Aug. 31–Sept. 2, 2010. LLNL-CONF-426266.

Khan, F., M. Gokhale, and C. Chua, 2010. *FPGA-based network traffic analysis using traffic dispersion patterns*. 20th Intl. Conf. Field Programmable Logic and Applications, Milano, Italy, Aug. 31–Sept. 2, 2010. LLNL-CONF-426380.

Li, L., B. A. Prakash, and C. Faloutsos. "Parsimonious linear fingerprinting for time series." *Proc. 36th Intl. Conf. Very Large Data Bases (VLDB10)*. LLNL-CONF-404625.

Merl, D., 2009. *Advances in Bayesian model-based clustering using particle learning*. LLNL-TR-421078.

Thompson, B., and T. Eliassi-Rad, 2009. *DAPA-V10: Discovery and analysis of patterns and anomalies in volatile time-evolving networks*. 1st Workshop on Information in Networks, New York, NY, Sept. 25–26, 2009. LLNL-CONF-416785.

Tong, H., et al., 2009. *BASSET: Scalable gateway finder in large graphs*. LLNL-TR-414380.

Tong, H., et al., 2009. *BridgeFind: Fast detection of top-K bridges in large graphs*. LLNL-TR-414449.

Tong, H., et al., 2008. "Fast mining of complex time-stamped events." *Proc. 17th ACM Conf. Information and Knowledge Management*. LLNL-CONF-405539.

Tong, H., et al., 2010. "On the vulnerability of large graphs." *Proc. 10th IEEE Intl. Conf. Data Mining*. LLNL-CONF-46445.

Ulmer, C., and M. Gokhale, 2010. *A configurable hardware document similarity classifier to detect Web attacks*. 18th Reconfigurable Architectures Workshop, Anchorage, AK, May 16–17, 2011. LLNL-CONF-420263.

Ulmer, C., et al., 2011. "Massively parallel acceleration of a document-similarity classifier to detect Web attacks." *J. Parallel Distr. Comput.* **71**(2), 225. LLNL-JRNL-422668.

Quantitative Analysis of Vector Field Topology—Peer-Timo Bremer (09-ERD-014)

Abstract

Today's scientific computer simulations produce data of increasing complexity, resulting in an increased need for qualitative and quantitative analysis of complex features of physical phenomena, as required to understand those phenomena in detail. Topology provides powerful tools to define and extract such features. We will focus on techniques to quantitatively analyze vector fields, such as earth's magnetic field and water flow in oceans, based on their topological structure. We will develop a mathematical framework for robustly extracting topology from sampled vector fields while maintaining rigorous error bounds. The extracted topology will allow quantitative analysis of topological structures. The hierarchical encoding we develop will allow us to analyze, simplify, and compare vector fields on multiple scales. These techniques will provide opportunities to find explicit definitions for secondary features such as vortices.

We will develop the computational theory necessary to generate complete topology of general vector fields using entirely combinatorial algorithms unaffected by numerical errors. Using metrics tailored to specific application domains, we will construct a hierarchical representation of the topology to permit multiscale analysis. Finally, we will use topological techniques to enhance the ability to track features in dynamic vector fields. The resulting tools will represent fundamentally new analysis capabilities directly applicable to the most ubiquitous form of simulated data.

Mission Relevance

Many relevant phenomena such as combustion, fluid flow, or magnetic fields are best described by vector fields. However, because of their inherent complexity, vector fields are often analyzed using derived scalar fields, which only partially describe these processes. Our direct quantitative analysis, simplification, and comparison of the structural properties of vector fields will provide LLNL with unique capabilities to more effectively analyze large simulations relevant to the national security mission areas of stockpile stewardship and global security. Our advances will also lead to new scientific insights.

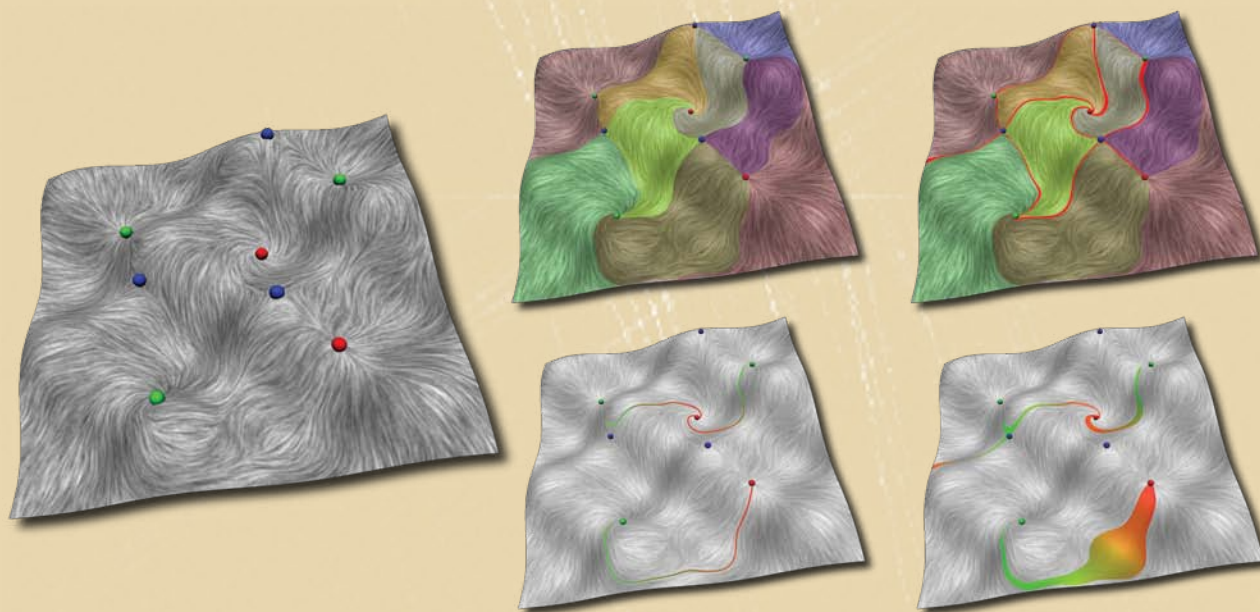
FY10 Accomplishments and Results

In FY10 we (1) developed a new mathematical theory for defining and extracting ridge lines, which includes a detailed classification, proofs of equivalence between different definitions, and a new definition that requires only first- rather than second-derivative estimation; (2) expanded the topological uncertainty work on vector fields, including a complete classification of all possible flow structures in

piece-wise linear flow, as well as a system to display uncertain vector field topology; and (3) developed several complementary Helmholtz–Hodge decomposition algorithms to analyze general flow fields.

Proposed Work for FY11

We will (1) implement a complete ridge-extraction framework, allowing the detection, simplification, and analysis of ridges in images with application in a wide range of fields; (2) extend the multiresolution vector field representation to include data uncertainty (as compared to computational uncertainty), allowing the processing and analyzing of uncertain flows; and (3) use the Helmholtz–Hodge decomposition to analyze two- and three-dimensional vector fields as two-scalar fields of gradient and rotational potential, combining the decomposition work with uncertainty quantification by expressing flow uncertainty as scalar uncertainty in the decomposition and combining the scalar field topology of the decompositions into a representation of flow topology.



Fuzzy vector field topology provides new insights into the inherent instability of vector field analysis. The colored dots represent critical points of a vector field—sources (blue), sinks (red), and saddles (green). The colored regions indicate source flow, and the narrow red regions are areas of boundary uncertainty given a certain amount of error in the computation or initial data. The rainbow regions are similar in that they describe streamline flow areas given a certain amount of uncertainty.

Rapid Exploitation and Analysis of Documents—David Buttler (09-ERD-017)

Abstract

Exploitation of unstructured document text is vital to the national intelligence mission. Millions of existing relevant documents and a rapidly increasing number of new ones must be quickly assessed. We will develop advanced analytic tools to rapidly triage documents so that analysts can focus on the most important ones. This proposal addresses specific research gaps in identification of concepts and automatic creation of a concept hierarchy for summarizing a corpus. We propose to develop cross-language topic hierarchies because documents of interest are often in foreign languages, where translation is a major bottleneck. Because analysts are overloaded with streams of documents, we will monitor analyst interests and provide a personal ranking system.

Our research focuses on understanding approaches and techniques that promote the efficient and effective discovery and analysis of large document sets, given the limitations of current natural language-processing technologies. We will work with intelligence analysts to identify conditions where different methods assist or fail in supporting their work. Furthermore, we will identify a number of targeted research activities that cover technology gaps in document exploitation. In particular, we will explore approaches that assist in the rapid exploitation and analysis of document corpora. We expect to dramatically improve the ability of analysts to discover the most relevant documents for a particular line of inquiry.

Mission Relevance

This effort performs the foundational research necessary to create a world-class information exploitation capability for LLNL's missions in national and homeland security by boosting ability to process the increasingly massive data sets collected for non-proliferation, intelligence, and military missions. We will develop new algorithms to organize vast document sets and alert analysts of new information relevant to their analytic tasks. This capability will have direct applications for Livermore programs in counterproliferation analysis that are of interest to the Department of Defense.

FY10 Accomplishments and Results

In FY10 we (1) created a technique to examine a domain-specific corpus and discover concepts and the links between them as enriched and guided by existing knowledge and relationships, (2) measured the effectiveness of personalization on the ranking of search results for targeted applications relevant to the intelligence community, (3) incorporated probabilistic models into personalization results, (4) created a technique to generate multilingual topic models from a parallel corpus, and (5) began optimizing and measuring the integration of topic models with our search interfaces, including term disambiguation.

Proposed Work for FY11

In FY11 we plan to (1) extend the performance of probabilistic topic models using new parallelization techniques, (2) create alternative clustering methods that are high performing and maintain document similarity cohesion without requiring a user to manually tune the number of clusters, and (3) create, for personalization, a system that generates profiles based on small collections of task-specific documents, which will allow users to find documents of interest based on existing domain knowledge they identify.

Publications

Pon, R. K., et al., 2010. "Measuring the interestingness of articles in a limited user environment." *Info. Process. Manage.* **47**, 97. LLNL-JRNL-407783.

Adding Validation and Novel Multiphysics Capabilities to the First-Principles Molecular Dynamics Qbox Code—Erik Draeger (09-ERD-019)

Abstract

The purpose of this project is to perform the research necessary to increase the accuracy and temperature and pressure range of first-principles molecular dynamics materials simulation codes such as Qbox, which currently relies on approximations that can break down at extreme temperatures and pressures. We will integrate Qbox with high-accuracy quantum Monte Carlo codes and develop automated

validation tools to quantitatively assess these approximations on the fly. We will also develop a flexible, parallel multiphysics framework to couple different quantum simulation codes to allow researchers to easily implement and test new multiphysics algorithms. Lastly, we will use this framework to develop new multiphysics methods to deal with extreme conditions such as quantum effects of light nuclei and electron exchange–correlation effects.

We expect this project to result in (1) rebuilt, sustainable quantum Monte Carlo capabilities; (2) robust, on-the-fly validation tools for Qbox; (3) a flexible multiphysics framework to simplify development of new multiphysics quantum algorithms; and (4) new multiphysics algorithms to extend predictive materials simulations capabilities. These results will allow us to perform validated, accurate calculations of materials at extreme conditions with unprecedented accuracy. They will also pave the way for new breakthroughs in predictive materials modeling.

Mission Relevance

Predictive materials simulation has long been a cornerstone of NNSA and LLNL missions. Qbox is currently being used for calculations in the Stockpile Stewardship Program and the National Boost Initiative to the limit of its current capabilities. Increasing the accuracy, validation capabilities, and range of accessible conditions would be of direct benefit to national security efforts. As a general materials simulation tool, new capabilities would also benefit many basic research efforts performed at Lawrence Livermore.

FY10 Accomplishments and Results

We (1) created CASINO-compatible Qbox checkpoints for conducting independent molecular dynamics simulations using the code MPI after determining that limitations in parallel remote method-invocation operations using the code Co-op would make the run-time integration of CASINO and Qbox inefficient for such simulations; (2) wrote a Co-op test code and measured parallel performance for different configurations; (3) continued our path-integral Monte Carlo simulations of hydrogen plasmas, which generated considerable interest; and (4) developed and implemented numerous algorithmic improvements into the path-integral code

to maximize both accuracy and efficiency for these systems and carried out a careful verification study.

Proposed Work for FY11

To bring this project to a successful conclusion, we will focus on systems in which our new simulation capabilities can make an immediate impact in highly relevant fields: hydrogen isotopes and plasmas at extreme conditions. Specifically, we will continue to develop new predictive capabilities for first-principles plasma and hydrogen simulations at conditions beyond the limits of stand-alone Qbox simulations. In addition, we will couple Qbox and our path-integral code using the qbLink interface to explore use of more sophisticated wave-function nodes to increase accuracy at conditions in which current nodal models fail. We expect to publish our algorithmic developments and new high-accuracy hydrogen simulation results in high-visibility journals.

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

Abstract

Role discovery arises in many intelligence and defense applications. Our objective is to develop algorithms that capture the formation and evolution of roles and functions in noisy and incomplete dynamic semantic graphs, which are used to uncover relationships hidden in streams of data from multiple sources. To model this complex process, new algorithms are needed that take into account both the heterogeneity and dynamicity in data. These new algorithms will generate statistical models that combine probabilistic predictive models (that handle data heterogeneity) with stochastic process models (that handle data dynamicity). For the first time, this work will unite two modeling categories on graphs. New statistical models will be judged based on their accuracy, run time, and space complexity and tested on publicly available as well as sponsor-provided data.

If successful, the work will provide viable solutions to some of the current analysis needs in cybersecurity as well as homeland and national security. In particular, the work will produce new algorithms that (1) model both the heterogeneity

and dynamicity in data, (2) allow analysts to directly examine the roles of entities in data sets, and (3) provide insights on the generative mechanisms of relationships. The discovered knowledge can subsequently be used for behavior modeling, anomaly detection, and other graph analytics problems. For instance, in the cybersecurity domain, the work will model the function of hosts over time to detect suspicious activities. These expected results are significant because they provide a different view of the asymmetric threats facing the nation.

Mission Relevance

This work supports LLNL missions in nonproliferation and homeland security and in advanced defense capabilities. By tracking the formation and evolution of roles (i.e., functions) in dynamic semantic graphs, the roles of entities of interest can be directly examined. This abstraction contributes to the understanding of hidden hostile elements and is well suited for identification of the asymmetric nature of threats faced in homeland and national security domains.

FY10 Accomplishments and Results

In FY10 we (1) developed discrete and continuous-time group-discovery algorithms for dynamic graphs; (2) implemented group-discovery inference on distributed-memory machines using the codes Hadoop and MapReduce; (3) developed a scalable hybrid community-discovery algorithm that takes advantage of hints and background information; (4) identified a bias in statistical tests for network classifiers that leads to incorrect conclusions and developed novel tests to correct for this bias; (5) developed a model of node and graph activity that uses ideas from combinatorial set-system discrepancy to flag deviations from expected behavior; (6) developed a model for inferring missing nodes and links in networks, utilizing Kronecker models and expectation maximization; (7) developed a model of real-world networks, called the “multiplicative attribute graph,” by extending Kronecker models to incorporate node attributes; (8) developed an iterative procedure to construct role discovery features using egonet structures; (9) validated all

methods empirically on real-world and synthetic data sets; and (10) published seven peer-reviewed publications, one of which was runner-up in a “best paper” competition.

Proposed Work for FY11

In FY11 we plan to (1) finish developing the various role-discovery algorithms on graphs from different domains, such as cybersecurity and social media, including role discovery with typed and typeless egonets, role discovery with discrete and continuous time, and recursive role discovery, in which the goal is to find the optimal role assignment for all nodes in the graph; (2) begin a comparative study of the algorithms; (3) develop models for multifaceted information diffusion and study their utility in role discovery; and (4) conduct, for each task, extensive empirical studies on publicly available data, which we have already identified, and determine commonalities. By the end of FY11 we expect to have a role-discovery prototype system for dynamic semantic graphs.

Publications

Eliassi-Rad, T., and K. Henderson, 2009. “Literature search through mixed-membership community discovery.” *Proc. 1st Workshop on Information in Networks*. LLNL-CONF-416981.

Eliassi-Rad, T., and K. Henderson, 2010. “Literature search through mixed-membership community discovery.” *Proc. 2010 Intl. Conf. Social Computing, Behavioral Modeling, and Prediction*, p. 70. LLNL-CONF-416981.

Gallagher, B., and T. Eliassi-Rad, 2010. “Leveraging label-independent features for classification in sparsely labeled networks: An empirical study.” *Lect. Notes Comput. Sci.* **5498**, 1. LLNL-JRNL-411529.

Henderson, K., and T. Eliassi-Rad, 2009. “Applying latent Dirichlet allocation to group discovery in large graphs.” *Proc. 24th Ann. ACM Symp. Applied Computing*, p. 1456. LLNL-CONF-408036.

Henderson, K., et al., 2010. "HCDF: A hybrid community discovery framework." *Proc. 2010 SIAM Intl. Conf. Data Mining*, p. 754. LLNL-CONF-422685.

Henderson, K., et al., 2009. *Best of both worlds: A scalable hybrid community discovery algorithm*. LLNL-TR-414387.

Kim, M., and J. Leskovec, 2010. *Multiplicative attribute graph model of real-world networks*. LLNL-SR-460642.

Kim, M., and J. Leskovec, 2010. *Network completion problem: Inferring missing nodes and edges in networks*. LLNL-MI-461042.

Miller, K., and T. Eliassi-Rad, 2009. *Continuous-time group discovery in dynamic graphs*. 23rd Ann. Conf. Neural Information Processing Systems, Whistler, Canada, Dec. 11, 2009. LLNL-CONF-461724.

Neville, J., et al., in press. "Correcting evaluation bias of relational classifiers with network cross validation." *Knowl. Inform. Syst.* LLNL-JRNL-455699.

Neville, J., B. Gallagher, and T. Eliassi-Rad, 2009. "Evaluating statistical tests for within-network classifiers of relational data." *Proc. 9th IEEE Intl. Conf. Data Mining*, p. 397. LLNL-CONF-417025.

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

Tong, H., et al., 2010. "BASSET: Scalable gateway finder in large graphs." *Proc. 14th Pacific-Asia Conf. Advances in Knowledge Discovery and Data Mining*, p. 449. LLNL-CONF-461610.

Tong, H., et al., 2008. "Fast mining of complex time-stamped events." *Proc. 17th ACM Conf. Information and Knowledge Management*, p. 759. LLNL-CONF-405539.

Modern Finite Elements for Lagrangian Hydrodynamics—Tzanio Kolev (09-ERD-034)

Abstract

The objective of this project is to develop new finite-element discretization algorithms for compressible Lagrangian shock hydrodynamics. Our methods will be more accurate and robust than the currently used computational schemes and address several longstanding issues with hydrodynamics simulation codes at LLNL, including symmetry preservation on unstructured grids, exact total energy conservation, artificial viscosity discretization in multiple dimensions, and the handling of hourglass-mode instabilities. This will be achieved by the application of modern finite-element technology for discretizing the Euler equations on a moving grid, coupled with new mathematical theory and numerical algorithms.

If successful, this project will produce new finite-element discretization schemes that will enable Lagrangian simulations with LLNL's hydrodynamics codes with a higher degree of fidelity than is currently possible. This research could also allow finite-element methodology, which has been very successful for elliptic problems, to be extended to general systems of hyperbolic conservation laws in a Lagrangian frame.

Mission Relevance

Hydrodynamics simulations are of critical importance in numerous LLNL applications, including stockpile stewardship, inertial-confinement fusion, and other mission-relevant efforts. The proposed research will develop finite-element simulations technology to improve the predictive capability of these simulations while requiring fewer user-adjustable parameters. This project therefore supports LLNL's missions in national and energy security.

FY10 Accomplishments and Results

We (1) further developed and extended our curvilinear high-order, finite-element method for solving Euler's equations in a moving Lagrangian frame,

based on a general framework that supports multiple discretization options in two dimensions (2D) and 3D; (2) demonstrated significantly improved robustness with respect to symmetry preservation and mesh imprinting, and verified high-order convergence on smooth problems; (3) developed new, more stable variants of the Runge–Kutta time-integration schemes, enabling us to exact total energy conservation on fully discrete levels and high-order convergence in space and time; (4) implemented and tested the methods in our object-oriented high-order, finite-element Lagrangian hydrocode BLAST; and (5) derived an extension of our finite-element approach to axisymmetric problems by a careful reduction of the 3D problem to a 2D variational form in a meridian cut of the domain, and demonstrated its robustness with respect to symmetry preservation and energy conservation.

Proposed Work for FY11

We will widen the applicability and improve the efficiency of our general high-order, finite-element approach for solving the Euler equations in a Lagrangian frame. Specifically, we will (1) extend the method to handle 3D problems by employing curved hexahedral zones, (2) consider the handling of materials with strength in our general discretization algorithm, (3) develop a parallel version of the finite-element approach and implement it in our research code to facilitate large-scale simulations, and (4) investigate performance-enhancing techniques and document tradeoffs between speed and robustness.

Publications

Dobrev, V. A., et al., 2010. *Curvilinear finite elements for Lagrangian hydrodynamics*. 42nd Mtg. Joint Working Group, June 21, 2010, Livermore, CA. LLNL-PRES-425542.

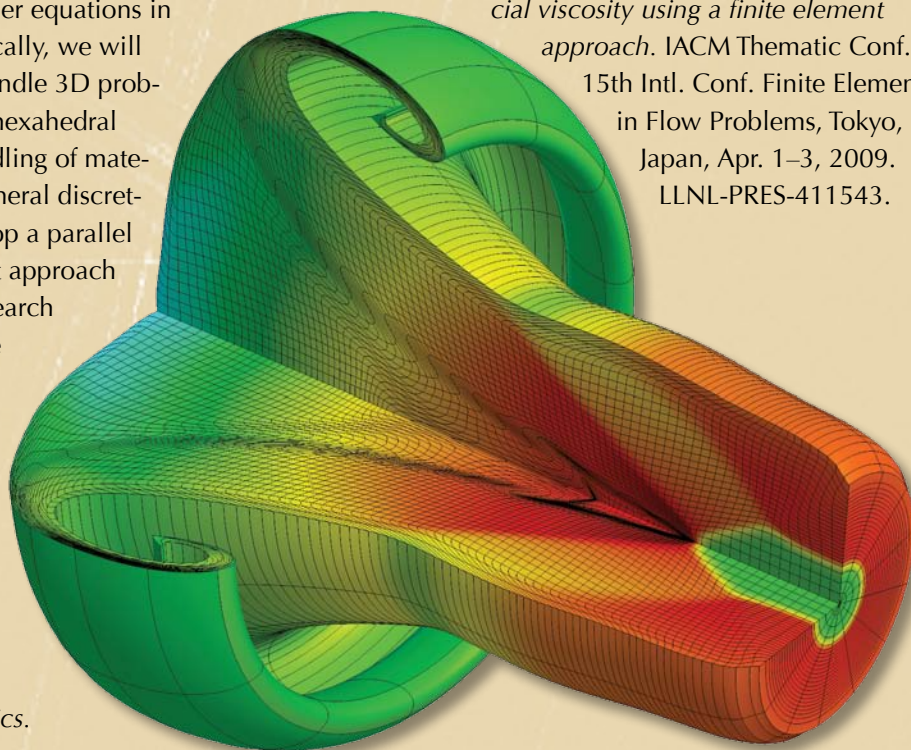
Dobrev, V. A., et al., 2010. “Curvilinear finite elements for Lagrangian hydrodynamics.” *Int. J. Numer. Meth. Fl.* **65**(11-12), 1295. LLNL-JRNL-422302.

Dobrev, V. A., et al., 2009. *Energy conserving finite element discretizations of Lagrangian hydrodynamics, part 1: Theoretical framework*. Numerical Methods for Multi-Material Fluids and Structures, Pavia, Italy, Sept. 21–25, 2009. LLNL-PRES-416883.

Dobrev, V. A., et al., 2009. *Energy conserving finite element discretizations of Lagrangian hydrodynamics, part 2: Examples and numerical results*. Numerical Methods for Multi-Material Fluids and Structures, Pavia, Italy, Sept. 21–25, 2009. LLNL-PRES-416822.

Kolev, T., and R. Rieben, 2009. “A tensor artificial viscosity using a finite element approach.” *J. Comput. Phys.* **228**, 8336. LLNL-JRNL-409868.

Kolev, T., and R. Rieben, 2009. *Tensor artificial viscosity using a finite element approach*. IACM Thematic Conf., 15th Intl. Conf. Finite Elements in Flow Problems, Tokyo, Japan, Apr. 1–3, 2009. LLNL-PRES-411543.



A curvilinear finite-element Lagrangian calculation of a shock triple-point interaction in axisymmetric coordinates. Note the robustness of the method with respect to highly deformed and stretched zones.

Lagrange Multiplier Embedded-Mesh Method—Michael Puso (09-ERD-044)

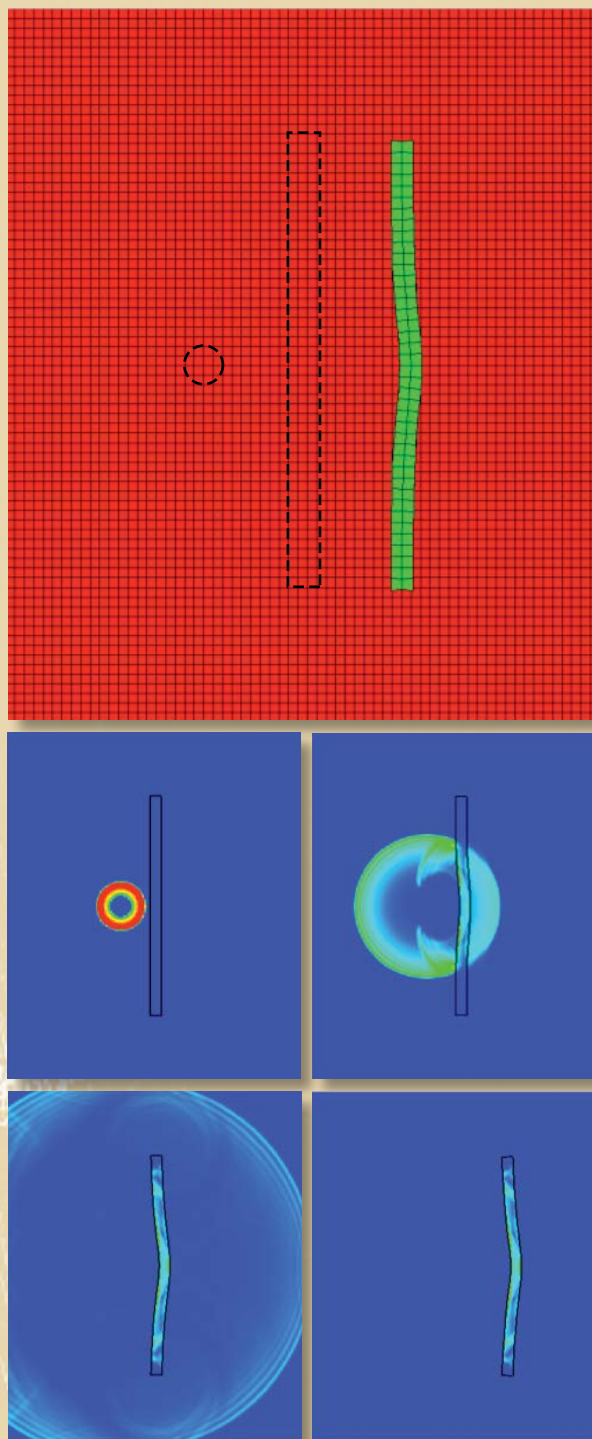
Abstract

Many engineering and physics analysis problems could be simplified by applying an “embedded” mesh (a secondary domain or mesh that is embedded in but independent of the primary computational mesh). For example, a blast problem with a shell structure overlapping a rectangular air grid typically requires a conforming mesh between the shell and air mesh. However, the analysis may fail because of mesh tangling, even with arbitrary Lagrange–Eulerian (ALE) codes. We propose to develop an embedded-mesh method with a shell (or solid) mesh independent of the rectangular air grid and with appropriate constraints applied at shell–air boundaries. Embedded-mesh methods were originally developed for finite-difference schemes. A new finite-element embedded-mesh scheme will be developed in this work that will efficiently allow monolithic coupling for explicit finite elements.

We will develop a computational tool in which an embedded mesh eliminates the need for a conforming mesh and thus requires no mesh motion for the types of problems considered. This general constraint tool will be built to interface with different LLNL codes such as the ALE3D and Diablo arbitrary Lagrange–Eulerian hydrodynamics codes and will be demonstrated on two model problems: the blast rupture of shell structures and moving solid conductors in air grids. The new method may drastically simplify model building and improve code robustness in many instances.

Mission Relevance

The results of this research effort could have fundamental impacts on combining physics such as fluid dynamics with structural mechanics. Specifically, the tools developed in this project will support LLNL’s national security and defense missions, such as work involving moving solid conductors for flux-compression generation and rail guns.



A circular charge is placed next to a submerged plate, with the initial plate and charge shown as dotted lines in the top image. The evolution of pressure in the fluid and plastic strain in the plate are shown at bottom after exposure to the underwater blast.

In addition, the proposed embedded-mesh method has applications for understanding the effects of high explosives, a core Livermore competency.

FY10 Accomplishments and Results

In FY10 we completed development of the FEusion embedded-mesh coupling software library to compute overlap of foreground and background meshes and resultant constraints for solids and fluids, and implemented the library into the DYNA3D, ALE3D, and NIKE3D codes. A fluid–structure interaction problem (shown in the figure on p. 155) was analyzed using the new embedded grid method and ALE3D. For this example, a 2-in. thick (Lagrangian) steel plate was exposed to an underwater blast in an Eulerian fluid. Unlike standard ALE methods, the background fluid mesh was stationary whilst the plate moves in the foreground (top image). We found that the pressures and displacements (bottom image) compared very well to standard ALE approaches. We then applied the method to much more complicated structures not amenable to standard approaches.

Proposed Work for FY11

We will (1) extend to three dimensions the theory modifications for handling fine-foreground and coarse-background meshes, (2) extend our finite-element method approach for handling overlapping materials to handle not just solid elements but also shell elements, (3) make additional modifications to ALE3D to allow fluid to pass by eroded elements to capture failure, and (4) make modifications to the implicit embedded implementation to handle embedded-mesh finite elements derived by Nédélec.

Publications

Laurse, T. A., M. A. Puso, and J. Sanders, in press. “Mortar contact formulations for deformable–deformable contact: Past contributions and new extensions for enriched and embedded interface formulations.” *Comput. Meth. Appl. Mech. Eng.* LLNL-JRNL-416574.

Towards Understanding Higher-Adaptive Systems—Brenda Ng (09-LW-030)

Abstract

Countering real-world adversaries such as terrorist networks and cyber attackers involves formidable challenges such as incomplete or imperfect information, misinformation, asymmetric players, and nonsequential or unknown sets of actions. This effort focuses on higher-adaptive systems, which can modify their structure or behavior in response to detection or regulation attempts, with the ultimate goal of enhancing adversarial modeling and response. Our plan is to develop three modules in a spiral lifecycle model, including an adversary and response system with knowledge representation of an observer system and decision control of an observer system. We will create a prototype system and iteratively improve upon its capabilities for learning and modeling of increasingly complex adversarial behaviors.

We will study passive adversaries with fixed dynamics as well as deceptively aggressive adversaries with adaptive dynamics. We expect to contribute to a computational framework for characterizing dynamically changing, deceptive adversarial systems, as well as deliver a software prototype of such a framework that includes state-of-the-art models and algorithms. This will enable even more adaptive and aggressive adversarial systems, such as those withholding resources and information from their opponents, which will help advance work in artificial intelligence and game theory and provide the basis for addressing significant national security threats.

Mission Relevance

This project supports the Laboratory’s national security mission by providing important knowledge and skills about real-world adversarial modeling and higher-adaptive systems, with applications for biological systems such as regulatory networks, law-enforcement problems such as money laundering and drug trafficking, and homeland security issues such as terrorist networks, cyber attacks, and proliferation of weapons of mass destruction.

FY10 Accomplishments and Results

This work was driven by real-world modeling needs where one individual intelligent component or “agent” is (1) uncertain about its environment, the state of which must be inferred through observations; (2) faced with an intelligent adversary, against whom to succeed it must anticipate counteractions, which entails also anticipating the adversary’s observations and beliefs; and (3) unsure about how its actions might affect the environment, which requires learning through trial and error. In FY10, we introduced a framework, the Bayes-adaptive interactive partially observable Markov decision process (BA-IPOMDP), which augmented the IPOMDP system we developed in FY09 with model-learning capabilities. This framework is novel in that agents model the beliefs as well as the learning processes of their adversaries. Thus, BA-IPOMDP agents are not only intelligent in making decisions, but are also adaptive in updating their perception of the environment. To our knowledge, this is the first multi-agent adversarial decision-making framework to explicitly incorporate learning, thus allowing for modeling of imperfect knowledge about the environment as well as model parameters, such as an agent’s probabilities for state transitions and observations. The successful completion of this

project is an enormous stride forward in bridging multi-agent decision theory to real-world adversarial modeling applications, especially those involving human agents. We are seeking further support from the Department of Homeland Security to conduct follow-on research and application efforts.

Publications

Boakye, K., et al., 2011. *Bayes-adaptive interactive partially observable Markov decision processes*. AAMAS 2011 10th Intl. Conf. Autonomous Agents and Multiagent Systems, Taipei, Taiwan, May 2–6, 2011. LLNL-CONF-455924-DRAFT.

Ng, B., et al., 2009. *Modeling money laundering via interactive partially observable Markov decision processes*. AAMAS 2010, 9th Intl. Conf. Autonomous Agents and Multiagent Systems, Toronto, Canada, May 10–14, 2010. LLNL-CONF-418110-DRAFT.

Ng, B., et al., 2010. “Towards applying interactive POMDPs to real-world adversary modeling.” *Proc. 22nd IAAI Conf. Innovative Applications of Artificial Intelligence*, Association for the Advancement of Artificial Intelligence, Menlo Park, CA, 1814. LLNL-CONF-426131.



Our computational framework can model intent to reason and learn about adversaries and environment, which is needed to anticipate opponent strategies in repeated interactions.

The Advance of Uncertainty Quantification Science—Richard Klein (10-SI-013)

Abstract

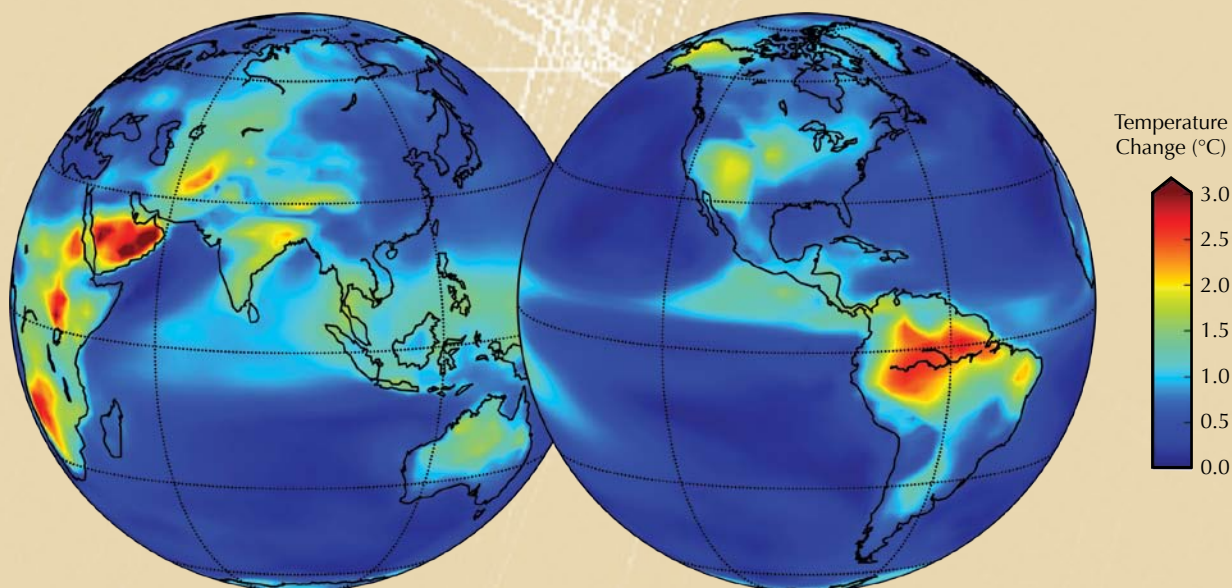
Uncertainty quantification deals with the propagation of uncertainty in multiphysics codes that depend in a highly nonlinear fashion on uncertainties in the underlying physics models, algorithms, databases, inputs, and output observables. We propose to build a focused multidisciplinary scientific effort that will investigate, develop, and apply uncertainty quantification science to high-impact scientific areas. We will make major advances in two leading areas of uncertainty quantification—high dimensionality and error and uncertainty propagation—by developing powerful intrusive and nonintrusive uncertainty quantification approaches. Finally, we will use Laboratory applications as a test bed for our new methodologies, with an initial focus on climate prediction.

If successful, we will make significant advances in uncertainty quantification science by (1) developing error and uncertainty propagation methods in multiphysics and multiscale codes, (2) tackling the “curse of high dimensionality” with the development of novel methods for dimensional reduction, and (3) developing an advanced computational

pipeline to enable complete uncertainty quantification workflow and analysis for ensemble runs at the extreme scale with self-guiding adaptation. We will apply these new methods to carry out uncertainty quantification for a coupled ocean–atmospheric model, yielding an adaptively constructed ensemble of simulations for past and future climate; characterize the uncertainty for important global climate variables; and carry out regional climate change uncertainty quantification, with a focus on precipitation and evaporation changes.

Mission Relevance

Our work for this project will support the Laboratory mission in enhancing the nation’s environmental security by focusing on reducing uncertainty in the parameters of climate models that cannot currently be constrained by available observations. Our research will also have a large impact in stockpile stewardship by providing methods that will enable increasingly precise uncertainty bounds to be placed on the performance of nuclear weapons. In addition, quantification and reduction of uncertainty in the inertial-confinement fusion design process will optimize target designs so that they are more likely to perform as intended and reduce damage in laser operations.



Sensitivity map showing the magnitude of changes in surface air temperature that can result when an uncertain climate-model parameter is altered.

FY10 Accomplishments and Results

We (1) developed and documented a standard set of linear advection, advection-diffusion, and inviscid and viscous Burgers' test problems for error estimation; (2) applied adjoint error estimation and direct error evolution methods to these problems, and then began analyzing the techniques to understand their limitations; (3) developed a method for the visual exploration of high-dimensional functions based on the Morse–Smale complex; (4) developed a non-parametric, piecewise regression method also based on the Morse–Smale complex; (5) developed an improved algorithm for approximating the Morse–Smale complex by shattering crystals; (6) carried out comparative studies of various variable-selection and various input dimension-reduction methods; (7) developed and tested a Gaussian adaptive-sampling method using local, radial-basis kernels and multiple sampling criteria; (8) developed an initial version of the statistical MARS response model and Gaussian process response model in Python and tested these methods using our ensemble of climate model simulations; (9) developed a uncertainty qualification dynamic scheduler, dynamic sample-point server, and support for third-party methods, thus providing the pipeline infrastructure needed to support the research of automated decision analysis and sample point selection technologies using adaptive-sampling refinement and dimensional reduction; and (10) completed over 2,300 present-day climate ensemble simulations using the Community Atmosphere Model, identifying and ranking important parameter uncertainties in the model using uncertainty qualification, assembling critical observational data sets to calibrate the ensembles, and achieving results that will be used to propagate uncertainties through future climate change simulations.

Proposed Work for FY11

In FY11 we will (1) investigate adjoint error estimates and direct-evolution methods for implicit and explicit discretizations of linear and nonlinear advection–diffusion equations, including the viscous

Burgers' equation; (2) compare contour-tree topological analysis with a pilot-estimation-advancing, high-dimensional level-set extraction method for adaptive-sample refinement strategies and explore alternative dimension-reduction strategies; (3) incorporate advances in dimensional reduction into the uncertainty quantification pipeline; and (4) use results of the uncertainty quantification of input parameters to conduct doubled carbon dioxide atmospheric simulations in order to characterize uncertainty in global climate sensitivity, identify important regional data sets, carry out specific regional uncertainty quantification, and prepare for coupled ocean–atmospheric uncertainty quantification with the Community Climate System Model.

Publications

Brandon, S., 2010. *The advance of UQ science and the LLNL UQ pipeline*. 15th Ann. Community Earth System Model Workshop, Breckenridge, CO, June 28, 2010. LLNL-PRES-438634.

Gerber, S., et al., 2010. "Visual exploration of high-dimensional scalar functions." *IEEE T. Vis. Comput. Gr.* **16**(6), 1271, LLNL-CONF-446831.

Gerber, S., et al., 2010. *Visual exploration of high-dimensional scalar functions*. IEEE 2010 Visualization, Information Visualization, and Visual Analytics Science and Technology Conf. (VizWeek 2010), Salt Lake City, UT, Oct. 24–29, 2010. LLNL-CONF-446831.

Hittinger, J. A., J. W. Banks, and C. S. Woodward, 2010. *Periodic hyperbolic and advection dominated model problems for a posteriori error estimation*. LLNL-TR-426285.

Johannesson, G., and A. Kupresanin, 2010. *Adaptive Bayesian calibration of computer models using sequential Monte Carlo*. American Statistical Association 2010 Joint Statistical Meetings (JSM 2010), Vancouver, Canada, July 31–Aug. 5, 2010. UCRL-PRES-418578.

Klein, R. I., et al., 2010. "Narrowing uncertainties." *Sci. Tech. Rev.*, July/Aug. 2010, 12. UCRL-TR-52000-10-7/8.

Lucas, D. D., 2010. *The LLNL climate UQ project: update and future directions*. 15th Ann. Community Earth System Model Workshop, Breckenridge, CO, June 28, 2010. LLNL-PRES-438116.

Lucas, D. D., et al., 2010. *The climate uncertainty quantification project at Lawrence Livermore National Laboratory: Initial analysis of the sensitivities and uncertainties in the Community Atmosphere Model*. Current Challenges in Computing Workshop: Climate Modeling, Napa, CA, Aug. 30–Sept. 1, 2010. LLNL-POST-450875.

Lucas, D. D., 2010. *The LLNL climate UQ project: Brief overview and preliminary results*. Community Earth System Model Atmosphere Model Working Group Mtg., Boulder, CO, Feb. 10–12, 2010. LLNL-PRES-423404.

Tannahill, J., 2010. *The LLNL climate UQ project: Overview and design*. 15th Ann. Community Earth System Model Workshop, Breckenridge, CO, June 28, 2010. LLNL-PRES-438071.

Tong, C., 2010. *A comparison of several computational methods for variable subset selection*. 2010 Society for Industrial and Applied Mathematics Ann. Mtg., Pittsburg, PA, July 12–16, 2010. LLNL-PRES-437131.

ExaCT: Exascale Computing Technologies—Bronis de Supinski (10-SI-014)

Abstract

We propose to prepare for the large-scale supercomputer systems anticipated in the near future, with capabilities of multiple petaflops (one thousand trillion floating point operations per second) and, in the longer term, of exaflops (one quintillion floating point operations per second) total performance.

This will herald a new era of predictive simulation. Specifically, our ExaCT (Exascale Computing Technologies) project will dramatically improve the scalability and performance of Laboratory applications, particularly in the presence of much more frequent soft faults such as bit flips, through innovative algorithms and automated adaptation to systems with huge numbers of nodes, each with much less memory and less memory bandwidth per core. Overall, we will create fundamentally new approaches not only to algorithmic design, including integrated fault-tolerance strategies, but also to debugging and large-scale performance automation.

Our ExaCT project will produce tools and strategies to diagnose and overcome difficulties arising in large-scale supercomputer systems. We will (1) identify models of fault vulnerability and design strategies to overcome it, (2) design and develop sparse linear solvers to address memory constraints, (3) explore automated code transformations that reduce memory bandwidth requirements and asynchronously compute load redistributions to improve performance on millions of cores, and (4) investigate a debugging methodology to locate the source of programming errors automatically and to track algorithmic behavior. Our work with application scientists will demonstrate enhanced productivity, enabling effective use of large-scale systems and thus providing critical predictive simulation capabilities.

Mission Relevance

This research supports LLNL's broad national and energy security missions by providing the needed underpinnings for predictive simulation on large-scale supercomputers through extensions to our world leadership in algorithmic design and systems software and tools and by directly applying them to simulation applications for materials modeling, fusion-energy science, and the physics relevant to stockpile stewardship.

FY10 Accomplishments and Results

In FY10 we (1) developed detailed models of existing sparse linear-solver algorithms and designed new algorithms more appropriate for multicore

systems, (2) designed mechanisms to automatically locate the source of errors in message-passing interface programs, (3) designed techniques to asynchronously compute load redistributions to the primary application, and (4) developed a detailed model of multilevel checkpoint systems.

Proposed Work for FY11

In FY11 we will (1) study the convergence properties of sparse linear-solver algorithms and refine our performance model of those algorithms, (2) test and refine mechanisms to automatically locate the source of errors in message-passing interface programs, (3) implement the techniques developed in FY10 to asynchronously redistribute computational load to the primary application, and (4) create a library of prototype, generic checkpoint compression tools.

Publications

Ahn, D. H., et al., 2009. *Scalable temporal ordering for large scale debugging*. SC2009, Computing for a

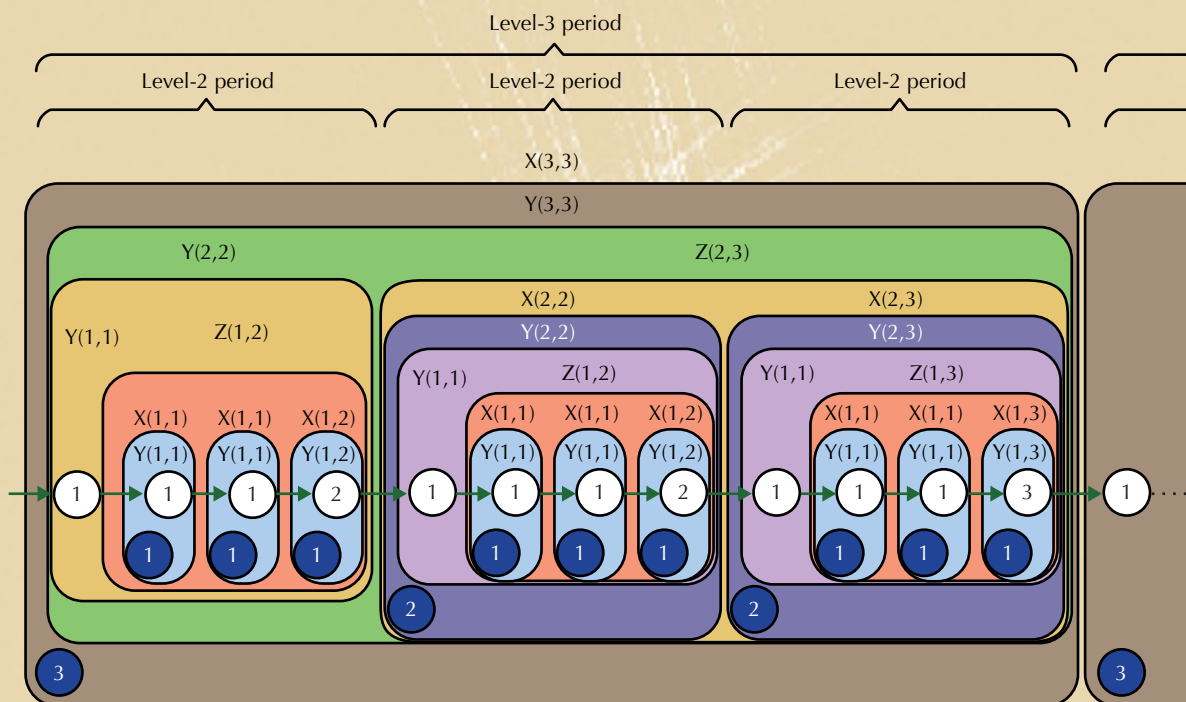
Changing World, Portland, OR, Nov. 14–20, 2009. LLNL-CONF-412227.

Baker, A. H., M. Schulz, and U. M. Yang, 2010. *On the performance of an algebraic multigrid solver on multicore clusters*. 9th Intl. Mtg. High Performance Computing for Computational Science (VecPar 2010), Berkeley, CA, June 22–25, 2010. LLNL-CONF-429864.

Baker, A. H., et al., 2010. *Multigrid smoothers for ultra-parallel computing*. LLNL-JRNL-435315.

Bronevetsky, G., et al., 2010. *AutomaDeD: Automata-based debugging for dissimilar parallel tasks*. 40th Ann. IEEE/IFIP International Conf. Dependable Systems and Networks (DSN 2010), Chicago, IL, June 28–July 1, 2010. LLNL-CONF-426270.

Bronevetsky, G., et al., 2010. *Statistical fault detection for parallel applications with AutomaDeD*.



We developed a Markov model of our multilevel checkpoint system that demonstrates our innovative software significantly increases effective system utilization.

IEEE Workshop on Silicon Errors in Logic—System Effects (SELSE 6), Stanford, CA, Mar. 23–24, 2010. LLNL-CONF-426254.

Gamblin, T., et al., 2010. *Clustering performance data efficiently at massive scales*. 24th Intl. Conf. Supercomputing (ICS 2010), Tsukuba, Japan, June 1–4, 2010. LLNL-CONF-422684.

Humphrey, A., et al., 2010. *Verification for portability, scalability, and grokkability*. EC² 2010: Workshop on Exploiting Concurrency Efficiently and Correctly, Edinburgh, U.K., July 20–21, 2010. LLNL-CONF-442476.

Moody, A., et al., 2010. *Modeling and design of a scalable multi-level checkpoint system*. SC2010, The Future of Discovery, New Orleans, LA, Nov. 13–19, 2010. LLNL-CONF-427742.

Vo, A., et al., 2010. *A scalable and distributed dynamic formal verifier for MPI programs*. SC2010, The Future of Discovery, New Orleans, LA, Nov. 13–19, 2010. LLNL-CONF-2475.

Yang, U. M., 2010. “On long range interpolation operators for aggressive coarsening.” *Numer. Lin. Algebra Appl.* **17**(2-3), 453. LLNL-JRNL-417371.

Parallel Discrete-Event Simulation of Cyber Attack and Defense Scenarios and Automated Rollback Code Generation—David Jefferson (10-ERD-025)

Abstract

Widespread cyber attacks that overwhelm Web sites are a prime national security concern, and a recent powerful attack that targeted government and private sites underscores how unevenly prepared the U.S. government is to block such multipronged assaults. We propose to develop a discrete-event

simulation using the NetWarp platform for executing cyber attack and defense code on a network of virtual machines. The code will be synchronized using a discrete-event simulator to accurately replicate, for the first time, the timing of events in the modeled system. In parallel, we will develop the BackStroke system to automatically generate a companion method that reverses unwanted side effects of specialized computer algorithms. This is a capability critical for “optimistic” parallel discrete-event simulation, and will be developed using LLNL’s ROSE compiler technology.

We expect to develop NetWarp as the first simulation platform to enable realistic studies of cyber attack and defense scenarios that are scalable and accurate in both behavior and performance. It will enable ensemble studies to optimize cyber defense systems against an array of attack codes, and do so without prior understanding of how the attack codes work. We envision that it will scale to at least 10,000 virtual nodes, possibly coupled to a much larger number of conventionally simulated nodes. By developing the BackStroke system, we will dramatically lower barriers to the use of optimistic parallel discrete-event simulation techniques. Programmers will not be forced to write inverse methods for every forward-event method, nor face the extremely difficult debugging otherwise required.

Mission Relevance

Our project supports the Laboratory’s mission to reduce or counter threats to national security by allowing us to simulate cyber attack and defense scenarios much more accurately, more quickly, and in some cases at a larger scale than ever before. In addition, these simulations can be done early, before the attack code is even understood. The BackStroke system will support several Laboratory missions because it is a fundamental improvement to the technology of optimistic parallel discrete-event simulation.

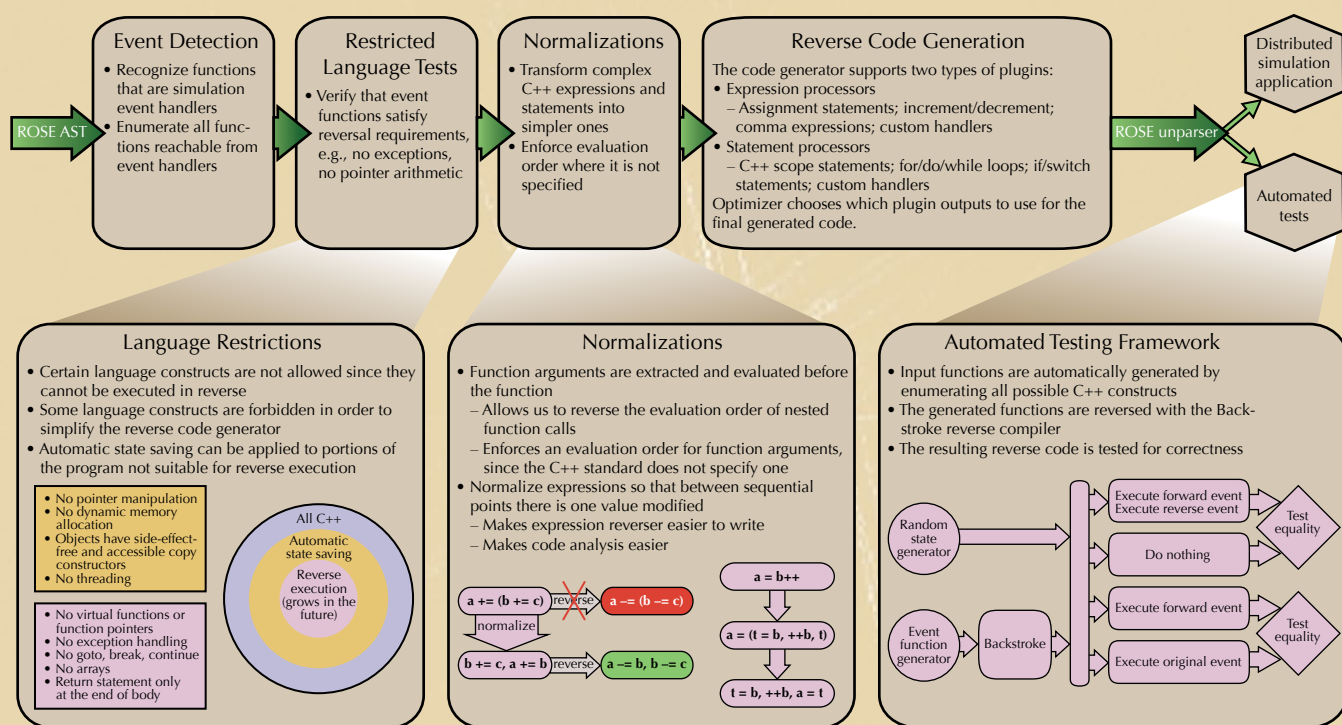
FY10 Accomplishments and Results

In FY11 we (1) defined a subset of the C++ language that automatically generates reverse code for BackStroke; (2) created a capability using the ROSE compiler to automatically reverse execution through state saving and restoration; (3) created a capability for more-sophisticated reverse code generation through value analysis and verified that BackStroke is exceeding its goals; (4) installed computers for the NetWarp platform and configured Xen virtual-machine monitors, allowing multiple operating systems to run concurrently on a host computer, with Linux running on virtual machines; and (5) evaluated the Xen scheduler and clock and network interfaces in preparation for modifying the system to work under a sequential discrete-event simulator.

Proposed Work for FY11

In FY11 we will (1) continue our proof-of-concept implementation of NetWarp on Linux networks or clusters at small scale; (2) complete the coupling of a discrete-event simulator to the Xen virtual-machine monitor to run Linux and Windows operating systems, as well as Linux or Windows router code and any applications or services that run over them; (3) extend our initial version of BackStroke so that it runs in conjunction with either the SPEEDES or ROSS parallel discrete-event simulators; and (4) demonstrate generation of inverse code using the ROSE capabilities for compiler control and data-flow analysis.

The Backstroke Framework



BackStroke uses ROSE to automatically generate reverse code for C++ methods as a means of speeding up optimistic parallel discrete-event simulations.

CgWind: A Parallel, High-Order Accurate Simulation Tool for Wind Turbines and Wind Farms—William Henshaw (10-ERD-027)

Abstract

Our objective is to develop a next-generation computational tool, called CgWind, for high-fidelity simulation of wind turbines with rotating blades and for the simulation of arrays of turbines in a wind farm, including the effects of topography and regional winds, through coupling to mesoscale atmosphere models. CgWind will solve the incompressible Navier–Stokes equations and will be based on the development of high-order accurate, compact approximations; nonlinear large-eddy simulation models for turbulent flows; adaptive mesh refinement; “matrix-free” multigrid algorithms; and parallel moving-grid-generation algorithms.

We expect that CgWind will be used by the wind turbine community to design, optimize, and predict the performance and power output of wind turbines and wind farms for energy generation. This tool will be orders of magnitude faster than existing approaches and will enable simulations that will provide new insight into the physics of these complex turbulent flow problems. CgWind will bridge the gap between the larger scale atmospheric modeling being performed at LLNL and turbine-scale flows, and therefore be an important component of an end-to-end wind-modeling capability. As part of this work, we will also develop new mathematics and algorithms such as fast, high-order accurate parallel matrix-free multigrid algorithms and fast, parallel moving-grid-generation algorithms.

Mission Relevance

This proposal supports the Laboratory’s energy and environmental security mission by enabling and enhancing the development of a clean and renewable wind energy source. This proposal also addresses the grand challenge goal of simulating high-Reynolds-number incompressible turbulent flows around complex and moving geometries and the multiscale coupling of very large-scale flows

(meteorological) with very small-scale flows (turbine-blade boundary layers) in support of LLNL’s cutting-edge science, technology, and engineering in the area of high-performance computing and simulation. The new parallel, high-order accurate matrix-free multigrid algorithms and moving-grid-generation algorithms developed under this proposal will impact various other simulation fields.

FY10 Accomplishments and Results

In FY10 we (1) developed a new high-order accurate, compact approximate-factorization scheme for the incompressible Navier–Stokes equations, using a new technique that significantly reduces the number of approximate factors that must be solved at each time step; (2) made a number of improvements to maintain time and spatial accuracy on overlapping grids and to make the scheme robust even for under-resolved flows; (3) verified the scheme with the method of manufactured solutions; (4) began developing a new fourth-order accurate, parallel, matrix-free multigrid algorithm for solving the pressure equation, developing the high-order smoothers and boundary conditions and developing parallel versions of all components, including the parallel generation of coarse grids; (5) constructed improved parallel grid generation and interpolation capabilities to support moving geometry problems; and (6) formed a calculation that demonstrates parallel moving-grid capabilities by simulating the flow past a pitching airfoil.

Proposed Work for FY11

In FY11 we will (1) continue improving our high-order compact schemes, including accurate treatment of no-slip wall boundary conditions and support for parallel computations and moving grids; (2) continue developing the high-order multigrid solver, including accurate treatment of Neumann boundary conditions in three dimensions; (3) make further improvements in parallel grid generation for moving-grid problems; (4) develop and incorporate large-eddy simulation turbulence models for overlapping grids; and (5) begin demonstration calculations of a turbine with moving blades.

Publications

Chand, K. K., and W. D. Henshaw, 2010. *CgWind: A composite grid simulation tool for wind energy applications*. 10th Symp. Overset Composite Grids and Solution Technology, NASA Ames Research Center, Moffett Field, CA, Sept. 20–23, 2010. LLNL-ABS-432826.

Chand, K. K., et al., 2010. *CgWind: A high-order accurate simulation tool for wind turbines and wind farms*. 5th Intl. Symp. Computational Wind Engineering (CWE2010), Chapel Hill, NC, May 23–27, 2010. LLNL-CONF-424863.

Binary Analysis—Daniel Quinlan (10-ERD-039)

Abstract

We propose to develop new binary analysis techniques for the analysis of software and, in particular, for the evaluation of specific behavioral properties that are critical for cyber security classification software. Our work will also address the use of parallel machines for analysis of binaries and result in tools for the analysis of binaries, comparative analysis, evaluation of properties, and application of formal-method technologies. We intend to leverage existing work in LLNL's open ROSE compiler infrastructure to support the development of specialized mixed static–dynamic analysis tools. This work will be used to build new forms of binary analysis and support domain-specific binary analysis tools.

We expect to develop new tools, new forms of binary analysis, external collaborations with industry and government, and new opportunities related to programs in cyber security. Our work is significant for both the Laboratory and throughout the DOE and elsewhere in the government. Our new tools will allow for a deeper look into binary forms for software and provide transparency to commercial off-the-shelf software—the most dominant type of software used within government and industry.

Mission Relevance

Our proposal is directly relevant to LLNL's strategic mission thrust in cyber and space security and intelligence. Our proposed research is focused on issues central to cyber security, building a research-level of expertise in binary analysis at LLNL, and especially the understanding of software and its use on Laboratory networks. An ability to analyze the software that defines network traffic will be key to understanding and predicting network behavior and providing situational awareness of ongoing network attacks in the future. Furthermore, the general identification of properties within binary software is one of a range of ways of establishing bounds on its capabilities.

FY10 Accomplishments and Results

In FY10 we developed (1) improved function recognition and disassembly in binaries to address the complexities of malware, which is significantly more complex than normal binaries generated from compiled software; (2) support for symbolic analysis of binaries as part of advancing more sophisticated state-of-the-art forms of static analysis; and (3) tools for mixed forms of static and dynamic analysis of binaries on a Windows infrastructure. This work was conducted in collaboration with the Department of Homeland Security's Computer Emergency Readiness Team (CERT) to ensure that the malware analysis tools we develop are applicable to challenges faced by government users.

Proposed Work for FY11

In FY11 we will (1) analyze CERT's malware database using some of the newest binary symbolic analysis tools built in FY10, (2) analyze sample malware using LLNL supercomputers, (3) define new formal-method analysis technologies and use these to explore function equivalence and techniques for vulnerability detection, (4) test our suite of binary analysis tools on problems posed by our collaborators at CERT to prepare for multiple government users, and (5) test our suite of analysis tools on

problems determined through collaborations with other government agencies.

Publications

Quinlan, D., and C. Cohen, 2010. "Discovery of C++ data structures from binaries." *Proc. 6th Ann. Workshop on Cyber Security and Information Intelligence Research*. LLNL-ABS-428049.

Uncertainty Visualization—Peter Lindstrom (10-ERD-040)

Abstract

This project will develop new techniques for data management and visualization of high-dimensional and high-volume data sets generated in petascale ensemble runs for uncertainty quantification. Our techniques will enable compressed data storage for post-simulation analysis without expensive reruns. This will provide unique visualization capabilities for online monitoring of ensembles to aid uncertainty quantification parameter sampling for exploration of high-dimensional merit functions and for displaying probability distributions resulting from invasive uncertainty quantification techniques. Our approach relies on wavelet statistics for concise feature description, data clustering, and highly compressed storage and on statistical summaries and new spatiotemporal interpolation schemes for visualizing complex and uncertain data.

We expect to enable offline data analysis and evaluation of new merit functions with two-orders-of-magnitude lossy but error-bounded compressed storage of time-varying simulation fields. Our methods will provide the first-ever automated tools for selective visualization of the range of behavior in huge ensembles to facilitate decision making with regards to early termination of runs and uncertainty quantification parameter selection, thereby reducing wasted computation time. We will also provide visual aids for understanding the complex relationships between high-dimensional input and output spaces and how sensitive the outcome of a simulation is to individual or combined parameter settings.

In combination, these techniques will provide entirely new capabilities critical to the success of the Laboratory's uncertainty quantification efforts.

Mission Relevance

Uncertainty quantification is a critical component of computer simulation across many mission-relevant applications, with an identified need in stockpile stewardship, climate modeling, and high-performance computing. By helping to create an advanced capability to manage, analyze, visualize, and ultimately gain insight from the complex and large quantities of data generated in uncertainty quantification codes, this project supports the Laboratory's missions in national and energy security.

FY10 Accomplishments and Results

In FY10 we developed compressed representations of three-dimensional fields defined on latitude-longitude grids such as time series from climate simulations. In particular, we (1) designed a new lossy compression scheme and demonstrated a tenfold improvement in rate distortion, (2) developed basis transformations to exploit correlations between fields for better compression, (3) designed a new family of biorthogonal wavelets with rational coefficients and improved filtering properties, (4) developed a new hybrid topological and geometric representation of high-dimensional scalar functions such as response surfaces from multiparameter uncertainty analysis—our novel two-dimensional representation accounts for geometric proximity and gradient behavior to better indicate shape and potential symmetry of the function, and (5) made theoretical advances in the identification of neighbors in sparsely sampled high-dimensional spaces to facilitate adaptive sampling and accurate reconstruction of scalar field topology.

Proposed Work for FY11

In FY11 we will (1) develop techniques for visualization of high-dimensional response functions, (2) design density estimation schemes based on wavelets, (3) develop compressed high-temporal-resolution probability density representations of time-varying fields, and (4) begin work on visualizing and

analyzing distribution fields for the qualitative and quantitative assessment of spatial uncertainty. The result of this work should be new capabilities for interpreting unknown relationships between uncertain inputs and outputs, as well as the ability to store and later query climate data at a temporal resolution (daily) more than ten times higher than currently possible and use the results to identify extreme climate events and transient and periodic phenomena that are not captured at seasonal timescales.

M3Net: Taxonomy Construction and Topic Mapping for Multimedia Message Manager Traffic—Douglas Poland (10-ERD-041)

Abstract

Intelligence analysts need to discover, access, and exploit intelligence information in a secure, tailored manner. Our objective is to connect analysts' domain models to multimedia message manager (M3) traffic in a way that allows them to more effectively exploit this vital data source. We are motivated by recent research in topic extraction, lexicon and taxonomy development, and faceted search. A pathway is needed for putting the power of these new text analytics at analysts' fingertips. To this end, we will construct a taxonomy known as M3Net from M3 data, and develop a dynamic update capability. We will then develop a methodology for mapping analyst models such as the existing FactWeave or Elecent software tools. Archived and incoming messages will be indexed via M3Net, and the mapped models will facilitate creation of domain-specific meta-indices that are instantiated as personalized facet structures.

We expect to develop an intuitive, multifaceted view of message traffic derived from analyst models of those messages for the intelligence community. Instead of a keyword-filtered list of hundreds of messages per day, our M3Net will connect analysts to the data they need and enable them to focus on higher-level analytics. If successful, this methodology will lend itself to fusion with other data sources and is a step towards plug-and-play model and data compatibility.

Mission Relevance

This project supports the Laboratory mission in national and global security. Success of M3Net will be a significant step toward the strategic mission thrust in cyber and space security and intelligence to enable end users to efficiently exploit intelligence information. In addition to advancing a more effective and efficient analytic paradigm at LLNL, with direct benefits to ongoing programs and sponsors, this project would establish the Laboratory as a leader in the development of new analytic technology that will be needed for national security.

FY10 Accomplishments and Results

We (1) developed an M3 message-parsing capability and assembled and ingested a test corpus, going through several iterations of tuning our keyword-, key-phrase-, and entity-extraction code guided by performance on our unclassified usage case; (2) performed baseline experiments in taxonomy construction, finding that even with heavy filtering of the corpus, the current state of the art—based on the University of California at Berkeley Castanet code—did not look promising; (3) developed and tested an alternative—a graph-based empirical approach to lexicon construction, which was shown to be much more flexible and robust; (4) conducted experiments in deploying the centerpiece subgraph algorithm against the test corpus, achieving promising results in filtering messages and structuring the results; (5) demonstrated the ability of our graph-based approach to capture associations between extracted entities and keywords and to be readily mapped to keyword- and key-phrase-based models; and (6) developed a meta-facet infrastructure based on the search server Solr coupled to our graph analytics, yielding a novel approach to scalable, dynamic corpus modeling.

Proposed Work for FY11

In FY11 we propose to (1) continue to focus on end-to-end experiments, using M3 data and our FY10 Psources, and develop precision and recall-like metrics for evaluating our lexicon acquisition, taxonomy mapping, and facet generation in the context of the usage cases; (2) address deficiencies

in lexicon acquisition (such as the amount of local syntax, semantics, and topics used), taxonomy mapping (word-sense disambiguation and taxonomy extension), and facet generation for both the corpus and a set of seed texts, including developing multi-layered graph construction and centerpiece subgraph algorithms; and (3) develop a Java- and Solr-based user-feedback model and interface to allow analysts to confirm or redirect the facet-generation process.

Eigensolvers for Large-Scale Graph Problems—Van Henson (10-ERD-054)

Abstract

The eigenvalues and eigenvectors of graph matrices are crucial to several applications—ranking graph nodes, clustering, identifying communities and common interests, and computing message times between nodes. We will produce scalable parallel algorithms for computing the eigenvalues and eigenvectors of matrices of extremely large graphs (with an N of billions) and for swiftly updating the eigensystems as the underlying graphs rapidly evolve. For the former, we will use graph characteristics such as power-law distributions to generate optimal search strategies and starting points. For the latter, we will restrict the computation to a carefully chosen d -dimensional subspace to capture the most significant variations in only $O(d^2)$ operations.

We expect to produce new mathematical knowledge about how the eigensystems of graph matrices are found and how they evolve, and about the nature of the graphs arising from networks and information-processing applications. We will produce research software implementing the scalable algorithms on large computer clusters such as Hera, develop an understanding of implementations for the BlueGene family of systems, and implement an eigensystem update under a streaming infrastructure. When hardened and productized, these tools will enable the application of popularity, clustering, community identification, commute time, and other important analytical tools for graphs whose sheer size has heretofore precluded such treatment.

Mission Relevance

Large-scale graphs are used in many cyber security and intelligence applications involving, for instance, the Internet, network intrusions, funding flows on financial networks, email message traffic, power grids, information propagation, information retrieval, and data mining, which this research can impact significantly.

FY10 Accomplishments and Results

We (1) performed scaling studies for parallel eigensolvers for preferential-attachment power-law graphs, with up to 1.3 billion vertices and 4 billion edges (using up to 512 Hera processors), and found these methods not scalable; (2) identified the matrix-vector multiplication (matvec) as the major barrier to scalability and devised and implemented two alternative storage and calculation schemes—preliminary tests indicate significant algorithmic speedup; (3) created and implemented two new serial multigrid-based eigensolvers and began testing, analysis, and parallelization—we discovered a new disaggregation method for approximating the eigenvalues of a power-law graph to arbitrary accuracy while simplifying and speeding the inter-processor communication in the parallel matvec; and (4) hired two postdoctoral researchers and two summer students, bringing to the Laboratory additional expertise in scalable computing.

Proposed Work for FY11

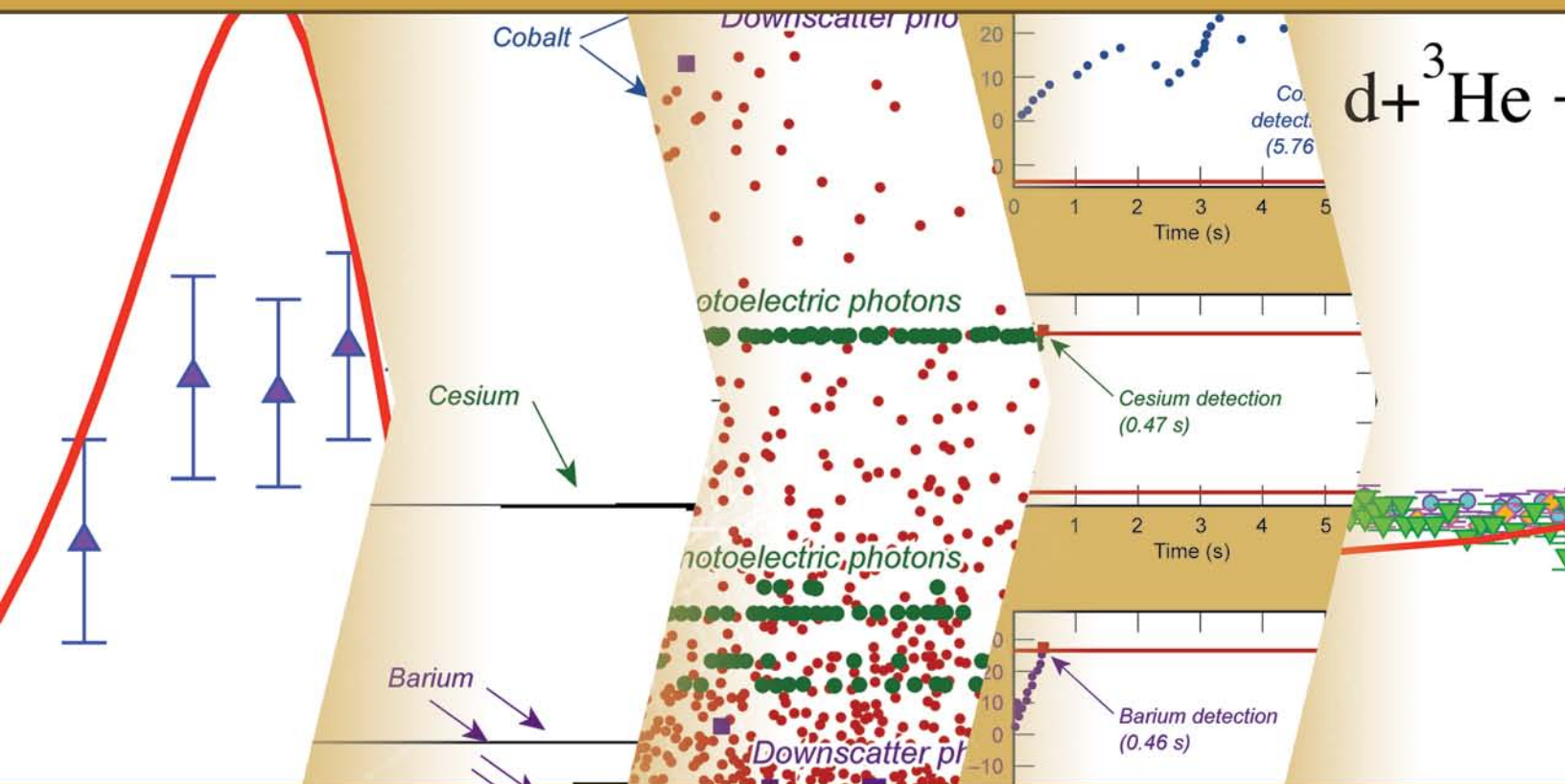
For FY11 we will (1) continue to analyze and improve standard parallel eigensolver packages, primarily by improving matvec for efficiency when applied to power-law graphs; (2) continue researching multilevel methods, improving and expanding multigrid-based eigensolver approaches; (3) begin parallelizing the multigrid-based eigensolvers; (4) determine how low-rank approximations of the graph Laplacian can be used to accurately compute commute times and implement the approximations in codes that can be used in allied projects; (5) implement an eigensolver on the Hadoop cluster; and (6) work with Sandia National Laboratories to implement and analyze low-rank updating methods

for eigensolvers and tensors on the Cray XMT shared-memory supercomputer.

Publications

De Sterck, H., V. E. Henson, and G. Sanders, 2010.
Multilevel aggregation methods for small-world graphs with application to random-walk ranking.
Intl. Workshop on Information Retrieval by Matrix Methods on Supercomputer Infrastructures, Tsukuba, Japan, June 1–4, 2010. LLNL-PROC-428196.

Winlaw, M., M. J. O'Hara, and V. E. Henson, 2010.
Nonnegative matrix factorization using bicliques.
SIAM Annual Meeting, Philadelphia, PA, July 12-16, 2010. LLNL-PRES-453094.



$d + {}^3\text{He} \rightarrow$

Nuclear Science
and Engineering

Detection, Classification, and Estimation of Radioactive Contraband from Uncertain, Low-Count Measurements—James Candy (07-ERD-019)

Abstract

The detection of smuggled special nuclear material (SNM) is a critical issue for homeland security as well as for nonproliferation efforts and the manufacturing, processing, and tracking of material. Today's high-speed, high-throughput computers enable physics-based statistical models that capture the essential signatures of radionuclides to be incorporated into a sequential scheme (a Bayesian sequential processor) capable of online, real-time operation. This project is focused on the detection, classification, and estimation of SNM from highly uncertain, low-count radionuclide measurements using a statistical approach based on Bayesian inference and physics-based signal processing. The effort will encompass theory, simulation, experiments, and application.

We expect to develop solutions for the reliable detection of a stationary as well as a moving SNM source, with a goal of 95% probability of detection 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 to a large variety of model-based problems in many other critical areas of Laboratory work, including defect detection in the Stockpile Stewardship Program, nonproliferation, and the manufacturing, processing, and tracking of SNM. Advanced signal- and image-processing techniques for the next generation of processors will evolve.

Mission Relevance

The detection of illicit SNM is a top priority of LLNL in furthering the national security mission. Radionuclide detection, classification, and identification are critical for detecting 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.

FY10 Accomplishments and Results

We developed a statistical radiation-detection software system (SRaDS). Specifically, we (1) theoretically developed an optimal physics-based decision function that incorporates both photoelectric and downscattered photons (Compton scattering); (2) applied these theoretical results to develop an algorithm capable of automatically detecting targeted SNM; (3) implemented a simple signal-processing transport model, enabling down-scatter photon discrimination; (4) estimated the required physics parameters—for instance, channel energy, inter-arrival parameters, and emission probabilities—using modern Bayesian sequential techniques such as Kalman and particle filters; (5) implemented a parallel, distributed algorithmic structure capable of being realized with field-programmable gate arrays to achieve high computational speeds; (6) applied the algorithmic structure to a set of controlled experimental data for high-purity germanium detectors; and (7) verified a detection probability of 98% for SRaDS, compared to 46% for the spectroscopy software analysis software GAMANAL (both yielded 0% false alarm rates). In summary, this project developed a novel sequential radiation detection software system, SRaDS, which demonstrated outstanding radionuclide detection performance with high reliability and short acquisition times. SRaDS is a breakthrough in detection processing that couples Bayesian statistical processors with physics-based models incorporating Compton down-scatter information. The next step is to evaluate this capability with moving containers.

Publications

Candy, J. V., et al., 2010. *Detection, classification and estimation of radioactive contraband from uncertain low-count measurements*. LLNL-TR-426278.

Candy, J. V., et al., 2010. "Model-based detection of radioactive contraband for harbor defense incorporating Compton scattering physics." *Proc. Oceans 2010 IEEE Sydney*. LLNL-CONF-425060.

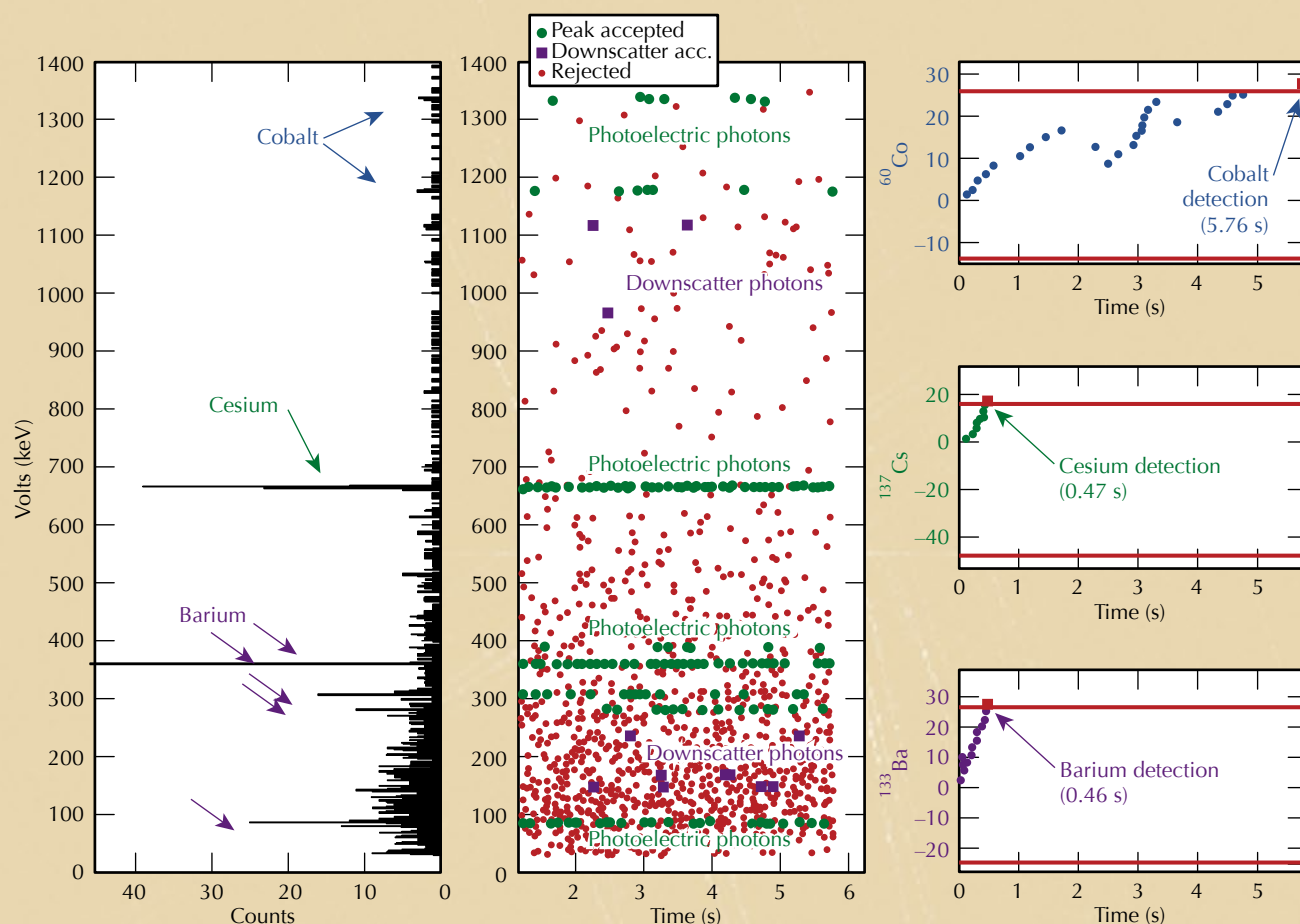
Candy, J. V., et al., 2009. "Physics-based detection of radioactive contraband: A sequential Bayesian approach." *IEEE Trans. Nucl. Sci.* **56**(6), 517. LLNL-JRNL-411357.

Candy, J. V., et al., 2009. "Radioactive contraband detection: A Bayesian approach." *Proc. MTS-IEEE Oceans 2009 Conf.* LLNL-CONF-411355.

Candy, J. V., et al., 2010. "Radioactive threat detection with scattering physics: A model-based application." *Proc. 2nd Intl. Workshop Cognitive Information Processing*. LLNL-CONF-423209.

Candy, J. V., et al., 2010. "Statistical radiation detection system (SRaDS)." *R&D 100 Mag.*, July 2010. LLNL-BR-425377.

Candy, J. V., et al., 2010. "Threat detection of radioactive contraband incorporating Compton scattering physics: A model-based processing approach." *IEEE Trans. Nucl. Sci.* **57**(6). LLNL-JRNL-422429.



Composite pulse-height spectrum. The second column shows the measured photon energies (arrivals) in red circles. The green circles and blue squares represent discriminator output. The third column shows decision functions and thresholds.

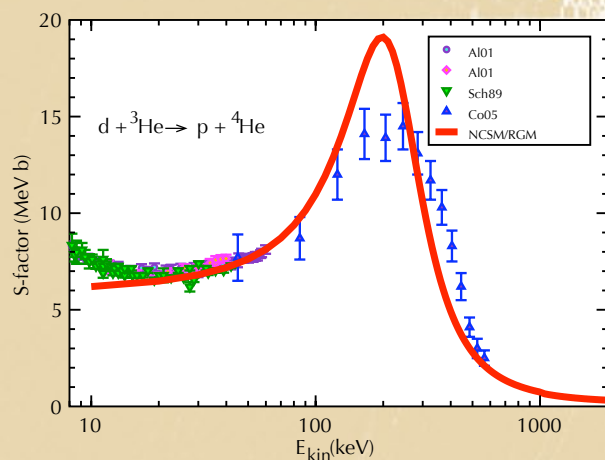
Chambers, D., 2008. "Signal-processing model for radiation transport." *IEEE Trans. Nucl. Sci.* **1**, 150. LLNL-TR-405952.

How Carbon and Oxygen Can Be Made in Stars: An Ab Initio Approach to Nuclear Reactions—Petr Navratil (09-ERD-020)

Abstract

Predictions of stellar and nucleosynthesis modeling depend strongly on knowledge of the reactions that produce carbon-12 and oxygen-16. These thermonuclear reactions determine the carbon-to-oxygen ratio during stellar helium burning, with far-reaching consequences for the production of all heavier species. Current knowledge about the reactions is insufficient, and a breakthrough can be reached only with a fundamental theory. We propose to develop an ab initio many-body nuclear reaction theory to accurately predict the rates of alpha-capture reactions responsible for production of the two elements. In this project, alpha-capture rates will be calculated from first principles by means of an ab initio no-core shell model combined with the resonating-group method.

We will systematically develop formalism and codes to treat the scattering on light nuclei of



Results for the astrophysical S-factor from the ab initio no-core shell model combined with the resonating-group method (NCSM/RGM) for the $^3\text{He}(d,p)^4\text{He}$ capture reaction, with comparison to beam-target measurements. Data curve up and deviate from theoretical results at low energy because of laboratory electron screening.

increasingly heavier projectiles and perform the first-ever ab initio calculations of $\text{D}(\text{T},\text{n})^4\text{He}$ and $^4\text{He}(^3\text{He},\gamma)^7\text{Be}$ cross sections as intermediate steps towards addressing the alpha-capture reactions leading to the formation of carbon-12 and oxygen-16. The successful completion of this project will result in (1) a long-awaited ab initio theory to explain alpha clustering in light nuclei and calculate cross sections of reactions important for astrophysics from first principles; (2) an improved accuracy of the $2\text{-}\alpha(\alpha,\gamma)^{12}\text{C}$ and $^{12}\text{C}(\alpha,\gamma)^{16}\text{O}$ reaction rates; and (3) an enhancement of the predictive capability in stellar modeling.

Mission Relevance

This project will establish the capability to perform calculations of light-ion reactions relevant to LLNL efforts in fusion energy generation and will result in a fundamental understanding of alpha clustering and improved alpha-burning cross sections for astrophysics, in support of the Laboratory's national security mission.

FY10 Accomplishments and Results

In FY10 we (1) developed the formalism for three-nucleon projectiles necessary to describe the $^4\text{He}(^3\text{He},\gamma)^7\text{Be}$ capture reaction including deriving expressions for the three-nucleon projectile-integration kernels and coding and testing the norm kernel; (2) began coding of the Hamiltonian kernel; (3) obtained intermediate results of ^3He -alpha and ^3H -alpha scattering calculations and ab initio $^4\text{He}(^3\text{He},\gamma)^7\text{Be}$ and $^4\text{He}(^3\text{H},\gamma)^7\text{Li}$ capture reaction calculations; (4) successfully completed D-alpha scattering and lithium-6 bound-state calculations; and (5) obtained the first ever ab initio calculations of the $\text{D}(\text{T},\text{n})^4\text{He}$ and $\text{D}(^3\text{He},\text{p})^4\text{He}$ reactions.

Proposed Work for FY11

In FY11 we will (1) develop the formalism for four-nucleon projectile formalism, extending our ab initio many-body nuclear reaction theory from the three-nucleon projectile capability developed in FY10, which will allow us to describe alpha-nucleus scattering and alpha clustering in light nuclei; (2) test the formalism in alpha-alpha scattering calculations; (3) study alpha clustering in carbon-12 and

oxygen-16; and (4) derive ab initio calculations of $^8\text{Be}(\alpha, \gamma)^{12}\text{C}$ and $^{12}\text{C}(\alpha, \gamma)^{16}\text{O}$ cross sections.

Publications

Navratil, P., and S. Quaglioni, 2009. "Applications of local chiral N^2LO three-nucleon interaction to nuclear structure and reactions." *Bull. Am. Phys. Soc.* **54**, DH.00008. LLNL-ABS-414346.

Navratil, P., and S. Quaglioni, 2009. "Towards the first ab initio calculation of the deuterium–tritium fusion." *Bull. Am. Phys. Soc.* **54**, DM.00005. LLNL-ABS-414340.

Navratil, P., S. Quaglioni, and R. Roth, in press. "Ab initio theory of light-ion reactions." *J. Phys. Conf.* LLNL-PROC-455934.

Navratil, P., R. Roth, and S. Quaglioni, 2010. "Ab initio many-body calculations of nucleon scattering on ^4He , ^7Li , ^7Be , ^{12}C and ^{16}O ." *Phys. Rev. C* **82**, 034609. LLNL-JRNL-439759.

Navratil, P., et al., 2009. "Recent developments in no-core shell model calculations." *J. Physics G: Nucl. Part. Phys.* **36**, 083101. LLNL-JRNL-411567.

Quaglioni, S., and P. Navratil, 2009. "Ab initio many-body calculations of nucleon-nucleus scattering." *Phys. Rev. C* **79**, 044606. LLNL-JRNL-409500.

Quaglioni, S., P. Navratil, and R. Roth, 2010. "Scattering of light nuclei." *EPJ Web Conf.* **3**, 01012. LLNL-PROC-421512.

Shock Temperatures from Neutron Resonance Spectroscopy—James McNaney (09-ERD-037)

Abstract

Temperature is a fundamental thermodynamic property, and accurate measurements are necessary to understand and predict processes involving thermal activation, such as chemical reactions, plastic flow, and phase transitions. However,

temperature is extremely difficult to measure during dynamic loading. Optical techniques such as pyrometry are widely used but cannot probe the bulk volume of opaque materials such as metals. We intend to develop neutron resonance spectrometry for measuring temperature dynamically and in situ during shock loading by developing a short-pulse laser-based neutron source.

Successful completion of this work would result in a high-fidelity, time-resolved temperature-measurement technique capable of probing the interior of a dynamically loaded material on a nanosecond timescale. Development of a high-fluence, single-shot, and laser-based neutron source would represent a significant achievement, while resonance spectrometry at the nanosecond timescale would represent a groundbreaking achievement. The technique would have diagnostic application in mid- to large-scale fusion-class laser facilities, and measurements made using this approach would lead to a better understanding of temperature-dependent material behavior in general.

Mission Relevance

Development of a neutron resonance spectrometry capability would be of high value to Laboratory efforts in both weapons and photon science, in support of the Stockpile Stewardship Program and the national and energy security missions. In particular, the proposed work would support advanced physical model development, improved materials property understanding, advanced experiments and diagnostics, and high-neutron-flux science. This capability would have significant impact on understanding many aspects of material behavior under dynamic loading conditions, including those relevant to LLNL fundamental high-energy-density research.

FY10 Accomplishments and Results

In FY10 we (1) demonstrated neutron production on the short-pulse Titan laser at LLNL over a range of conditions and neutron converter materials, (2) developed an optimization method to obtain maximal neutron yield on short-pulse laser systems, (3) developed a scaled-up experiment for the OMEGA EP laser at the University of Rochester, and

(4) began a collaboration with the OMEGA facility to speed the development of time-resolved neutron-detection methodologies necessary for spectrometry measurements.

Proposed Work for FY11

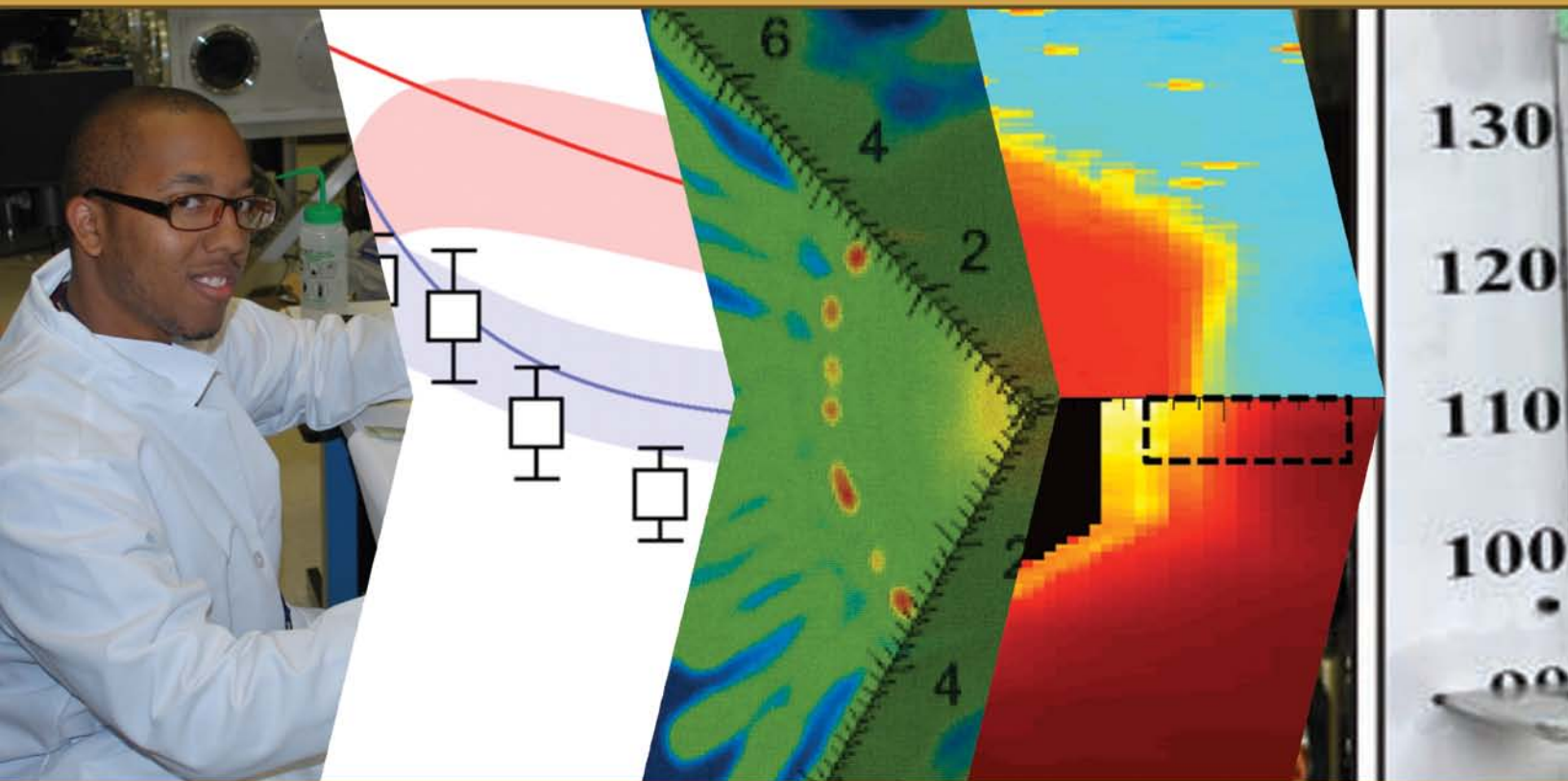
In FY11 we will demonstrate the feasibility of shocked neutron resonance spectrometry measurements by achieving multiple technical goals. Specifically, we will (1) develop the ability to measure epithermal neutrons in the presence of short-pulse laser-based prompt radiation, (2) demonstrate sufficient epithermal neutrons to characterize static neutron-absorption resonance, and (3) perform a credible laser-based material dynamics experiment for temperature measurement.

Publications

Higginson, D. P., et al., 2010. "Laser-generated neutron source for neutron resonance spectroscopy." *Phys. Plasma*. **17**, 100701. LLNL-JRNL-428631.

Higginson, D. P., et al., 2009. *Laser-generated proton beam optimization for (p,n) neutron production*. 51st Ann. Mtg. APS Division of Plasma Physics, Atlanta, GA, Nov. 2–6, 2009. LLNL-POST-418832.

Higginson, D. P., et al., 2009. *Manipulation of laser-generated proton beam energy distribution for (p,n) neutron production*. 51st Ann. Mtg. APS Division of Plasma Physics, Atlanta, GA, Nov. 2–6, 2009. LLNL-ABS-414877.



Physics

Fast-Ignition Proof-of-Principle Experiments—Pravesh Patel (08-SI-001)

Abstract

We propose to investigate the feasibility of a new laser ignition approach of fast ignition, which directly compresses the fusion fuel to high densities and then ignites it with a separate laser beam. This challenging approach offers the potential for large advances in efficiency over central hot-spot ignition that is being studied in the Stockpile Stewardship Program. We will perform integrated fast-ignition experiments that will measure and optimize the laser-to-ignition hotspot-energy-coupling efficiency for a fuel assembly required for high-gain fast ignition. Our work will define requirements for fast ignition and provide the pathway to robust 100-MJ-yield platforms for experimental access to extreme high-energy-density environments.

This project will define the requirements for high-gain fast ignition for future fusion-class laser systems. In particular, we will optimize isochoric fuel assembly in the presence of a cone and understand and optimize both ultra-intense laser-plasma interactions and energy transport by relativistic electrons to measure the short-pulse energy required to obtain high-gain fast ignition. We will resolve the key physics uncertainties in fast ignition, which will have broad implications for high-energy-density science.

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 missions in stockpile stewardship and energy security and allow access to new regimes of excited-state nuclear physics and basic science. In addition, increased gain from fast ignition will enable an inertial fusion path to energy security for the nation.

FY10 Accomplishments and Results

In FY10 we (1) designed and fabricated targets for two experimental campaigns on the National Ignition Facility (NIF) to test different compression schemes—single-shock and four-shock drive—and to study hohlraum energetics and the symmetry of the implosion of a spherical fast-ignition capsule; (2) developed a two-dimensional cone-in-shell

implosion with 500-kJ laser drive, producing target yields of 20 MJ; (3) developed an integrated point design using particle-in-cell, hybrid transport, and radiation-hydrodynamic codes to model fuel compression, fast electron generation and transport, and core heating, showing that at ignition scale, the fast electron beam is produced with a high intrinsic divergence, resulting in extremely high ignition energies on the order of 1 MJ of incident laser energy; (4) designed experiments on the OMEGA laser at the University of Rochester to validate new tuning strategies for single-shock compression targets; (5) designed radiography experiments to characterize fuel assembly around the cone tip; and (6) successfully tested the technique on the OMEGA laser and demonstrated its feasibility for NIF's advanced radiographic capability. This project has produced a significant new capability for the advanced, self-consistent simulation of fast-ignition inertial-confinement fusion. A new program has been founded in the DOE Office of Fusion Energy Sciences to develop the fast-ignition concept as a potential advanced ignition target scheme for inertial fusion energy.

Publications

Akli, K. U., 2009. *Measurements of high-intensity, short-pulse laser-generated electron beam flux*. IFSA2009, 6th Intl. Conf. Inertial Fusion Sciences and Applications, San Francisco, CA, Sept. 6–11, 2009. LLNL-ABS-412303.

Akli, K. U., et al., 2010. "A dual-channel x-ray spectrometer for fast ignition research." *J. Instrum.* **5**, P07008. LLNL-JRNL-428255.

Amendt, P., 2010. *Radiation-hydrodynamics simulations of fast-ignition compression experiments on the National Ignition Facility*. LLNL-ABS-444094.

Beg, F. N., 2010. *Fast electron transport in laser-driven shock heated warm dense matter relevant to fast ignition*. 52nd Ann. Mtg. APS Division of Plasma Physics, Chicago, IL, Nov. 8–12, 2010. LLNL-ABS-459921.

Chen, C. D., et al., 2009. "Bremsstrahlung and K-alpha fluorescence measurements for inferring conversion efficiencies into fast ignition

relevant hot electrons." *Phys. Plasma*. **16**, 082705. LLNL-JRNL-415191.

Chen, C. D., et al., 2010. *Bremsstrahlung measurements of hot electron divergence and coupling efficiency in planar and conical geometries*. 52nd Ann. Mtg. APS Division of Plasma Physics, Chicago, IL, Nov. 8–12, 2010. LLNL-ABS-445273.

Chen, C. D., et al., 2010. "Suprathermal electron generation in fast ignition relevant short-pulse laser plasma interactions." *Proc. 2010 IEEE Intl. Conf. Plasma Science*. LLNL-ABS-422852.

Chrisman, B., et al., 2010. *Ionization and Z effects in cone wire experiments*. 52nd Ann. Mtg. APS Division of Plasma Physics, Chicago, IL, Nov. 8–12, 2010. LLNL-ABS-443203.

Friesen, H., 2010. *Simultaneous investigation of hot-electron transport and preplasma formation in cone-wire targets*. 52nd Ann. Mtg. APS Division of Plasma Physics, Chicago, IL, Nov. 8–12, 2010. LLNL-ABS-451971.

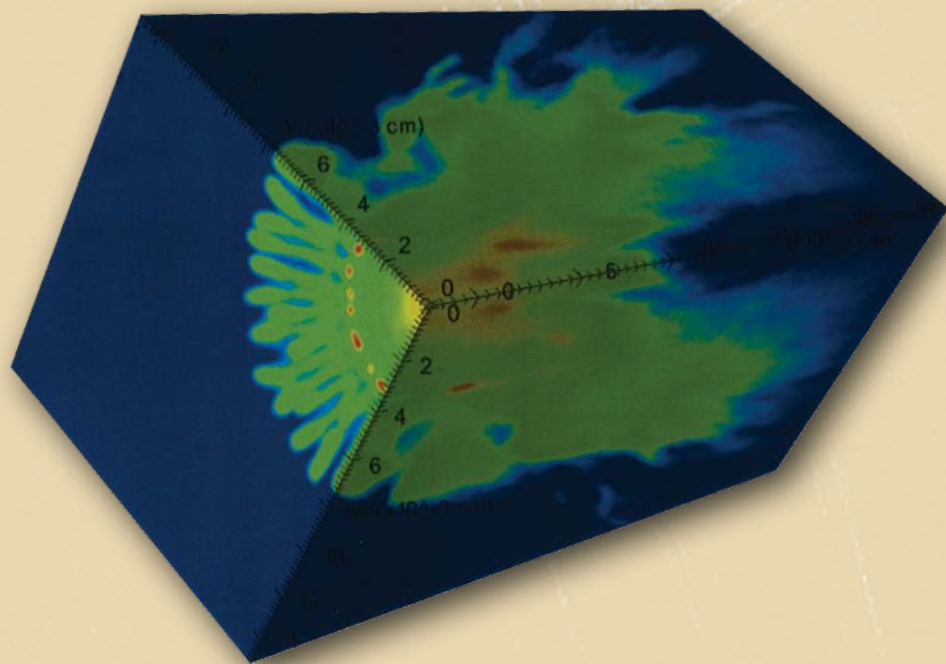
Hey, D. S., 2010. *Compton radiography of directly driven fast ignition implosions on Omega*. 11th Intl. Workshop on Fast Ignition of Fusion Targets, Shanghai, China, Oct. 17–21, 2010. LLNL-ABS-445274.

Higginson, D. P., 2010. *Fast ignition relevant hot electron coupling at 1ω and 2ω* . 52nd Ann. Mtg. APS Division of Plasma Physics, Chicago, IL, Nov. 8–12, 2010. LLNL-ABS-442571.

Homoelle, D., 2010. *Progress of the fast ignition drive optics upgrade to the ARC beamline on NIF*. 2010 Conf. Intl. Committee on Ultrahigh-Intensity Lasers, Watkins Glen, NY, Sept. 26–Oct. 1, 2010. LLNL-ABS-428065.

Kemp, A. J., 2010. *Focusing of picosecond laser pulses in cone geometries*. 52nd Ann. Mtg. APS Division of Plasma Physics, Chicago, IL, Nov. 8–12, 2010. LLNL-ABS-442498.

Kemp, A. J., 2009. *Full-scale kinetic modeling of short-pulse interaction and electron transport in*



A three-dimensional integrated simulation of a fast-ignition target performed with coupled radiation-hydrodynamics (HYDRA) and hybrid electron-transport (ZUMA) codes. The color scale represents the electron energy-deposition rate (eV/cm/μsec), from 0 (blue) to 8.5^{11} (red).

cone target experiments. 2nd Intl. Conf. High Energy Density Physics, Austin, TX, May 19–22, 2009. LLNL-ABS-411899.

Kemp, A. J., B. Cohen, and L. Divol, 2010. "Integrated kinetic simulation of laser-plasma interactions, fast electron generation and transport in fast ignition." *Phys. Plasma*. **17**, 056702. LLNL-JRNL-420456.

Kemp, A. J., et al., 2010. *Interaction of intense laser pulses with plasma gradients at fast-ignition scales*. 52nd Ann. Mtg. APS Division of Plasma Physics, Chicago, IL, Nov. 8–12, 2010. LLNL-ABS-442499.

Larson, D. J., et al., 2010. *Hybrid simulations for magnetized fast ignition targets and analyzing cone-wire experiments*. 52nd Ann. Mtg. APS Division of Plasma Physics, Chicago, IL, Nov. 8–12, 2010. LLNL-ABS-443231.

Ma, T., 2009. *Effects of laser prepulse on hot electron production and transport in hollow cone targets*. 16th Intl. Conf. Atomic Processes in Plasmas, Monterey, CA, 2009. LLNL-ABS-409819.

Ma, T., 2009. *Laser-to-fast-electron conversion efficiency scaling with prepulse in cone targets*. IFSA2009, 6th Intl. Conf. Inertial Fusion Sciences and Applications, San Francisco, CA, Sept. 6–11, 2009. LLNL-ABS-412205.

Ma, T., et al., 2009. *Study of hot electron production and transport as a function of preplasma filling of hollow cone targets*. 36th Intl. Conf. Plasma Science and 23rd Symp. Fusion Engineering, San Diego CA, May 31–June 5, 2009. LLNL-ABS-409816.

Mackinnon, A. J., et al., 2009. *Progress in fast ignition studies with electrons and protons*. APiP2009, 16th Intl. Conf. Atomic Processes in Plasmas, Monterey, CA, Mar. 22–26, 2009. LLNL-ABS-409835.

MacPhee, A. G., 2009. *Explaining the effects of laser pre-pulse on hot electron generation in cones*. 6th Intl. Conf. Inertial Fusion Sciences and Applications, San Francisco, CA, Sept. 6–11, 2010. LLNL-ABS-412374.

Ovchinnikov, V. M., 2010. *Recent measurements of the effects of cones on hot electron divergence*. LLNL-ABS-459371.

MacPhee, A. G., et al., 2009. "Limitation on pre-pulse level for cone-guided fast-ignition ICF." *Phys. Rev. Lett.* **104**, 055002. LLNL-JRNL-416502.

Patel, P. K., 2009. *Design of fast ignition core heating experiments with full scale hydrodynamic fuel assembly*. IFSA2009, 6th Intl. Conf. Inertial Fusion Sciences and Applications, San Francisco, CA, Sept. 6–11, 2009. LLNL-ABS-413395.

Sawada, H., et al., 2010. *Bremsstrahlung measurements for fast electron characterization at Omega EP*. 52nd Ann. Mtg. APS Division of Plasma Physics, Chicago, IL, Nov. 8–12, 2010. LLNL-ABS-446053.

Shay, H. D., et al., 2010. "Design considerations for a cone in a fast ignition capsule." *J. Phys. Conf. Ser.* **244**, 022061. LLNL-PROC-417877.

Strozzi, D. J., 2010. *Modeling of electron-driven fast ignition at ignition scale*. 40th Ann. Anomalous Absorption Conf., Snowmass Village, CO, June 13–18, 2010. LLNL-ABS-429632.

Tabak, M., 2010. *Assembling fuel in fast ignition cone-shell targets for good transport coupling*. 52nd Ann. Mtg. APS Division of Plasma Physics, Chicago, IL, Nov. 8–12, 2010. LLNL-ABS-441691.

Tabak, M., et al., 2010. "Features of a point design for fast ignition." *J. Phys. Conf. Ser.* **244**, 022066. LLNL-ABS-412196.

Tommasini, R., 2010. *Compton radiography: A novel diagnostic for implosions*. 14th Intl. Workshop Radiative Properties of Hot Dense Matter, Marbella, Spain, Oct. 4–8, 2010. LLNL-ABS-455131.

Wei, M. S., 2010. *Investigation of dependence of laser absorption and energy coupling on target material*. LLNL-ABS-459920.

Westover, B., et al., 2010. *Short-pulse laser-produced electron temperature, divergence and conversion efficiency measurements using multiple x-ray*

spectrometers. 52nd Ann. Mtg. APS Division of Plasma Physics, Chicago, IL, Nov. 8–12, 2010. LLNL-ABS-451971.

Nonequilibrium Electron Dynamics in Warm Dense Matter—Yuan Ping (08-ERD-005)

Abstract

Recent discoveries in the behavior of warm dense matter cannot be explained by existing theory, which ignores nonequilibrium and nonadiabatic effects. Our goal is to understand dynamic electron behavior under nonequilibrium extreme conditions and to advance condensed matter theory beyond adiabatic approximation. This will be an integrated experimental and theoretical effort, which will overcome a fundamental barrier in condensed matter physics by measuring temporal evolution of the electron density of states and introducing nonequilibrium electron distribution and nonadiabatic electron–phonon coupling in calculations. Measurements will be made using optical and x-ray probes, and theory development will be based on an extension of the Ehrenfest theorem, which is the expectation value of the Heisenberg equation of motion.

We will obtain temporal evolution of carrier density and dielectric function from optical measurements and the N-edge absorption structure from

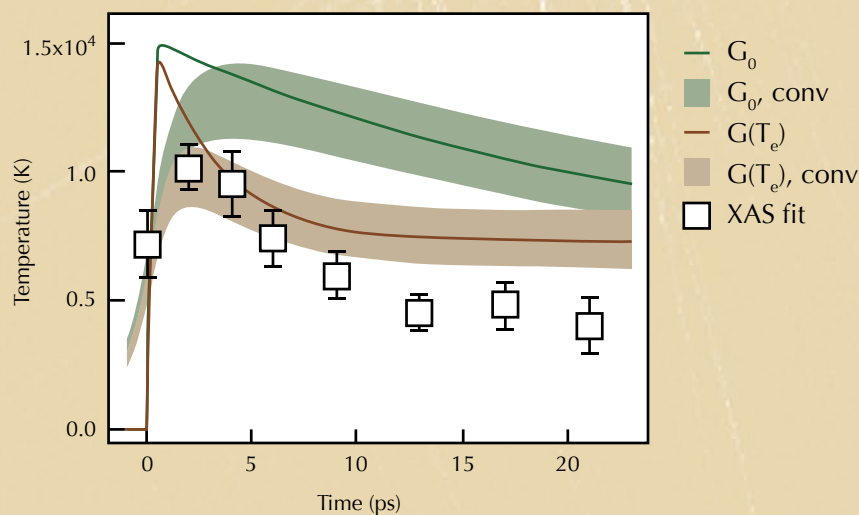
x-ray measurements. These will be the first data on the behavior of electron density of states under nonequilibrium extreme conditions, serving not only as a phenomenological guide to model development, but also as a quantitative benchmark of theory. Our theory effort will yield calculations of nonequilibrium 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.

FY10 Accomplishments and Results

We (1) completed time-resolved x-ray absorption spectroscopic measurements and obtained high-quality data for laser-heated copper, which, in combination with theoretical calculations of x-ray absorption cross-sections, represent the first evidence of a temperature-dependent electron–phonon coupling rate; (2) found the electron–phonon



Temporal evolution of equilibrium electronic energy (T_e). The calculations using a T_e -dependent electron–phonon coupling coefficient G (brown) show better agreement with the experimental data (squares) than does a constant G (green).

coupling rate to be enhanced at an elevated equilibrium electronic energy, so that the electrons are cooler than expected using a constant coupling rate; (3) researched the ballistic transport of excited electrons—the key process for isochoric heating—instead of selective excitation, after determining that because of poor contrast, measurements made with an 800-nm pump were sensitive to the pulse shape of the laser, which was difficult to control; and (4) conducted measurements using a novel front-and-back Fourier domain interferometry, discovering reduced ballistic distance of electrons at high energy densities (above 5 MJ/kg). This project led to the discovery of a temperature-dependent electron–phonon coupling rate, which has already had a profound impact on modeling and understanding high-energy-density matter, and to collaborations in the field with the Stanford Linear Accelerator Center, Lawrence Berkeley National Laboratory, and Florida State University. In addition, our novel diagnosing techniques have already been adopted for experiments on the x-ray free-electron laser at the Stanford Linear Accelerator Center.

Publications

Cho, B. I., et al., 2010. *Electronic structure of warm dense copper studied by ultrafast x-ray absorption spectroscopy*. LLNL-JRNL-455938.

Ping, Y., et al., 2010. “Warm dense matter created by isochoric laser heating.” *High Energy Density Phys.* **6**, 246. LLNL-PROC-419545.

Studying Reactions of Excited Nuclear States—Lee Bernstein (08-ERD-008)

Abstract

The formation of heavy elements in astrophysical environments involves reactions of both ground and excited nuclear states in high-energy-density plasmas. Inertial-confinement fusion lasers offer an unprecedented opportunity to observe reactions in excited nuclear states because of the exceptionally short “burn” time and nuclear–plasma interactions

that occur in the plasma environment. We will study nuclear–plasma interactions in a high-energy-density plasma and the effect of the population of excited nuclear states on nucleosynthesis reactions through an accelerator-based nuclear science program. In addition, we will develop a plan for a new class of scientific experiments investigating these nuclear states at Livermore’s National Ignition Facility (NIF).

This project will result in an increased understanding of both nuclear–plasma interactions and the effects that excited nuclear states, through these interactions, have on reactions in both stellar and stockpile stewardship environments. We will also produce a plan for performing astrophysically relevant excited-state reaction experiments using fusion-class lasers. This work will be coordinated with a program to develop nuclear diagnostic capability for fusion-class lasers and act to integrate the scientific capabilities needed for our unique work into the diagnostics being developed. In addition, it will 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 the reactions of nuclei in excited states will improve the interpretation of radiochemical data, which are a key nuclear weapons diagnostic used in both stockpile stewardship and nonproliferation applications. Our research also supports the Laboratory’s mission in frontier science by improving the interpretation of radiochemical data relevant to the formation of elements in astrophysical environments.

FY10 Accomplishments and Results

In FY10 we devised a method for measuring neutron capture cross sections in NIF experiments through observation of the statistical gamma rays emitted following neutron capture using gas Cherenkov detectors in a gamma reaction history system. Because NIF will enable measurements of nuclear reactions at the temperatures, densities, and ionization states similar to those that occur in stars, NIF scientists will be able to study the stellar s-process, a series of slow neutron-capture reactions and

beta decays that synthesize half the nuclei above iron. The development of this technique provided the technical basis for the very first approved shot-time proposal for a NIF nuclear physics experiment to measure astrophysically relevant neutron spectra using gamma reaction history. In addition, we participated in the first-ever workshop on neutron-capture nucleosynthesis with NIF, which was attended by 40 scientists from 5 different international nuclear science institutions. This workshop, together with two white papers describing collaborative nuclear physics work using NIF, has helped cement future collaborations. Overall, this project resulted in a peer-reviewed plan for performing, and the first data from, nuclear physics experiments using NIF. In the coming year we will continue our collaborative work with faculty and staff from GSI Helmholtz Centre for Heavy Ion Research in Germany, the CEA Alternative Energies and Atomic Energy Commission in France, and Notre Dame and Ohio universities in the U.S. We will provide the technical capabilities needed to propose new nuclear physics experiments at NIF, beginning with a workshop in the United Kingdom in March 2011.

Publications

Bernstein, L. A., 2010. *Neutron capture measurements using the National Ignition Facility*. LLNL-PROP-457055.

Bernstein, L. A., 2010. *Nuclear excitation in plasma environments*. LLNL-PROP-457810.

Bernstein, L. A., 2010. *Nuclear physics at the National Ignition Facility: Physics at the atomic/nuclear interface*. LLNL-ABS-423420.

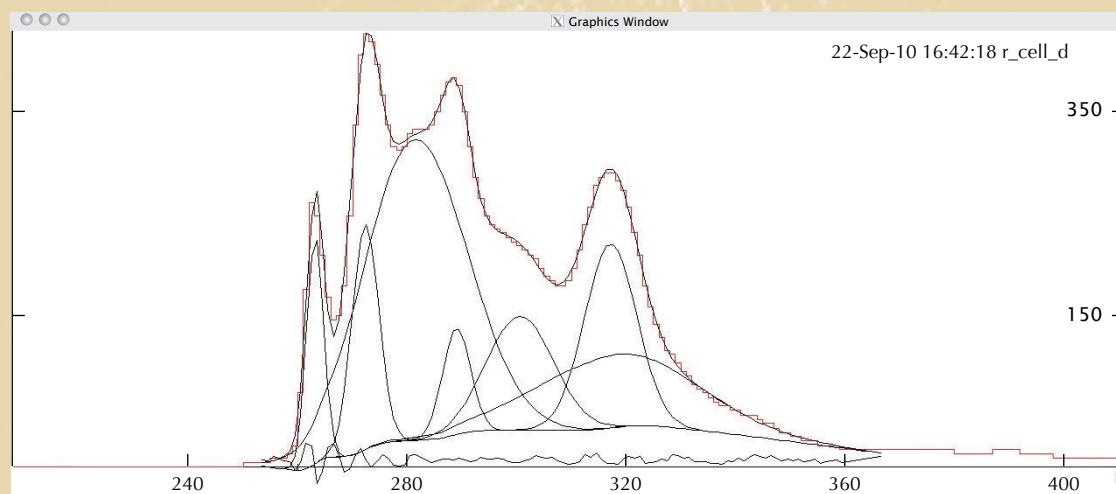
Bernstein, L. A., et al., 2009. *Reactions on nuclei in high energy density plasmas*. 2nd Workshop Level Density and Gamma Strength, Oslo, Norway, May 11–15, 2009. LLNL-ABS-412220.

Bernstein, L. A., 2010. *Realistic stellar nucleosynthesis studies involving nuclear excitation via atomic–nuclear interactions in high energy density plasma environments*. LLNL-PROP-424305.

Bernstein, L. A., et al., 2009. *Studying reactions on excited states using NIF*. Fall Mtg. American Chemical Society, Washington, DC, Aug. 16–20, 2009. LLNL-ABS-411365.

Bernstein, L. A., 2010. *Using NIF to study the interaction of hot nuclear matter with neutron-rich plasmas*. LLNL-ABS-463533.

Wiedeking, M., et al., 2009. *Determining lifetimes of highly excited nuclear states*. LLNL-PRES-417198.



First gamma reaction history data showing neutron-induced reactions on material near the National Ignition Facility target chamber center. The peak furthest to the left represents the production of neutrons from the fusion of deuterium and tritium.

Exploration of Laser–Plasma Interactions for High-Performance Laser-Fusion Targets—David Strozzi (08-ERD-017)

Abstract

We will use kinetic simulation and analytical theory to study nonlinear laser–plasma interactions relevant to advanced, future laser-fusion targets. For many planned laser applications, laser–plasma interactions such as Raman and Brillouin scattering are expected to be in a nonlinear regime, and uncertainty regarding these interactions has led to several conservative design choices. Better understanding of the interactions may relax these constraints and expand future laser capabilities such as enabling the use of higher-energy “green” laser light. For our project, we will use the three-dimensional (3D) particle-in-cell code Z3, the 1D Eulerian Vlasov code Sapristi, and, if available, a 2D Vlasov code currently in development.

Our research will advance the knowledge of nonlinear laser–plasma effects, including particle trapping and the Langmuir decay instability. 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 laser target 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.

FY10 Accomplishments and Results

In FY10 we (1) continued collaborating with France’s Atomic Energy Commission on a nonlinear adiabatic theory of stimulated Raman scattering (SRS), which compared well with Vlasov simulations and resulted in several publications; (2) conducted Vlasov studies of SRS re-amplification by crossing lasers and found gains at or below the linear level; (3) modeled backward Raman amplifier experiments and conducted particle-in-cell modeling of seeded SRS and of the density gradients of SRS-generated energetic electrons; (4) derived and published a fully relativistic theory of Thomson scattering, which agreed well with Jupiter laser experiments; (5) applied a threshold condition for two-plasmon decay to ignition plasmas to explore a reduced instability threshold for obliquely incident light resulting from electric-field swelling; and (6) applied our electron-trapping metric, based on competition with collisions and geometric loss, to SRS in ignition designs. We found Langmuir decay instability less important than trapping in such conditions. This project has increased our understanding of nonlinear and relativistic laser–plasma interactions and enhanced our capacity to model them with kinetic and other codes. The National Ignition Campaign has expressed interest in applying some of these achievements to ignition experiments.

Publications

Benisti, D., et al., 2010. “Self-organization and threshold of stimulated Raman scattering.” *Phys. Rev. Lett.* **105**, 015001. LLNL-JRNL-426616.

Divol, L., et al., 2010. “Hot electron measurements on NIF: Energetics and preheat.” *Bull. Am. Phys. Soc.* **55**(15), NO5.00013. LLNL-PRES-461699.

Ellis, I. N., et al., 2010. “The onset of inflation and the effects of seed pulses on SRS.” *Bull. Am. Phys. Soc.* **55**(15), XP9.00020. LLNL-POST-461293.

Kruer, W. L., et al., 2010. “Assessing the 2 ω instability and other preheat considerations in ignition-scale hohlraums.” *J. Phys.: Conf. Ser.* **244**, 022020. LLNL-ABS-412267.

Langdon, A. B., et al., 2010. *Theory of superhot electron spectra generated by Raman scatter*. 40th Ann. Anomalous Absorption Conf., Snowmass, CO, June 13–18, 2010. LLNL-PRES-408405.

Palastro, J. P., et al., 2010. "Fully relativistic form factor for Thomson scattering." *Phys. Rev. E* **81**, 036411. LLNL-JRNL-418764.

Regan, S. P., et al., 2010. "Suprathermal electrons generated by the two-plasmon-decay instability in gas-filled hohlraums." *Phys. Plasmas* **17**, 020703. LLNL-JRNL-404583.

Strozzi, D. J., et al., 2009. "Role of electron trapping in SRS on NIF ignition targets." *Bull. Am. Phys. Soc.* **54**, LLNL-PRES-413928.

Strozzi, D. J., et al., 2010. "Eulerian-Lagrangian kinetic simulations of laser-plasma interactions." *Eulerian Codes for the Numerical Solution of the Kinetic Equations of Plasmas*. Nova Science Publishers, Hauppauge, NY. LLNL-BOOK-411147.

Wang, T.-L., et al., 2010. "Particle-in-cell simulations of kinetic effects in plasma-based backward Raman amplification in underdense plasmas." *Phys. Plasmas* **17**, 023109. LLNL-JRNL-424086.

Innovative Divertors for Future Fusion Devices—Dmitri Ryutov (08-ERD-019)

Abstract

This project aims 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 below 10 MW/m². 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 as well as a scheme to reduce impulsive heat loads. 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's BOUT boundary plasma turbulence and UEDGE plasma transport simulation 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 Development Facility, as well as for future commercial reactors. We will devise appropriate tests on existing fusion devices at Princeton and General Atomics, and plan to produce journal publications, patents, and preliminary design specifications. Successful project completion will provide the solution of a problem of critical importance for toroidal fusion reactors, and LLNL will be well positioned to become a leader in one of the key areas of fusion research at a time when funding of U.S. projects is expected to increase after completion of the ITER international 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 resource limitations. In addition, the proposed research and development in fusion energy will lead to significant progress in plasma physics and material science, which supports the Laboratory's mission in stockpile stewardship.

FY10 Accomplishments and Results

In FY10 we (1) studied the drift orbits, showing that prompt ion losses from our snowflake divertor provide additional control over the electric field inside the separatrix and stability of the edge plasma; (2) used the UEDGE code to analyze the interplay of the snowflake geometry and the processes of radiation and partial detachment of the divertor plasma from the end plates; (3) continued implementing tilted end-plate boundary conditions in the BOUT code; (4) collaborated with Princeton to successfully experiment with the snowflake configuration on the National Spherical Torus Experiment facility, demonstrating a dramatic reduction of heat flux on the divertor plates, accompanied by reduction of

impurities in the core plasma; (5) collaborated with General Atomics to develop a convenient representation of the snowflake magnetic field; and (6) further analyzed the induced current technique, including accounting for asymmetries of the heat flux. This successful project has established novel techniques for reducing heat loads on plasma-facing components in tokamaks. Already, a strongly favorable effect of the snowflake configuration on bursty-edge heat loads has been demonstrated at Switzerland's TCV tokamak, in agreement with our predictions. Candidates for future experiments following from this project include the concept of induced convection and using currents driven through the scrape-off layer to control non-axisymmetric-edge magnetic fields.

Publications

Joseph, I., 2009. "Driving toroidally asymmetric current through the tokamak scrape-off layer, part II: Magnetic field structure and spectrum." *Phys. Plasmas* **16**, 052511. LLNL-JRNL-412074.

Joseph, I., 2009. *Driving toroidally asymmetric current through the tokamak scrape-off layer to suppress edge localized modes*. Intl. Sherwood Fusion Theory Conf., Denver, CO, May 3–5, 2009. LLNL-ABS-409785.

Joseph, I., 2010. "Magnetic perturbation spectrum produced by non-axisymmetric scrape-off layer current and the X-point shadow." *Contrib. Plasma Phys.* **50**(3-5), 331. LLNL-JRNL-416576.

Joseph, I., and T. D. Rognlien, in press. "Assessment of thermo-electric techniques for scrape-off layer current drive in flux-tube geometry." *J. Nucl. Mater.* LLNL-JRNL-433553.

Joseph, I., et al., 2010. *Driving toroidally asymmetric current through the tokamak scrape-off layer to control edge-localized instabilities and equilibrium profiles*. 23rd IAEA Fusion Energy Conf., Daejeon, Korea, Oct. 11–16, 2010. LLNL-CONF-456824.

Joseph, I., R. H. Cohen, and D. D. Ryutov, 2009. "Driving toroidally asymmetric current through the tokamak scrape-off layer, part I: Potential for ELM suppression." *Phys. Plasmas* **16**, 052510. LLNL-JRNL-411897.

Rognlien, T. D., et al., 2010. *Advances in understanding tokamak edge/scrape-off layer transport*. 23rd IAEA Fusion Energy Conf., Daejeon, Korea, Oct. 11–16, 2010. LLNL-POST-458732.

Ryutov, D. D., 2009. *The dynamics of coherent scrape-off layer structures in a snowflake divertor*. 50th Ann. Mtg. Division of Plasma Physics, Dallas, TX, Nov. 17–21, 2008. LLNL-ABS-405443.

Ryutov, D. D., and M. V. Umansky, 2010. "Ion drifts in a snowflake divertor." *Phys. Plasmas* **17**, 014501. LLNL-JRNL-418155.

Ryutov, D. D., M. A. Makowski, and M. V. Umansky, 2010. "Local properties of the magnetic field in a snowflake divertor." *Plasma Phys. Contr. Fusion* **52**, 105001. LLNL-JRNL-426717.

Ryutov, D. D., et al., 2008. "A snowflake divertor: A possible way of improving the power handling in future fusion facilities." *Proc. 2008 Fusion Energy Conf.* LLNL-CONF-407193.

Umansky, M. V., et al., 2009. "Analysis of geometric variations in high-power tokamak divertors." *Nucl. Fusion* **49**, 075005. LLNL-JRNL-410565.

Umansky, M. V., et al., 2010. "Edge plasma in a snowflake divertor." *Contrib. Plasma Phys.* **50**, 350. LLNL-CONF-416151.

Zweben, S. J., R. H. Cohen, and D. D. Ryutov, 2009. "Local scrapeoff layer control using biased electrodes in NSTX." *Plasma Phys. Contr. Fusion* **51**, 105012. LLNL-JRNL-414426.

High-Temperature Thermal X-Radiation Sources at Short-Pulse Lasers—Marilyn Schneider (08-ERD-024)

Abstract

Data from experiments measuring the material properties of dense matter at high temperatures and in local thermodynamic equilibrium are important to the advancement of high-energy-density science. Such data benchmark the radiation-transport, opacity, equation-of-state, and atomic physics codes used to simulate astrophysical objects, weapons, and inertial-confinement fusion targets. This study creates a thermal x-ray radiation source by heating a few microns of bulk material to high temperatures. The bulk material can be heated by the heat wave diffusing into it, by refluxing of hot electrons, or by return currents balancing the charge of escaping hot electrons. The source will be optimized by maximizing the conversion of short-pulse laser energy into thermal x rays.

If successful, this project will impact high-energy-density physics by (1) determining the fundamental physics of heating of bulk material by short-pulse lasers, (2) developing the ability to use the high radiation field in the thermal source as a broad-band backlighter for short-pulse laser experiments that probe the configurations and charge states of materials under extreme conditions, and (3) coupling the short-pulse laser heating of bulk materials with long-pulse lasers to produce a true “hot” hohlraum



Graduate student Kelly Cone adjusts a soft x-ray spectrometer inside the target chamber of Livermore's petawatt-class Titan laser.

at laser facilities. These achievements will open the door to experimental platforms that generate new data for benchmarking plasma physics codes.

Mission Relevance

This project will enable laboratory-based experiments on materials important to the Stockpile Stewardship Program. Our research also supports the LLNL mission in frontier science and technology by optimizing the conversion of laser energy into x rays, which is a fundamental high-energy-density physics problem.

FY10 Accomplishments and Results

In FY10 we (1) measured the heating of layered copper and plastic targets at Livermore's COMET (Compact Multipulse Terrawatt) and Janus laser facilities using a soft x-ray spectrometer coupled to an x-ray streak camera, which was used to examine the back side of the target and observe a time-dependent shift in the L-edge spectrum of copper; (2) modeled this experiment with Livermore's HYDRA radiation hydrodynamic code in collaboration with Colorado State University and produced plasma maps of density, temperature, and ionization state versus time, which will be analyzed using the thermodynamic equilibrium radiation transport code Cretin to produce x-ray spectra for comparison with the experiment; and (3) investigated if structured targets can increase conversion of laser energy into soft x-rays—the RADEX code was used to model the structured targets, and we concluded that near-equilibrium regions of high density and temperature are formed for certain structured targets. This is an important guide for future experiments. Our project provided a basic set of data on soft x-ray production from short pulse lasers as a function of laser conditions and target types, and we intend to seek collaborators for future research.

Publications

Cone, K. V., 2009. *Development of a hot, thermal x-radiation source using short pulse lasers*. IFSA 2009, 6th Intl. Conf. Inertial Fusion Science and Applications, San Francisco, CA, Sept. 6–11, 2009. LLNL-PROP-413345.

Cone, K. V., et al., 2010. "Development of a time-resolved soft x-ray spectrometer for laser produced plasma experiments." *Rev. Sci. Instrum.* **81**, 10E318. LLNL-CONF-431867.

Magee, E. W., et al., 2010. "Calibration of a high resolution grating soft x-ray spectrometer." *Rev. Sci. Instrum.* **81**, 10E314. LLNL-JRNL-451153.

Park, J., et al., 2010. "Calibration of a flat field soft x-ray grating spectrometer for laser produced plasmas." *Rev. Sci. Instrum.* **81**, 10E319. LLNL-CONF-431711.

Stafford, D., 2009. *Time integrated soft x-ray imaging in high intensity laser experiments*. Master's thesis, University of California at Davis, Sept. 4, 2009. LLNL-TH-416616.

Advanced Computational and Experimental Analysis of Plasma Equations of State and Transport—Brian Wilson (08-ERD-027)

Abstract

We propose to develop, apply, and experimentally validate a finite-temperature, multi-ion-center code for understanding amorphous warm dense systems such as shock-heated aluminum, foams, and plasma mixtures. This work will significantly advance the study of warm dense matter by including multicenter scattering effects in finite-temperature ensembles. As a consequence, both equilibrium and macroscopic transport quantities will be calculated in the warm dense matter regime.

Our novel computational approach will greatly improve our ability to calculate and understand the equilibrium and transport properties of warm dense plasma systems at a fundamental level. More realistic treatment of continuum lowering and pressure ionization in simple systems such as aluminum—as well as complex mixtures such as copper–beryllium ablaters 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

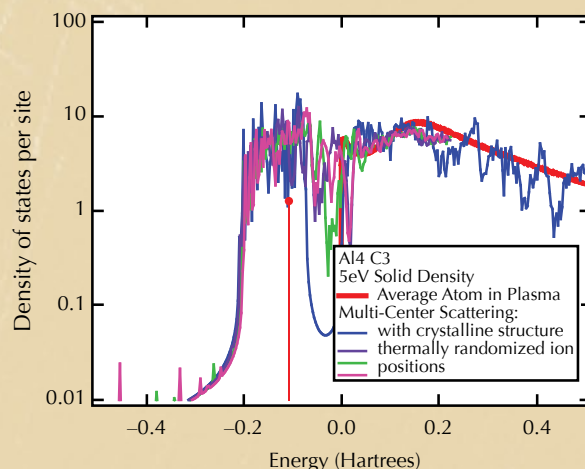
states, will be a widely applicable advance in the general ability to measure microscopic features of shocked systems.

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.

FY10 Accomplishments and Results

We completed an improved method to initialize ion configurations to facilitate ease of simulations. Specifically, we (1) completed a Voronoi polyhedral integration scheme—necessary to perform required integrals over individual scattering centers, such as needed for a Poisson solver—and tested it on an analytic electronic charge model; (2) incorporated and tested a new variational definition of energy-zero for the Korringa–Kohn–Rostoker multiple scattering potential; (3) improved the analysis code, both for density of states and Bloch spectral calculations; (4) included an improvement to the complex-energy contour integration to address extreme temperatures; and (5) tested an implementation of contour



The density of states of aluminum carbide at solid density and a temperature of 5 eV. The plot highlights the effects of multi-atom scattering and noncrystalline order.

integration in the code MPI. One next step would be to incorporate the MPI contour integration implementation into future releases to permit parallel calculations over the “energy grid” (the contour integration) and k-space grid, with savings of 6 to 20 times of each ensemble run. In summary, this project has resulted in an advanced multicenter scattering electronic structure code with applications in the warm dense matter regime.

Publications

Wilson, B., D. Johnson, and A. Alam, 2010. *Multicenter electronic structure calculation for plasma equation of state*. LLNL-PRES-456332.

Impurity and Alloying Effects on Material Strength from First Principles—Robert Rudd (08-ERD-035)

Abstract

We will pioneer the theory and computational framework for a predictive description of impurity and alloying effects on the constitutive behavior of materials under extreme deformation based on first principles. To date, strength modeling at LLNL using ab initio methods has focused exclusively on pure, pristine materials. This proposal will begin to develop the capability for predictive strength modeling of alloyed or “dirty” materials, using quantum mechanical techniques to study three strength-related phenomena: solute mobility, impurity strengthening, and alloy core-structure modification. The project will

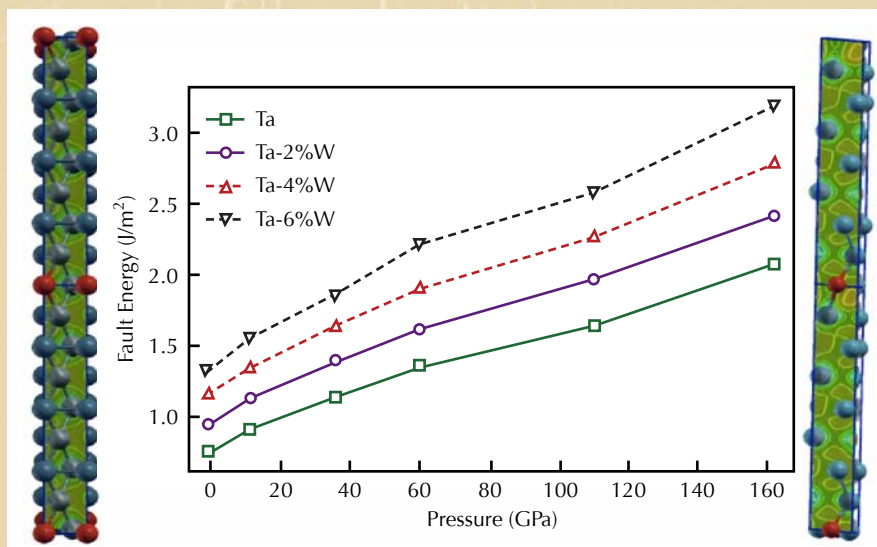
be both computational and experimental, with development and application of novel ab initio theory and advanced diamond-anvil cell experiments to produce validated models.

We will develop the basic science of how alloying and impurities affect strength through modified interatomic interactions. Success will entail calculation of the effect of alloying and impurities on solute mobility, impurity strengthening, and alloy core modification. Diamond-anvil cell experiments will provide validation for impurity strengthening and help develop techniques for strengthening—other results will be validated with existing experimental data. The significant benefit of these achievements will be an ability to model the effect of isostructural alloying and impurities on strength from first principles. We expect to publish results of our findings in high-profile peer-reviewed journals.

Mission Relevance

Computational modeling of equation of state and related constitutive properties is a core competency of Lawrence Livermore. Although 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 stock-pile science.

The generalized stacking fault energy of tantalum (Ta) alloyed with tungsten (W) as computed from first principles, along with the charge density around the Ta (blue) and W (red) atoms at different levels of slip.



FY10 Accomplishments and Results

In FY10 we continued to develop theoretical and experimental techniques for determining the strength of metal alloys at pressures up to a few megabars. Specifically, we (1) conducted large-scale density functional theory calculations of the energies of tantalum–tungsten dislocation cores, (2) used these calculations to determine the Peierls stress, (3) used density functional theory to calculate the row deformation energy in tantalum–tungsten alloys and compared these and the core calculations with our prior gamma surface results, and (4) conducted diamond-anvil cell experiments at the Advanced Photon Source at Argonne National Laboratory in which we measured the strength of tantalum–tungsten and vanadium alloys at high pressure (up to ~70 GPa) using the pressure gradient technique. We characterized samples by transmission electron microscopy after pressurization and deformation to determine dislocation densities and other indications of deformation mechanisms. In summary, this project produced a new capability to determine and understand the strength of metal alloys and other impure materials at high pressure. This capability is slated to be used in stockpile stewardship work at LLNL under the NNSA's Science Campaign and the Advanced Simulation and Computing Program.

Publications

Klepeis, J.-H. P., et al., 2010. "Diamond anvil cell measurement of high-pressure yield strength of vanadium using in situ thickness determination." *Phys. Rev. B* **81**, 134107. LLNL-JRNL-414905.

Lee, B., R. E. Rudd, and J. E. Klepeis, 2010. "Using alloying to promote the subtle rhombohedral phase transition in vanadium." *J. Phys. Condens. Matter* **22**, 465503. LLNL-JRNL-433876.

Rudd, R. E., and J. E. Klepeis, 2008. "Multiphase improved Steinberg–Guinan model for vanadium." *J. Appl. Phys.* **104**, 093528. LLNL-JRNL-406789.

Analysis of Plasma Microturbulence Simulations in Three Dimensions Plus Time—William Nevins (08-ERD-048)

Abstract

Plasma microturbulence is the dominant mechanism of heat loss in tokamaks and will affect the fusion gain of magnetic fusion reactors. A fundamental issue is energy flow—turbulent energy is produced by instabilities at low radial wave numbers. Waves, or the organized motion of plasmas, are very important because they can transport energy (heat) across magnetic field lines from the superhot reactor core to the tokamak's walls. The conventional theory is that the turbulent 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. We will develop and employ a 3D-plus-time analysis capability to investigate an alternate hypothesis—that turbulent energy is scattered to, and damped at, high parallel wave numbers.

We will develop a 3D-plus-time data-analysis capability and use it to explore the hypothesis of energy flow in plasma microturbulence, resulting in a data-analysis code and publications describing the code and 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.

FY10 Accomplishments and Results

In FY10 we (1) implemented 3D-plus-time data-analysis algorithms on parallel computers and analyzed electromagnetic data sets from the DOE Scientific Discovery through Advanced Computing Program Center for the Study of Plasma Microturbulence; (2) demonstrated that plasma

microturbulence breaks magnetic surfaces, resulting in tangling of the magnetic field on the microscale; and (3) demonstrated that the electron heat transport in these simulations was nearly identical to analytic predictions of heat transport in stochastic magnetic fields. The successful conclusion of this project advanced the state of the art in analyzing large 3D-plus-time data sets produced by gyro-kinetic simulations of plasma microturbulence. In particular, our research enabled study of the microstructure of the magnetic field at unprecedented time resolution, resulting in the demonstration that magnetic stochasticity is a routine consequence of plasma microturbulence.

Publications

Hatch, D. R., et al., 2010. *Role of subdominant stable modes in plasma microturbulence*. LLNL-JRNL-463759.

Nevins, W. M., and E. Wang, 2009. *Analysis of 3D plus time microturbulence simulation data*. Transport Task Force Workshop, San Diego, CA, May 28–June 1, 2009. LLNL-PRES-412568.

Nevins, W. M., E. Wang, and J. Candy, 2010. *Magnetic stochasticity in gyrokinetic simulations of plasma microturbulence*. Joint Varenna–Lausanne Intl. Workshop Theory of Fusion Plasmas, Varenna, Italy, Aug. 30–Sept. 3, 2010. LLNL-PRES-427508.

Nevins, W. M., E. Wang, and J. Candy, 2010. *Magnetic stochasticity in gyrokinetic simulations of plasma microturbulence*. LLNL-JRNL-463238.

Nevins, W. M., et al., 2009. *Turbulence driven magnetic reconnection*. 51st Ann. Mtg. Division of Plasma Physics, Atlanta, GA, Nov. 2–6, 2009. LLNL-PRES-418962.

Wang, E., and W. M. Nevins, 2009. *Radial propagation in the ITC CYCLONE base case*. 51st Ann. Mtg. Division of Plasma Physics, Atlanta, GA, Nov. 2–6, 2009. LLNL-POST-419067-DRAFT.

Wang, E., et al., 2010. *Electron heat transport from stochastic fields in gyrokinetic simulations*. LLNL-JRNL-463114.

Wang, E., et al., 2010. *Magnetic stochasticity in gyrokinetic simulations of plasma microturbulence*. 52nd Ann. Mtg. Division of Plasma Physics, Chicago, IL., Nov. 8–12, 2010. LLNL-PRES-459138.

Cryogenic Bolometers for Double-Beta Decay Experiments—Nicholas Scielzo (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 establish the absolute scale of neutrino masses. We will perform data analysis, produce a tellurium dioxide crystal bolometer, and develop background-reduction techniques that will improve the performance of CUORE and thus improve its sensitivity to detecting neutrinoless double-beta decay.

We will analyze our existing data from the CUORICINO experiment (a pilot-scale experiment for CUORE) to observe or establish the world's most sensitive limits on the rate of zero-neutrino double-beta decay and two-neutrino double-beta decay of tellurium-130 to both the ground and excited states of xenon-130, as well as the two-neutrino electron capture and beta-plus decay of tellurium-120. We will develop procedures for producing tellurium dioxide crystals to meet CUORE's stringent requirements on radio-purity, uniformity, and surface finish. We expect to identify materials with lower radioactive contamination than those used previously. In addition, we will prepare scientific papers and technical reports summarizing the results of each of these studies, and expect these efforts to position LLNL as a leader in the CUORE project.

Mission Relevance

This project will provide expertise with large cryogenic bolometers that will be useful in many future nuclear and high-energy-physics projects in support of stockpile stewardship. Low-background counting techniques that will be refined as part of this effort also will be of relevance for detecting minute amounts of radioactive materials in a wide variety of settings in support of Laboratory missions in nonproliferation and counterproliferation. In addition, this project will attract highly qualified student researchers to the Laboratory.

FY10 Accomplishments and Results

In FY10 we (1) designed and fabricated a device to use tellurium dioxide crystals as bolometers and verified better-than-expected performance; (2) further improved bolometer detector performance by lowering backgrounds intrinsic to the detector through careful studies of the materials used in crystal production, which will greatly increase the sensitivity of the apparatus to double-beta decay and other rare decay modes; and (3) after determining that a significant improvement in decay-rate constraints could be made, studied the decay modes of the double-electron capture and electron capture and positron emission of the tellurium-120 nucleus—in place of the search for double-beta decay of tellurium-130 to excited states of xenon-130—leading to discovery of tellurium-120 decay-rate constraints more sensitive by three to four orders of magnitude. Follow-on work would be necessary to study constraints on tellurium-130 decays to the excited states of xenon-130. This project developed new techniques to vastly improve the sensitivity of bolometric techniques to rare radioactive decays, including the long-sought-after neutrinoless double-beta decay, by reducing detector backgrounds, improving detector instrumentation techniques, and developing analysis tools to determine the source of any remaining backgrounds and the sensitivity to various scientific signals of interest. With increased support from the Office of Science, we will take a significant leadership role in the international effort to develop cryogenic bolometer arrays for double-beta decay searches. Our tellurium dioxide bolometer device was chosen for CUORE-0 and CUORE, and

assembly of the CUORE-0 array has already begun. Finally, as a result of this project, the postdoctoral researcher working on this project was selected to a leadership position as the CUORE-0 experimental coordinator.

Publications

Andreotti, E., et al., 2010. *Search for beta-EC double beta decay of ^{120}Te* . LLNL-JRNL-461978.

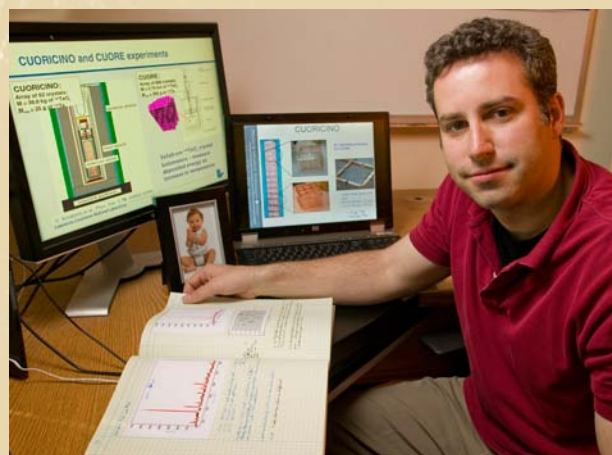
Andreotti, E., et al., 2010. “Muon-induced backgrounds in the CUORICINO experiment.” *Astropart. Phys.* **34**, 18. LLNL-JRNL-421925.

Arnaboldi, C., et al., 2010. “Production of high-purity TeO_2 single crystals for the study of neutrinoless double beta decay.” *J. Crystal Growth* **312**, 2999. LLNL-JRNL-462009.

Arnaboldi, C., et al., 2008. “Results from a search for the neutrinoless double beta decay of Te-130 .” *Phys. Rev. C* **78**, 041601. LLNL-JRNL-408037.

Barghouty, A. F., et al., 2010. *Measurements of proton-induced radionuclide production cross sections to evaluate cosmic-ray activation of tellurium*. LLNL-JRNL-462152.

Correll, D., and P. Kotta, eds., 2009. *Lawrence Fellow hunts for extremely rare phenomenon*. LLNL-AR-433076.



Nicholas Scielzo arrived as a Lawrence Fellow to lead the LLNL effort to improve sensitivity of cryogenic bolometers to rare phenomena such as double-beta decay.

Dolinski, M. J., 2008. *Neutron interactions in the CUORE neutrinoless double beta decay experiment*. LLNL-TH-408040.

Foggetta, L., et al., 2010. *Composite macro-bolometers for the rejection of surface radioactive backgrounds in rare-event experiments*. LLNL-JRNL-462678.

Norman, E. B., 2009. "Prospects for and status of CUORE—the Cryogenic Underground Observatory for Rare Events." *AIP Conf. Proc.* **1165**, 411. LLNL-PROC-414765.

Pedretti, M., et al., 2009. "A ton-scale bolometric detector for the search for neutrinoless double beta decay." *AIP Conf. Proc.* **1185**, 562. LLNL-JRNL-421922.

Pedretti, M., et al., 2008. "CUORE Experiment: The search for neutrinoless double beta decay." *Int. J. Mod. Phys. A* **23**, 3395. LLNL-JRNL-414692.

Stoyer, M. A., et al., 2010. "Nuclear physics and heavy element research at Lawrence Livermore National Laboratory." *Russ. Chem. Rev.* **78**, 1145. LLNL-CONF-413183.

Partition-of-Unity Finite-Element Method for Large-Scale Quantum Molecular Dynamics on Massively Parallel Computational Platforms—John Pask (08-ERD-052)

Abstract

First-principles quantum mechanical materials calculations now account for a significant fraction of large-scale computations. However, these calculations are highly computer-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 quantum mechanical simulations using modern partition-of-unity techniques and eigensolvers in finite-element analysis. Initial results suggest a potential order-of-magnitude improvement over current state-of-the-art approaches. We will

demonstrate the unique power of our method by performing large-scale 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 quantum mechanical calculations by an order of magnitude or more. This would change the way the largest, most complex quantum mechanical simulations are performed and enable a range of investigations not possible before, with corresponding impacts on the understanding and prediction of complex materials properties of both metals and insulators at ambient and extreme conditions.

Mission Relevance

This project will advance quantum mechanical materials calculations in general and will have a particular impact on stockpile stewardship by providing key understanding and predictions of current and future stockpile materials.

FY10 Accomplishments and Results

In FY10 we (1) further optimized parallel-computer quantum molecular dynamics simulations by moving from the prototype Open Multi-Processing programming interface to the MPI (Message Passing Interface) protocol used to program parallel computers, and completed test calculations verifying the correctness and scaling of the new MPI code; (2) developed a new finite-element eigensolver that is four times faster than the current state of the art in collaboration with the University of California at Davis; (3) initiated a related collaboration with the Naval Research Laboratory on high-order real-space methods for the Kohn–Sham problem (related to the investigation of atomic electronic structure in condensed matter); and (4) completed the application of our prototype code to molecular dynamics simulations of d- and f-electrons in metals. The successful conclusion of this project enabled development of a new method for large-scale quantum molecular dynamics simulations of condensed matter at extreme conditions, demonstrating an order-of-magnitude advance over current state-of-the-art methods based on plane waves. The method and prototype

code developed here now serve as the basis for the large-scale production code currently under development for applications to complex condensed matter systems at extreme conditions, and in particular, to significant stockpile-stewardship issues.

Publications

Pask, J. E., N. Sukumar, and S. E. Mousavi, in press. "Linear scaling solution of the all-electron coulomb problem in solids," *Int. J. Multiscale Comput. Eng.* LLNL-JRNL-427628.

Sukumar, N., and J. E. Pask, 2009. "Classical and enriched finite element formulations for Bloch-periodic boundary conditions." *Int. J. Numer. Meth. Eng.* 77, 1121. LLNL-JRNL-403676.

Measurement and Prediction of Laser-Induced Damage in the Presence of Multiple Simultaneous Wavelengths—Mike Nostrand (08-ERD-054)

Abstract

Accurate predictions of laser-induced optical damage are critical for enhancing performance and enabling timely recycling of optics for efficient laser operation. Predictions of damage in high-energy laser systems based on small-scale laboratory experiments have been poor in the past. We will create an improved predictive capability with measurements and modeling that give attention to the effects of multiple wavelengths and pulse-shape variations. This will include studies of behavior in mitigated damage sites and damage probability of process-induced flaws. We will collect laser damage data and develop a predictive capability for describing the damage expected on a fusion-class laser beam line and compare our predictions against laser observations.

We will create the capability to precisely predict the highest level of laser performance that can be achieved at acceptable cost. (Less-accurate predictions would necessitate a larger safety margin and hence reduced laser performance.) We will also determine iterative feedback between predictive performance modeling, full-aperture damage

observations, and the physical mechanisms underlying optical damage. This feedback will provide further understanding of damage mechanisms, thus providing better insight for improved optics performance and, therefore, improved laser performance.

Mission Relevance

By developing protocols to extend the useful lifetime of critical silicon dioxide and crystalline potassium dihydrogen phosphate and deuterated potassium dihydrogen phosphate 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.

FY10 Accomplishments and Results

We have (1) developed single-wavelength growth rules that predict damage growth rates for pulses with durations between 1 and 15 ns; (2) discovered and quantified a strong but previously unknown effect of site size on growth behavior, and determined that the size of initiated damage sites is governed by a laser-driven solid-state absorption front—these findings can be used to determine the growth of damage site cores for pulses of arbitrary shape for intensities less than 6 GW/cm²; (3) extended the multiple-wavelength growth rules to include flat-in-time pulses of various shapes between 1 and 10 ns in duration; (4) documented the damage initiation behavior of scratches as a function of their width and treatments developed in a related LDRD project on the "Chemical and Structural Modification and Figure Control during Glass Polishing;" and (5) developed the tool OpticsX to automate online damage predictions and used it to evaluate the lifetimes of the wedge focus lens and grading debris shield in NIF final optics assemblies for use in repair and replacement decisions for hundreds of shots. A follow-on LDRD has been initiated to study and understand the stochastic nature of laser-induced damage revealed in this work.

Publications

Abdulla, G., et al., in press. "Effective and efficient optics inspection approach using machine learning." *Proc. SPIE*. LLNL-PROC-462149.

Carr, C. W., J. D. Bude, and P. P. Demange, 2010. "Laser-supported solid-state absorption fronts in silica." *Phys. Rev. B* **82**, 184304. LLNL-JRNL-423847.

Carr, C. W., et al., 2010. "Temperature activated absorption during laser-induced damage: The evolution of laser-supported solid state." *Proc. SPIE* **7842**, 78420N. LLNL-PRES-456675.

Kegelmeyer, L. M., 2010. *Applying avatar machine learning to NIF optics inspection analysis*. Conf. Intelligent Data Understanding, Mountain View, CA, Oct. 6, 2010. LLNL-PRES-458291.

Liao, Z. M., et al., 2010. "Predicting laser-induced bulk damage and conditioning for deuterated potassium di-hydrogen phosphate crystals using absorption distribution model." *Optic. Lett.* **35**, 2538. UCRL-JRNL-423636.

Liao, Z. M., et al., 2009. "Using absorption distribution model to predict optimal laser conditioning for DKDP crystals." *Nonlinear optics: Materials, fundamentals and applications*, paper NWC7. Optical Society of America, Washington, DC. LLNL-PRES-414644.

Negres, R. A., et al., 2010. "Growth behavior of laser-induced damage on fused silica optics under UV, ns laser irradiation." *Optic. Express* **18**, 19966. LLNL-JRNL-439171.

Negres, R. A., et al., 2009. "The effect of pulse duration on the growth rate of laser-induced damage sites at 351 nm on fused silica surfaces." *Proc. SPIE* **7504**, 750412. LLNL-CONF-420370.

Norton, M. A., et al., in press. "Determination of laser damage initiation probability and growth on fused silica scratches." *Proc. SPIE*. LLNL-PROC-462148.

Suratwala, T. I., et al., in press. "HF-based etching processes for improving laser damage resistance of fused silica optical surfaces." *J. Am. Ceram. Soc.* LLNL-JRNL-425118.

Mesoscale Studies of Hydrodynamic Instability Growth in the Presence of Electric and Magnetic Fields— Peter Amendt (08-ERD-062)

Abstract

Recent proton backlighting data on laser-driven imploded capsules and rippled foils indicate the presence of strong self-generated electric (~ 1 -GV/m) and magnetic (~ 1 -MG) fields. Understanding their origin could be relevant to planned demonstrations of inertial-confinement fusion. Elucidating the nature of the fields and their effects on interfacial instability growth will require an approach that departs from standard single-fluid hydrodynamics and instead treats the system as an aggregate of coupled electron-ion fluids—that is, as a plasma. This project will explore such plasma effects on important hydrodynamic instabilities such as Rayleigh–Taylor and Richtmyer–Meshkov, as well as hohlraum dynamics.

We expect to provide an evaluation of electric and magnetic field effects in imploding systems, an understanding of their origin and magnitude, and suggested remedial measures if the effects are deemed significant. Initially, we will evaluate methods to understand the underlying physics—both analytically and computationally—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 national security mission relevance.

Mission Relevance

This project supports LLNL's energy security mission by furthering the goal of robust ignition designs for inertial-confinement fusion, and also supports the national security mission by impacting investigations of high-energy-density imploding systems.

FY10 Accomplishments and Results

In FY10 we (1) succeeded in developing a plasma-based theory of barotropic diffusion (pressure-gradient driven diffusion that is particularly important across shock fronts) in the presence of self-generated electric fields; (2) applied our model to an

implosion database of thermonuclear fuel mixtures, achieving anomalously low neutron yields and large x-ray image sizes compared with predictions that do not include self-generated electric fields; (3) summarized our results in a manuscript published in *Physical Review Letters*; (4) garnered national and international attention in this area of research, culminating in several invited talks; and (5) obtained first results with a hybrid particle-in-cell code to assess from first principles the structure of a plasma shock wave.

Proposed Work for FY11

In the first four months of FY11 (after which this project is scheduled to end), we will emphasize documenting and finalizing our understanding of barotropic diffusion in thermonuclear mixtures. We will also extensively use the collisional particle-in-cell Large Scale Plasma code to corroborate or modify our theory of barotropic diffusion and to understand shock-front morphology. We anticipate an invited talk at the annual American Physical Society Division of Plasma Physics meeting, leading to additional documentation in the peer-reviewed literature and an opportunity to showcase this work to the scientific community.

Publications

Amendt, P. A., 2008. "Effects of ionization gradients on inertial confinement-fusion capsule hydrodynamic stability." *Phys. Rev. Lett.* **101**, 115004. LLNL-JRNL-403824.

Amendt, P. A., et al., 2009. "Electric field and ionization-gradient effects on inertial-confinement-fusion implosions." *Plasma Phys. Contr. Fusion* **51**(12), 12404. LLNL-CONF-413857.

Amendt, P. A., et al., 2010. "Plasma barodiffusion in inertial-confinement-fusion implosions: Application to observed yield anomalies in thermonuclear fuel mixtures." *Phys. Rev. Lett.* **105**, 115005. LLNL-JRNL-416704.

Li, C. K., et al., 2009. "Observations of electromagnetic fields and plasma flow in hohlraums with proton radiography." *Phys. Rev. Lett.* **102**, 205001. LLNL-JRNL-410658.

Li, C. K., et al., 2009. "Pressure-driven MHD interchange instabilities in laser-produced HED plasmas." *Phys. Rev. E* **80**, 016407. LLNL-JRNL-423131.

Li, C. K., et al., 2009. "Proton radiography of dynamic electric and magnetic fields in high-energy-density plasmas." *Phys. Plasma.* **16**, 056304. LLNL-JRNL-423130.

Li, C. K., et al., 2009. "Study of direct-drive capsule implosions in inertial confinement fusion with proton radiography." *Plasma Phys. Contr. Fusion* **51**, 014003. LLNL-JRNL-423129.

Nuclear Astrophysics at the National Ignition Facility: Feasibility of Studying Reactions of the Stars on Earth—Richard Boyd (08-ERD-066)

Abstract

Our objective is to develop the technical approach for nuclear astrophysics experiments to be conducted at the National Ignition Facility (NIF) to study nucleosynthesis in stars and stellar evolution. Because these experiments can only be performed at NIF at its full energy, our work will focus on studies that must precede these experiments. Target simulations will be performed using the radiation-hydrodynamics HYDRA code for several nuclear 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. Concomitant theoretical studies will also be pursued in Big Bang nucleosynthesis to examine unresolved issues about primordial element abundances by including reactions involving short-lived nuclei for which there is little laboratory data.

This project will yield the optimal designs of laser target pellets for several experiments, along with an estimate of reaction yields, which will determine the feasibility of each experiment and which will be optimized by varying parameters such as pellet design, laser energy, and laser profile. We will also determine the diagnostics required for future shots, including if existing diagnostics will provide the required information in experiments. If new

diagnostic devices are required, their properties will be determined, which would lay the groundwork for future design work. Publications would result from the theoretical work; this could have revolutionary physics impact by supporting the potential need to investigate new particle physics to resolve problems about lithium abundance.

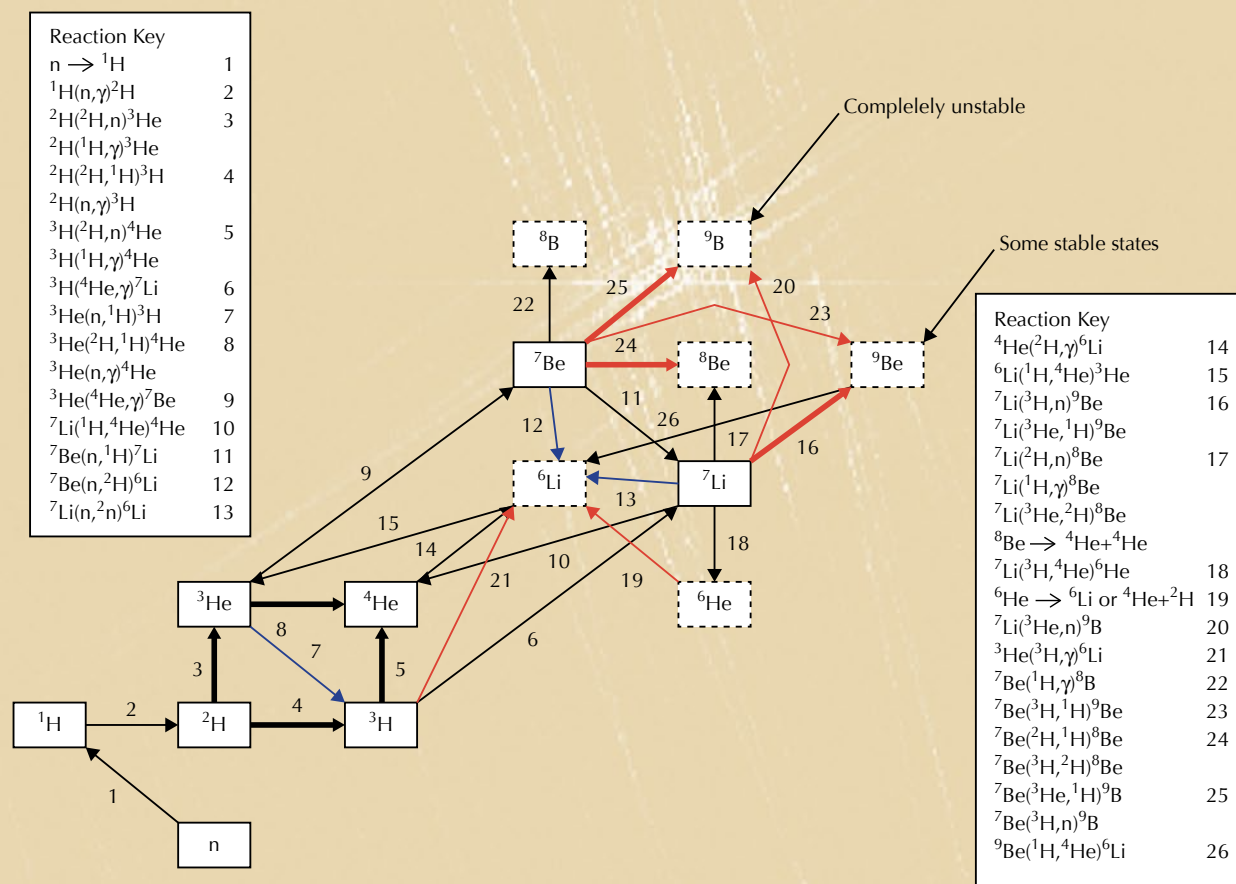
Mission Relevance

The project furthers the Laboratory's national security mission by paving the way for NIF astrophysics experiments that will lead to advances in understanding nuclear reactions relevant to stockpile stewardship. It also supports the Laboratory's commitment to pursuits in frontier science to advance scientific discovery.

FY10 Accomplishments and Results

In FY10 we studied nuclear reactions of astrophysical interest that were being considered for experiments at NIF. The *Physics Today* article we

published concluded that those that involved detection of neutrons appear to be feasible. However, our simulations of NIF shots showed that nearly all of the reactions that we had originally considered will not be possible with the current shot strategies. The yields were simply insufficient or the backgrounds were too high to produce a detectable level of reaction products. It may well be that new strategies being developed such as fast ignition or shock ignition will produce yields that could enable the experiments, but these scenarios are insufficient to produce measurable results with existing detection devices. We also performed a theoretical study of Big Bang nucleosynthesis in which we added consideration of the reactions of many additional short-lived nuclei for which laboratory data are sparse. This refocus of efforts to study nuclear reactions of the very lightest nuclei makes effective use of NIF while, for the moment, reactions involving heavier nuclei (except in the cases that involve neutrons) are on hold pending new shot scenarios. (Simulations of



Reaction network used in our Big Bang nucleosynthesis calculations. The boxes indicate nuclei and the lines indicate reactions that connect them. Red lines indicate reactions that were added to the code, and blue lines indicate reactions that were potentially affected by nonthermal particles.

reactions that were originally proposed can be revisited when the new shot scenarios are better developed.) As published in *Physical Review D*, our work on theoretical Big Bang nucleosynthesis strongly suggests either that one of the measurements of primordial lithium abundances is in error, or that new physics may be necessary to correctly describe the Big Bang abundances.

Publications

Boyd, R. N., 2009. "The National Ignition Facility: Studying the stars in the laboratory." *Proc. Sci. (NIC X)*198. LLNL-PRES-420500.

Boyd, R. N., L. Bernstein, and C. Brune, 2009. "Studying nuclear astrophysics at NIF." *Phys. Today* **62**(8), 60. LLNL-JRNL-414484.

Boyd, R. N., et al., 2010. "New nuclear physics for Big Bang nucleosynthesis." *Phys. Rev. D* **82**, 105005. LLNL-JRNL 446832.

Moses, E. I., et al., 2009. "The National Ignition Facility: Ushering in a new age for high energy density science." *Phys. Plasma*. **16**, 041006. LLNL-JRNL-406652.

Study of Kelvin–Helmholtz Instability in High-Energy-Density Hydrodynamic Processes—Hye-Sook Park (08-ERD-069)

Abstract

An unanswered question in high-energy-density hydrodynamics is how the Kelvin–Helmholtz instability can be studied in a controlled fashion. The successful fielding of a controlled Kelvin–Helmholtz experiment would provide a valuable demonstration of the ability to pursue a number of scientific experiments on future fusion-class lasers, including eventual supernova studies. In this project, we will conduct Kelvin–Helmholtz and related supernova experiments on the OMEGA laser at the University of Rochester and the National Ignition Facility (NIF) laser at Livermore, leveraging LLNL expertise in target design, simulation, diagnostics, and other fields. This project will be conducted in collaboration with the University of Michigan.

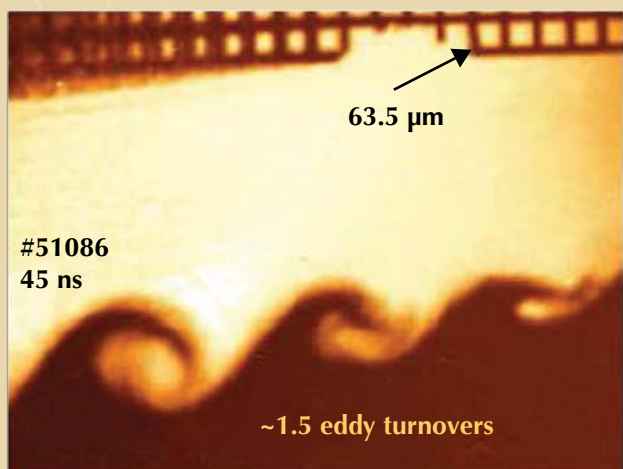
If successful, this project will deliver an x-ray radiograph of the rolled-up vortex of a material during a controlled Kelvin–Helmholtz instability, determining whether hydrodynamics experiments can resolve multiple interspersed layers of x-ray-absorbing and transmitting materials or if these layers are too adversely affected by turbulent mixing and the recently observed phenomenon of mass stripping to serve as valid diagnostics. After experiments on OMEGA and modeling and simulation of the results, we will have a better understanding of how to implement a supernova experiment on NIF. Our experiments and modeling will provide diagnostic requirements for new types of astrophysics experiments on NIF and show where the transition to turbulence occurs in Kelvin–Helmholtz vortex roll-ups.

Mission Relevance

Understanding Kelvin–Helmholtz instability is central to many hydrodynamic processes important to the Stockpile Stewardship Program. This project supports the Laboratory's national security mission by potentially producing an entirely new type of experimental data for the validation of stockpile stewardship codes.

FY10 Accomplishments and Results

In FY10 we (1) performed a second series of Kelvin–Helmholtz experiments on the OMEGA laser to understand the sensitivity of Kelvin–Helmholtz evolution to the mediating environment, using three different foam densities (50, 100, and 200 mg/cm³) and observing many turbulent features, such as striations in the foam area, which were likely a result of shock tube instability; (2) began interpreting the data along with the results of two-dimensional hydrodynamics simulations; (3) performed two successful NIF shots in collaboration with the University of Michigan to demonstrate backlighter brightness and hohlraum drive performance, showing that backlighter brightness meets the requirements for Rayleigh–Taylor supernova experiments and demonstrating that the hohlraum can deliver the radiation temperature (>300 eV) required for studying radiative effects on a supernova environment; and (4) continued studying how to diagnose dynamic features in high-density materials.



Radiographic images from laser-driven Kelvin–Helmholtz experiments using 100-mg/cm³ foam, suggesting a transition from a smooth to a more turbulent flow.

Proposed Work for FY11

In FY11 we will (1) perform another set of Kelvin–Helmholtz experiments on the OMEGA laser to study the effects of multimode initial perturbations, interface roughness, and the driven transition to turbulence; (2) develop the spectroscopic tagging of localized regions of targets to trace the deep nonlinear and turbulent mixing of material arising from Kelvin–Helmholtz instability; (3) continue collaborating with the University of Michigan to develop the first NIF experiments to study the effect of intense, shock-generated radiation preheat on the evolution of hydrodynamic instabilities at scaled intrastellar interfaces; and (4) design the first Kelvin–Helmholtz experiment for NIF, aimed at generating and diagnosing the development of turbulence at the interface.

Publications

Harding, E. E., et al., 2009. “Observation of a Kelvin–Helmholtz instability in a high-energy-density plasma on the OMEGA laser.” *Phys. Rev. Lett.* **103**, 045005. LLNL-POST-417686.

Hurricane, O. A., et al., 2009. “A high-energy-density shock-driven Kelvin–Helmholtz shear

layer experiment.” *Phys. Plasmas* **16**, 056305. LLNL-JRNL-410680.

Hurricane, O. A., et al., 2010. *Blast-wave-driven Kelvin–Helmholtz shear layers in a laser drive high-energy-density plasmas*. 8th Intl. Conf. High-Energy-Density Laboratory Astrophysics, Pasadena, CA, Mar. 15–18, 2010. LLNL-PROC-463635.

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/cm³ and directly measure density from broadening of the Compton-scattered spectrum. Our approach combines the recently demonstrated x-ray scattering technique with K-alpha radiation produced with an ultrashort-pulse laser from 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 producing and x-ray scattering 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 x-ray scattering techniques for fusion-class lasers and at the same time provide a critical test for hydrodynamic and equation-of-state modeling important to high-energy-density physics in support of stockpile stewardship. This project will also train the next generation of young scientists in a field of high importance to the Laboratory.

FY10 Accomplishments and Results

In FY10 we completed all milestones proposed for this project. Specifically, we (1) characterized shock-compressed boron and isochorically heated cryogenic hydrogen with x-ray scattering methods; (2) observed, in the vicinity of the Fermi momentum, dispersion-less collisionally damped plasmons, indicating a strongly coupled electron liquid—these observations agree with calculations that include the Born–Mermin approximation to account for electron–ion collisional damping and local field corrections reflecting electron–electron correlations;

(3) experimentally induced hydrogen plasma to a nonthermal state with an electron temperature of 13 eV and ion temperature below 0.1 eV; and (4) modeled the data using impact ionization cross sections based on classical free-electron collisions. The successful conclusion of this project enabled spectrally resolved x-ray scattering to diagnose high-energy-density plasmas. This technique is ready for use at the next generation of laser and free-electron laser facilities where the scientific community will adopt spectrally resolved x-ray Thomson scattering for basic science applications.

Publications

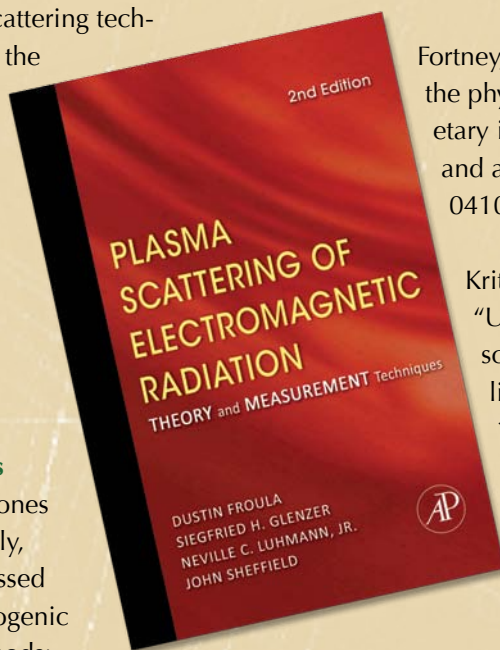
Faeustlin, R. R., et al., 2010. “Observation of ultrafast non-equilibrium collective dynamics in a warm dense hydrogen plasma.” *Phys. Rev. Lett.* **104**, 125002. LLNL-JRNL-419394.

Fortney, J. J., et al., 2009. “Frontiers of the physics of dense plasmas and planetary interiors: Experiments, theory, and applications.” *Phys. Plasma.* **16**, 041003. LLNL-JRNL-407191.

Kritcher, A. L., et al., 2009. “Ultrafast K alpha x-ray Thomson scattering from shock compressed lithium hydride.” *Phys. Plasma.* **16**, 1. UCRL-JRNL-227913.

Lee, H. J., et al., 2009. “X-ray Thomson-scattering measurements of density and temperature in shock-compressed beryllium.” *Phys. Rev. Lett.* **102**, 115001. LLNL-JRNL-406683.

Neumayer, P., et al., 2010. “Plasmons in strongly coupled shock-compressed matter.” *Phys. Rev. Lett.* **105**, 075003. LLNL-JRNL-431571.



LLRD research on x-ray scattering in warm dense matter has been featured in the new textbook, Plasma Scattering of Electromagnetic Radiation.

Proton Fast Ignition—Pravesh Patel (08-ERI-004)

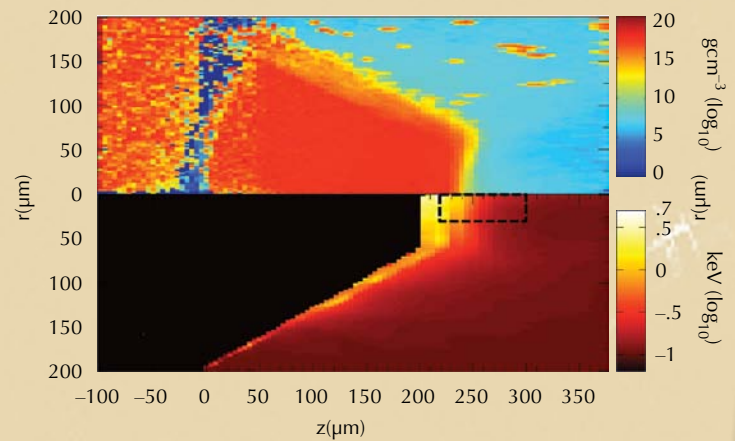
Abstract

We will explore proton fast ignition for inertial-fusion energy, from its conceptual phase to proof-of-principle subscale demonstration experiments. We intend to perform systematic experiments on Livermore's 350-J Titan laser and University of Rochester's 5.2-kJ OMEGA Extended Performance (EP) laser to determine optimal laser and target design parameters for subscale proton fast ignition, validate LLNL's short-pulse integrated modeling capability, and resolve outstanding physics issues related to proton conversion efficiency scaling, ballistic focusing, and stopping in dense plasma. The final deliverable will be an integrated demonstration experiment using the 30-kJ OMEGA implosion facility and a 5.2-kJ ignitor pulse to establish the viability of full-scale proton fast ignition on fusion-scale lasers.

Through experiments and modeling, we will establish the feasibility of full-scale proton fast ignition. The outstanding physics issues we will 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 hydrodynamic, particle-in-cell and hybrid particle-in-cell 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 proof-of-principle proton fast-ignition experiment on OMEGA EP would be of momentous significance for the entire U.S. fast-ignition endeavor.

Mission Relevance

This project will provide the scientific groundwork for demonstration of proton fast ignition on fusion-class fast-pulse lasers, in support of the Laboratory's missions in national and energy security.



Particle-in-cell simulation of a proton-drive fast-ignition target. Proton beam density is shown (top) along with heating of compressed fuel (bottom).

FY10 Accomplishments and Results

We achieved both of our proposed primary deliverables for FY10. Firstly, we performed an experiment on the 200-TW Trident laser at Los Alamos National Laboratory to study proton focusing with a new deflectometry diagnostic technique that uses radiography through a mesh to measure proton trajectories from an arbitrary shaped target surface. High-density carbon hemispherical shells were used as targets, and focal distances and spot sizes of the proton beam were measured. Both open- and closed-cone geometries were used—the closed cones representing a more realistic fast-ignition-like geometry. Excellent agreement was obtained with the modeling results of the large-scale plasma code. Secondly, we produced a first-revision proton fast-ignition point design based on the modeling of an ignition-scale proton beam accelerated from a hemispherical foil. Energy deposition of the protons in a 40- μm ignition region at best focus was computed. Initial estimates indicate that ignition energies required for proton fast ignition may be comparable to the mainline electron fast-ignition concept. The successful conclusion of this project has provided a detailed understanding of the dynamics of ultra-intense laser-generated proton beam focusing and

application to fast ignition. This project has been successfully transferred to a new DOE Office of Fusion Sciences Program on Ion and Proton Fast Ignition.

Publications

Bartal, T., 2010. *Proton beam focusing using novel structured targets*. 52nd Ann. Mtg. APS Division of Plasma Physics, Chicago, IL, Nov. 8–12, 2010. LLNL-ABS-442914.

Bartal, T., 2009. *The effect of hemispherical target diameter on proton focusing*. 51st Ann. Mtg. APS Division of Plasma Physics, Atlanta, GA, Nov. 2–6, 2009. LLNL-ABS-414851.

Bellei, C., 2010. *LSP simulations of proton-drive fast ignition*. 52nd Ann. Mtg. APS Division of Plasma Physics, Chicago, IL, Nov. 8–12, 2010. LLNL-ABS-459994.

Hey, D., 2009. *Laser-accelerated proton conversion efficiency thickness scaling*. IFSA 2009, 6th Intl. Conf. Inertial Fusion Sciences and Applications, San Francisco, CA, Sept. 6–11, 2009. LLNL-ABS-412620.

Mackinnon, A. J., 2009. *Progress in fast ignition studies*. APiP 2009, 16th Intl. Conf. Atomic Processes in Plasmas, Monterey, CA, Mar. 22–26, 2009. LLNL-ABS-409835.

Plasma Waveguide for Electron Acceleration—Laurent Divol (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 and 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.

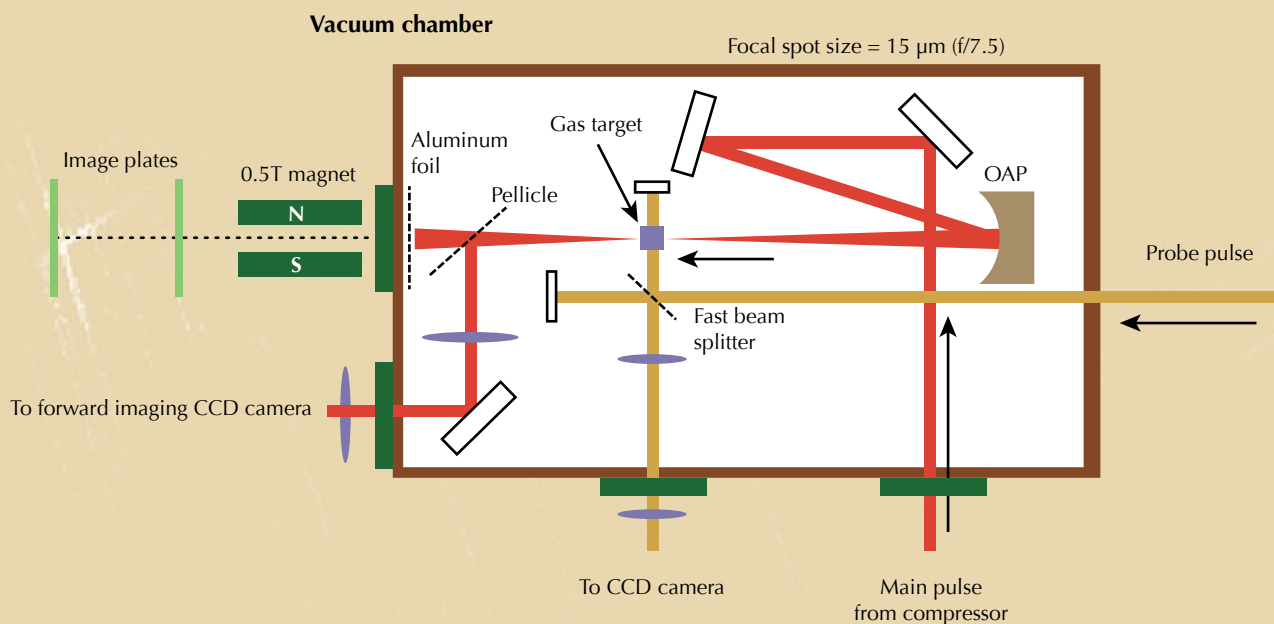
We will demonstrate a plasma channel that is inherently scalable to produce greater than 10-GeV electrons and the next generation of high-power, short-pulse laser beams. Our novel concept will not only be scalable to electron beam energies found in conventional accelerators, but will also provide a short-pulse 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 in advanced laser technologies.

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 frontier science high-energy-density physics investigations and weapons and biological studies.

FY10 Accomplishments and Results

In FY10 we focused our effort on use of the Callisto laser system at LLNL's Jupiter Laser Facility. Specifically, we demonstrated (1) after much improvement to the laser, self-guiding laser beams over a distance of 1.4 cm with peak electron energy limited by the self-trapping threshold; (2) the acceleration of electrons up to 1.3 GeV using ionization-induced injection; and (3) for the first time, staging of two gas cells—one providing injection of electrons in the laser wakefield and the second providing acceleration length with self-guided laser propagation. Overall, we had great successes on the Callisto laser in the self-guided regime of laser wakefield acceleration. However, control and characterization of a magnetically controlled waveguide proved difficult on the Janus laser, and we were unable to field this system on Callisto. Our experimental gas target and diagnostic setup developed under this LDRD and improvements to the Callisto laser system will be used in a future collaboration with the University of California at Los Angeles.



The three primary diagnostics in our successful demonstration of self-guided laser wakefield acceleration included a forward electron spectrometer using a 0.5-T permanent magnet, Michelson interferometry, and a forward image of the spot at the exit plane.

Publications

Froula, D. H., et al., 2009. "Magnetically controlled plasma waveguide for laser wakefield acceleration." *Plasma Phys. Contr. Fusion* **51**, 024009. LLNL-JRNL-403962.

Froula, D. H., et al., 2009. "Measurements of the critical power for self-injection of electrons in a laser wakefield accelerator." *Phys. Rev. Lett.* **103**(21), 215006. LLNL-PRES-410631.

Leurent, V., et al., 2008. "Study of x-ray radiation from a laser wakefield accelerator." *Advanced accelerator concepts: Proc. 13th Advanced Accelerator Concepts Workshop*, vol. 1086, p. 235. AIP Conf. Proc., Melville, NY. LLNL-PROC-406432.

Pollock, B. B., et al., 2008. "Multicentimeter long high density magnetic plasmas for optical guiding." *Rev. Sci. Instrum.* **79**, 10F550. LLNL-CONF-403602.

Pollock, B. B., et al., 2009. *Two-screen method for determining electron beam energy and deflection from laser wakefield acceleration*. 23rd Particle Accelerator Conf. PAC09, Vancouver, Canada, May 4–8, 2009. LLNL-PRES-410652.

Ralph, J., et al., 2010. "Laser wakefield acceleration at reduced density in the self-guided regime." *Phys. Plasma*. **17**, 056709. LLNL-JRNL-413708.

Ross, J. S., et al., 2009. *Thomson scattering measurements in the collective and non-collective regime in laser produced plasmas*. OMEGA Laser Facility Users Group 2009 Workshop, Rochester, NY, Apr. 29–May 1, 2009. LLNL-POST-412466.

Visco, A., et al., 2009. "Temporal dispersion of a spectrometer." *Rev. Sci. Instrum.* **79**, 10F545. LLNL-CONF-403770.

Precision Mono-Energetic Gamma-Ray Science for NNSA Missions—Christopher Barty (09-SI-004)

Abstract

We propose to study compact, mono-energetic gamma-ray (MEGa-ray) science for four high-impact NNSA missions: (1) isotope-specific nuclear resonance fluorescence imaging of stockpile and ignition components, (2) isotopic assays of fission products

and for nuclear waste stream applications, (3) isotopic radiography and quantitative assays of DOE legacy waste, and (4) isotope-specific flash radiography of multicomponent turbulent hydrodynamic experiments and ignited plasmas. We will demonstrate the world's first MEGA-ray system capable of meeting these needs and provide a dramatic new ability for scientific investigation of photonuclear interactions.

We expect to develop short-pulsed laser-based MEGA-ray sources for the static, isotope-specific imaging and assaying of highly enriched uranium, as well as for applications in stockpile stewardship, legacy waste, and dynamic nuclear resonance fluorescence imaging. The flash isotope radiography we

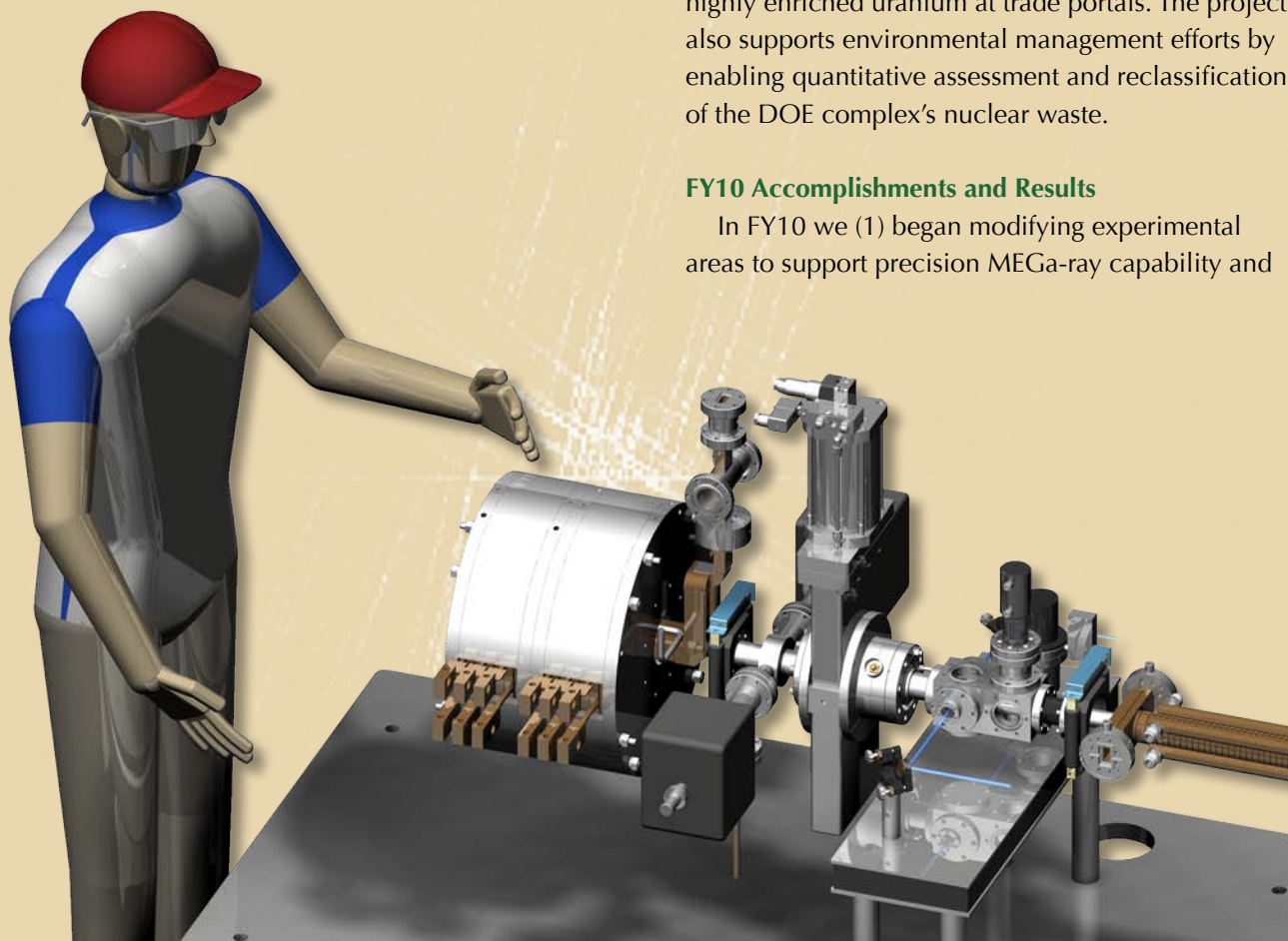
envision would allow time-resolved observation of the turbulent mixing of stockpile-relevant materials using isotope tracer layers. With a modular compact design, the robust MEGA-ray source would also enable portable isotope radiography tools for other national and homeland security applications.

Mission Relevance

This project supports the Laboratory's national security mission by developing a new and potentially revolutionary dynamic, isotope-specific radiography capability for stockpile stewardship and fundamental weapons physics by increasing the proliferation resistance of the nuclear fuel cycle with precision isotopic monitoring and by demonstrating the potential for MEGA-ray sources for detection of highly enriched uranium at trade portals. The project also supports environmental management efforts by enabling quantitative assessment and reclassification of the DOE complex's nuclear waste.

FY10 Accomplishments and Results

In FY10 we (1) began modifying experimental areas to support precision MEGA-ray capability and



Rendering of the precision MEGA-ray (mono-energetic gamma-ray) photo-gun developed in collaboration with the SLAC National Accelerator Laboratory. The new technology will generate an ultrabright beam of gamma rays (extremely high-energy photons) for use in studying the nuclei of individual isotopes.

completed modifications to the laser and magnet test laboratories; (2) designed a state-of-the-art 5.59-cell X-band-frequency photo-gun; (3) procured the solid-state modulator to drive a SLAC National Accelerator Laboratory XL4 klystron; (4) fabricated precision copper parts for the six T53 X-band accelerator sections; (5) designed a magnet lattice for the X-band accelerator, including a chicane to block Bremsstrahlung produced by dark current; (6) completed design of the photocathode fiber-laser front end, including ultraviolet-ray generation; (7) designed joule-level pulse compression for the interaction laser; (8) began design of the laser-transport system leading to the photocathode and interaction region as well as design of the radiofrequency compression and distribution system; (9) established a test bed for X-band-frequency measurements and component characterization; and (10) optimized gamma-ray generation physics using advanced electron-beam, gamma-ray, and laser codes.

Proposed Work for FY11

In FY11 we will (1) complete the fiber-based ultraviolet laser optimized for the X-band-frequency photo-gun; (2) complete fabrication, cold testing, tuning, and conditioning (to 200 MV/m) of the 5.59-cell X-band-frequency photo-gun, which will generate 250 pCi at 7 MeV with submicron normalized emittance; (3) complete the diode-pumped, joule-class, 120-Hz interaction laser system, which will generate 10-ps pulses via hyper-chirped-pulse amplification; (4) create a high-fidelity Compton model that includes, for the first time, three-dimensional nonlinear effects and a novel concept to use nuclear resonance fluorescence for in situ, picosecond-scale temperature probing; (5) conduct integrated X-band-laser system tests; and (6) redesign and rebuild the X-band sections for precision MEGa-ray technology.

Publications

Albert, F., 2009. *Characterization and applications of a bright tunable, MeV class Compton scattering gamma-ray source*. CLEO/ IQEC 2009, Conf. Lasers and Electro-Optics and Intl. Quantum Electronics Conf., Baltimore, MD, May 31–June 5, 2009. LLNL-PRES-4138.

Albert, F., 2009. *Characterization and applications of T-REX: LLNL's bright, tunable, laser-based gamma-ray source*. LLNL-POST-413803.

Albert, F., 2009. *Isotope specific detection with T-REX: LLNL's bright, tunable, laser-based mono-energetic gamma-ray (MEGA-ray) source*. Special Topics in Homeland Nuclear Security Workshop, Berkeley, CA, July 23, 2009. LLNL-PRES-415031.

Albert, F., et al., 2010. *Advanced Compton scattering light source R&D at LLNL*. Intl. Conf. Ultrafast Phenomena, Snowmass Village, CO, July 18–23, 2010. LLNL-CONF-424003.

Albert, F., et al., 2009. *Characterization and applications of T-REX, an ultrabright, laser-based, gamma-ray light source*. UFO/HFSW 2009, UltraFast Optics and High Field Short Wavelength Mtgs., Arcachon, France, Aug. 31–Sept. 4, 2009. LLNL-PRES-416231.

Albert, F., et al., 2009. *Characterization of a tunable, laser-based, MeV-class Compton scattering light source*. LLNL-JRNL-414424.

Albert, F., et al., 2010. "Compton scattering sources and applications at LLNL." *Advanced Accelerator Concepts: 14th Advanced Accelerator Concepts Workshop*, AIP Conf. Proc. vol. 1299, p. 550. LLNL-ABS-429019.

Albert, F., et al., 2010. "Isotope-specific detection of low-density materials with laser based monoenergetic gamma-rays." *Optic. Lett.* **35**, 354. LLNL-TR-411369.

Albert, F., et al., 2009. *Properties and applications of monoenergetic gamma-rays from laser-Compton scattering*. 51st Ann. Mtg. APS Division of Plasma Physics, Atlanta, GA, Nov. 2–6, 2009. LLNL-PRES-419113.

Anderson, S. G., et al., 2009. *Design of a 250 MeV, X-band photoinjector linac for a precision Compton-scattering based gamma-ray source*. PAC09, Particle

Accelerator Conf., Vancouver, Canada, May 4–8, 2009. LLNL-ABS-409324.

Anderson, S. G., et al., 2009. *Observation of nonlinear space-charge induced phase space wave-breaking and emittance growth in a high-brightness photoinjector*. PAC09, Particle Accelerator Conf., Vancouver, Canada, May 4–8, 2009. LLNL-ABS-409323.

Barty, C. P. J., 2009. *Mono-energetic gamma-ray (MEGA-ray) sources and nuclear applications*. LEI 2009, Light at Extreme Intensities, Brasov, Romania, Oct. 16–21, 2009. LLNL-ABS-418058.

Chu, T. S., et al., 2010. “500 MW X-band RF system of a 0.25 GeV electron LINAC for advanced Compton scattering source application.” *Proc. 1st Intl. Particle Accelerator Conference (IPAC’10)*, Kyoto, Japan, p. 3798. LLNL-ABS-421110.

Chu, T. S., et al., 2009. *Precision 0.5 GW X-band RF system for advanced Compton scattering source*. 12th Ann. Directed Energy Symp., San Antonio, TX, Nov. 2–6, 2009. LLNL-PRES-419532.

Gibson, D. J., 2009. *Development and applications of laser-based mono-energetic gamma-rays (MEGA-rays)*. LEOS 2009, 22nd Mtg. IEEE Lasers and Electro-Optics Society, Belek-Antalya, Turkey, Oct. 4–8, 2009. LLNL-PRES-417742.

Gibson, D. J., et al., 2009. *Commissioning a tunable MeV-level Compton-scattering-based gamma-ray source*. LLNL-JRNL-414643.

Gibson, D. J., et al., 2009. *Commissioning of a Compton-scattering based gamma-ray source*. 51st Ann. Mtg. APS Division of Plasma Physics, Atlanta, GA, Nov. 2–6, 2009. LLNL-POST-418356.

Gibson, D. J., et al., 2010. “Design and Operation of a tunable MeV-level Compton-scattering-based (gamma-ray) source.” *Phys. Rev. Spec. Top. Accel. Beams* **13**, 070703. LLNL-JRNL-414643.

Gibson, D. J., et al., 2009. *Demonstration and optimization of a drive laser for an X-band photoinjector*. PAC09, Particle Accelerator Conf., Vancouver, Canada, May 4–8, 2009. LLNL-CONF-412435.

Hartemann, F. V., 2008. *Compton scattering overview*. Compton Sources for X/Gamma Rays: Physics and Applications, Alghero, Sardinia, Italy, Sept. 7–12, 2008. LLNL-PROC-409586.

Hartemann, F. V., 2010. *Overview of Compton scattering light sources and applications*. 48th ICFA Advanced Beam Dynamics Workshop Future Light Sources, Mar. 1–5, 2010, Stanford, CA. LLNL-ABS-424344.

Hartemann, F. V., and F. Albert, 2009. *Design of a 2 MeV Compton scattering gamma-ray source for DNDO missions*. LLNL-TR-416320.

Hartemann, F. V., et al., 2009. *Compact, tunable Compton scattering gamma-ray sources*. FEL09, Free Electron Laser Conf., Liverpool, UK, Aug. 23–28, 2009. LLNL-PROC-416016.

Hartemann, F. V., et al., 2009. *Development of a precision tunable gamma-ray source driven by a compact X-band linac*. PAC09, Particle Accelerator Conf., Vancouver, Canada, May 4–8, 2009. LLNL-PROC-412716.

Hartemann, F. V., et al., 2010. *LLNL’s precision Compton scattering light source: Status and applications*. 52nd Ann. Mtg. APS Division of Plasma Physics, Chicago, IL, Nov. 8–12, 2010. LLNL-ABS-426225.

Hartemann, F. V., et al., 2009. *MeV mono-energetic gamma ray Compton scattering source R&D*. 51st Ann. Mtg. APS Division of Plasma Physics, Atlanta, GA, Nov. 2–6, 2009. LLNL-PRES-419112.

Hartemann, F. V., et al., 2010. “Overview of mono-energetic gamma-ray sources and applications.” *Proc. 1st Intl. Particle Accelerator*

Conference (IPAC'10), Kyoto, Japan, p. 2129.
LLNL-ABS-421111.

Hartemann, F. V., et al., 2010. *Velociraptor: LLNL's precision Compton scattering light source*.
LLNL-ABS-425969.

Marsh, R., 2009. *Development and applications of laser-based mono-energetic gamma-rays (MEGA-rays)*. CLIC09 Workshop, Geneva, Switzerland, Oct. 12–16, 2009. LLNL-PRES-417819.

Messierly, M., et al., 2010. *Advances in energetic short-pulse fiber lasers*. Frontiers in Optics, Rochester, NY, Oct. 24–28, 2010.
LLNL-ABS-439553.

Shverdin, M., et al., 2009. *Compact laser technology for Compton scattering sources*. 51st Ann. Mtg. APS Division of Plasma Physics, Atlanta, GA, Nov. 2–6, 2009. LLNL-PRES-418797.

Shverdin, M. Y., et al., 2009. *Compact laser technology for monoenergetic gamma-ray Compton source*. Nonlinear Optics, Honolulu, HI, July 12–17, 2009.
LLNL-CONF-411293.

Shverdin, M., et al., 2009. *Gamma-ray flux enhancement via high energy pulse recirculation*. Special Topics in Homeland Nuclear Security Workshop, Berkeley, CA, July 23, 2009. LLNL-PRES-414776.

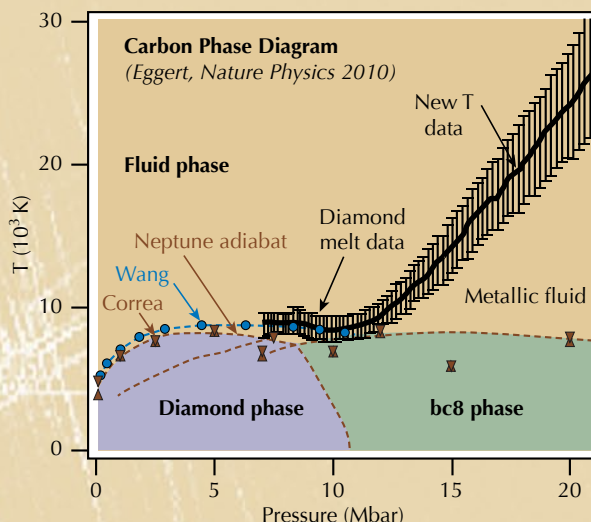
Shverdin, M., et al., 2010. "Laser technology for precision monoenergetic gamma-ray source R&D at LLNL." *Proc. 1st Intl. Particle Accelerator Conference (IPAC'10)*, Kyoto, Japan, p. 2126.
LLNL-PROC-428250.

Wu, S. S. Q., et al., 2009. *Nonlinear vacuum polarization in intense blackbody radiation and its effects on the radiation spectrum*. 51st Ann. Mtg. APS Division of Plasma Physics, Atlanta, GA, Nov. 2–6, 2009. LLNL-PRES-419099.

Physics and Chemistry of the Interiors of Large Planets: A New Generation of Condensed Matter—Gilbert Collins (09-SI-005)

Abstract

We propose to employ Livermore's advanced laser facilities to systematically characterize condensed matter at extreme conditions of gigabar pressures and over tenfold compression. This research focuses on establishing a new generation of experiments accessing the unexplored regime of ultrahigh compression, with applications that range from understanding the origin and evolution of planets to testing and significantly extending fundamental theories of condensed matter. Our effort will form a community of the world's leading scientists in condensed matter and planetary science.



Phase diagram for high-pressure carbon, with new temperature–pressure data compared with simulations. The black line denotes our new experimental shock-temperature data. The blue circles and blue dashed line represent the melt curve from density functional theory calculations from Wang, et al., that include diamond and liquid phases. The brown triangles that bracket the phase transitions and the brown dashed lines represent similar calculations by Correa, et al., that include the diamond, bc8, and fluid phases. Our measurements did not identify multiple solid phases—whether diamond, bc8, or both—as predicted by theory. The graphite phase is omitted for clarity.

We expect to develop a new scientific frontier of extreme states of matter from ultradense condensed matter to burning plasmas. We will determine key constraints on planetary and stellar evolution models using hydrogen, helium, and mixtures at more than tenfold compression, from a low-temperature isentrope to a burning plasma. We will determine whether hydrogen becomes a Wigner crystal, a superconductor, or a superfluid at extreme densities, as well as characterize iron at the low-temperature and ultrahigh-pressure conditions expected to exist at the core of extrasolar super-Earth planets. In addition, we will produce the first data on chemistry in the gigabar regime and determine the fundamental nature and key physics of burning plasmas.

Mission Relevance

To successfully maintain an aging stockpile, the nation needs new predictive capabilities. Of particular importance to the Stockpile Stewardship Program is the development of advanced capabilities to predict physical properties of matter under an extremely broad range of dynamic conditions—specifically, equation-of-state and constitutive models. Our project will fully develop required experimental capabilities as well as provide important data on metals and hydrogenic liquids in support of the Laboratory's mission in national security.

FY10 Accomplishments and Results

In FY10 we (1) discovered a new polymeric phase of carbon at pressures of 11 to 20 Mbar and temperatures of 1 to 2 eV—the highest pressure–melt curve ever recorded—and verified that temperature decreases with increasing pressure, similar to ice at near-atmosphere pressures, and that with current isentrope models of Neptune, the core of Neptune is potentially largely composed of solid diamond; (2) discovered that helium metallizes at approximately 2 g/cm³, a significantly lower density than predicted with traditional band-structure or ab initio calculations; (3) performed high-precision equation-of-state experiments on carbon and hydrogen mixtures to 10 Mbar; (4) developed new techniques to explore warm dense matter by isochoric heating; (5) discovered a

first-order liquid–liquid transition in magnesium silicate; (6) measured the melt curve of magnesium oxide to 5 Mbar; (7) determined that the structure of iron at Earth core pressures (~4 Mbar) and up to 6 Mbars is hexagonal closely packed, in contrast to previous predictions; (8) showed that helium–hydrogen mixtures behave as an ideal mixture deep in the interior of Jupiter; and (9) collected the highest pressure deuterium equation-of-state data ever recorded, at France's Laser Integration Line.

Proposed Work for FY11

In FY11 we propose to (1) use recent advances in ramp compression to design and field the highest-pressure solid-state experiments ever performed; (2) design, field, and use new diagnostic techniques at the National Ignition Facility to explore a new ultradense matter regime—namely, diffraction for determining structure at terapascal (≥ 10 Mbar) pressures, x-ray absorption for temperature and coordination at terapascal conditions, stimulated Raman to determine the nature of chemical bonds at hundred-fold compression, and broadband reflectance for the electronic structure of ultradense matter; (3) compress hydrogen to densities at which the interatomic spacing is comparable to the de Broglie wavelength, at which quantum mechanical effects are very strong and current theories have conflicting predictions; and (4) design and begin experiments to explore burning plasma elements crucial to advanced fusion concepts.

Publications

Celliers, P. M., et al., 2010. "A high-resolution two-dimensional imaging velocimeter." *Rev. Sci. Instrum.* **81**, 35101. LLNL-JRNL-414901.

Celliers, P. M., et al., 2010. "Insulator-to-conducting transition in dense fluid helium." *Phys. Rev. Lett.* **104**, 184503. LLNL-JRNL-417413.

Hicks, D. G., et al., 2008. "High-precision measurements of the diamond Hugoniot in and above the melt region." *Phys. Rev. B* **78**, 174102. LLNL-JRNL-406173.

Hicks, D. G., et al., 2009. "Laser-driven single-shock compression of fluid deuterium from 45 to 220 GPa." *Phys. Rev. B* **79**, 14112. LLNL-JRNL-402514.

McWilliams, R. S., et al., 2010. "Strength effects in diamond under shock compression from 0.1 to 1 TPa." *Phys. Rev. B* **81**, 14111. LLNL-JRNL-418469.

From Super-Earths to Nucleosynthesis: Probing Extreme High-Energy-Density States of Matter with X Rays—Bruce Remington (09-SI-010)

Abstract

We propose to develop advanced x-ray diagnostic systems to investigate materials at ultrahigh pressures (>10 Mbar), such as those found at the cores of newly discovered "super-Earth" exoplanets, and plasmas at ultrahigh densities (>100 g/cm³), as in nuclear burn in stars and supernovae. We will develop three types of diagnostic capabilities, including a lattice diagnostic, an ultrafast x-ray diagnostic for investigating nuclear burn, and a multiframe, single line-of-sight imager. We will also validate these capabilities through experiments at laser and calibration facilities. This project will enable precision science to be conducted on matter under the most extreme conditions of

density and temperature accessible, which is important to both basic and applied science.

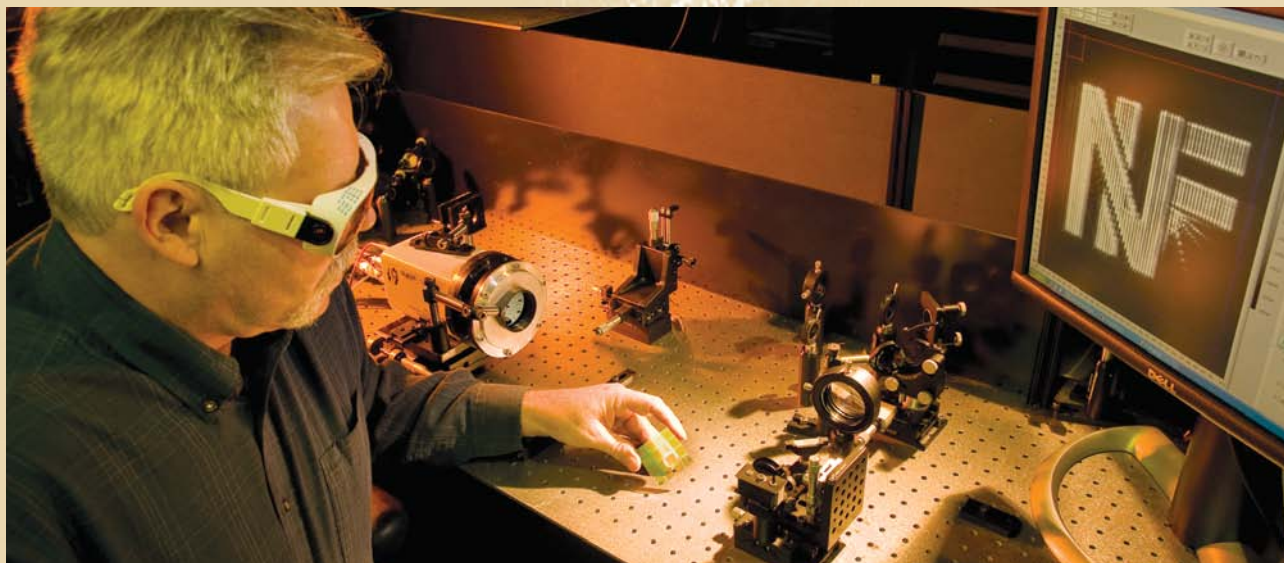
We expect to develop advanced x-ray diagnostic systems to study extreme high-energy-density states of matter. These new capabilities will make it possible to probe super-Earth core conditions with a dynamic lattice-level diffraction diagnostic at 100 times higher pressures and 4 times higher x-ray energies than is currently possible. These capabilities will also enable researchers to probe nucleosynthesis plasma conditions by dynamic characterization of hot, dense burning plasmas at 100 times higher densities and with 100,000 times higher yield than is currently possible.

Mission Relevance

By developing capabilities to measure material phase and lattice response at ultrahigh pressures and conditions in burning plasmas at ultrahigh densities, which are relevant to stockpile stewardship and high-energy-density science, this project supports the Laboratory's national security mission.

FY10 Accomplishments and Results

In FY10 we (1) demonstrated, for the first time, dynamic Bragg diffraction at about 20 keV in a shocked molybdenum crystal, and dynamic Laue diffraction at 10 to 30 keV in a shocked tantalum



Our LDRD project led to a 2010 R&D 100 award for the grating-actuated transient optical recorder (GATOR), which is designed to acquire sequential images of x rays or optical light in a trillionth of a second or faster during experiments at the National Ignition Facility.

crystal, using the OMEGA and OMEGA EP lasers at the University of Rochester; (2) demonstrated a 1-ps imaging time response to optical radiation with a proton-implanted gallium arsenide converter used in our ultrafast imaging x-ray diagnostic, GATOR (grating-actuated transient optical recorder), which was recognized with an R&D 100 Award in 2010; (3) studied the optical response of three new semiconductors with band gaps in the visible spectral region and showed that zinc selenide produced excellent high-speed images, qualifying it as a promising material for x-ray detection with a 530-nm probe beam—the use of a green probe beam would reduce the cost and complexity and may increase the sensitivity of the x-ray detection system; and (4) completed design of a proof-of-principle x-ray test for FY11 at Livermore's Callisto laser, and began optical testing of the detector system for the scheduled x-ray experiment.

Proposed Work for FY11

In FY11 we will (1) demonstrate high-energy x-ray diffraction and acquire dynamic data sensitive to defect density in driven materials, (2) finalize the selection of optimal spectral features to measure electron temperatures and densities in burning plasmas, (3) build an ultrafast x-ray diagnostic prototype and demonstrate it with proof-of-principle experiments on short-pulse lasers, and (4) complete the design concept for a 64-by-64-pixel sensor and readout electronics for a multiframe single-line-of-sight camera suitable for use on burning plasmas.

Publications

Meissner, C., 2010. "High-speed imager for fast, transient events at NIF." *Sci. Tech. Rev.*, Oct./Nov. 2010, 10. UCRL-TR-52000-10-10/11.

Maddox, B. R., in press. "Absolute measurements of x-ray backlighter sources at energies above 10 keV." *Phys. Plasma*. LLNL-463438.

Remington, B. A., 2009. *Progress towards materials science above 1000 GPa (10 Mbar) on the NIF laser*. 9th Intl. Conf. Mechanical and Physical Behaviour

of Materials under Dynamic Loading, Brussels, Belgium, Sept. 7–11, 2009. LLNL-CONF-411555.

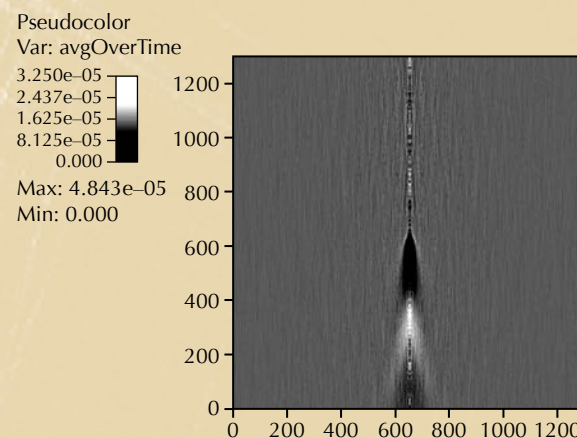
Rudd, R. E., 2009. "High-rate plastic deformation of nanocrystalline tantalum to large strains." *Mater. Sci. Forum* **3**, 633. LLNL-JRNL-410397.

The Microphysics of Burning, Hot Dense Radiative Plasmas—Frank Graziani (09-SI-011)

Abstract

We intend to develop a detailed microphysical understanding of the physics of burning, hot dense radiative plasmas by building a validated state-of-the-art *N*-body simulation capability. The extreme conditions of these plasmas mean that experimental data for validation are difficult to obtain. What is needed for this data-starved environment is a quantitative way of telling whether or not the physics used to describe burning, hot dense radiative plasmas is correct. We will address this critical need by building a world-class massively parallel *N*-body simulation capability in conjunction with experimental validation experiments. The microphysics of burning, hot dense radiative plasmas will be simulated without the assumptions that underlie current

DB: /nfs/dvstmp/gromit/Plasma/hdrp/surh/09_15_10/linkFarm/pwake_0/pwake_0.*database



A two-million-particle molecular dynamics simulation of the wake of a high-energy charged particle traversing and depositing energy in a plasma.

models used to calculate inertial-confinement fusion or astrophysical problems.

We expect to (1) develop an N -body simulation capability using molecular dynamics to investigate the properties of hot dense matter undergoing thermonuclear burn; (2) employ the new simulation capability to test microphysical foundations of widely accepted theoretical models; and (3) validate the new simulation capability using the ultrashort-pulse lasers Titan at Livermore, the OMEGA laser at the University of Rochester, and the Linac Coherent Light Source at Stanford.

Mission Relevance

The results obtained with this project directly address the issue of predictive capability, which is at the core of the Stockpile Stewardship Program. Furthermore, the validated simulation capability for burning, hot dense radiative plasmas that we will develop will extend LLNL's world leadership in high-energy-density physics to include not only experimental expertise but computational modeling as well. It will help establish LLNL as the world center for high-energy-density physics in support of the Laboratory's mission in fundamental science breakthroughs.

FY10 Accomplishments and Results

In FY10 we (1) collected stopping-power data from the Jupiter laser and structure data from Linac Coherent Light Source; (2) performed molecular dynamics (MD) simulations of the experiments, obtaining results consistent with the data but demonstrating the need to fully implement the atomic physics capability of domain decomposition MD; (3) began a detailed investigation of the statistical potentials used in domain decomposition MD, which we compared in detail to quantum Monte Carlo and the hyper-netted chain model approach, deriving a new set of potentials, which improved our results; (4) used domain decomposition MD to conduct a detailed study of stopping power in one- and two-component plasma materials; (5) developed kinetic-theory MD code to hopefully solve the time-scale hierarchy problem in plasmas, in which time-scales can differ by up to eight orders of magnitude;

(6) implemented simple versions of kinetic-theory MD and conducted a theoretical derivation of its formalism using Wigner functions, providing a rigorous foundation for the approach, which will be further pursued in FY11; and (7) strengthened the theoretical footing of the electron-ion coupling problem with a formalism that provided deep insights into the efficacy of statistical potentials for dynamic MD applications.

Proposed Work for FY11

In FY11 we will (1) apply our simulation capability to problems relevant to inertial-confinement fusion and stockpile stewardship, (2) build upon a new method of treating electrons at large time-scales to begin investigating thermonuclear burn in the presence of high-atomic-number dopants, (3) compare these results to radiation-hydrodynamic codes, and (4) obtain validation data from the Linac Coherent Light Source to compare simulation to data and test the atomic physics capability of the code.

Publications

Benedict, L. X., et al., 2009. "Molecular dynamics simulations of electron-ion temperature equilibration in an SF₆ plasma. *Phys. Rev. Lett.* **102**, 205004. LLNL-JRNL-412459.

Glosli, J., and D. Richards, 2010. "Beyond homogeneous decomposition: Scaling long-range forces on massively parallel systems." *Proc. SC '10: Conf. High-Performance Computing Networking, Storage, and Analysis*. LNL-CONF-423472.

Glosli, J. N., et al., 2009. "Molecular dynamics simulations of temperature equilibration in dense hydrogen." *Phys. Rev. E* **78**, 025401. LLNL-JRNL-401466.

Hau-Riege, S. P., et al., 2010. "Near-ultraviolet luminescence of N₂ irradiated by short x-ray pulses." *Phys. Rev. Lett.* **105**, 043003. LNL-CONF-423472.

Hau-Riege, S. P., 2010. *Ultrafast probing of the x-ray-induced lattice and electron dynamics in graphite at atomic resolution*. LLNL-TR-458811.

More, R., and F. Graziani, 2010. *Emission of visible light by hot dense metals*. 19th Intl. Toki Conference (ITC19) on Advanced Physics in Plasma and Fusion Research, Toki City, Japan, Dec. 8–11, 2009. LNL-CONF-423472.

More, R., et al., 2009. "Radiation in particle simulation." *High Energy Density Phys.* **6**, 29. LLNL-PROC-413971.

Shepherd, R. 2010. "An imaging proton spectrometer for short-pulse laser plasma experiments." *Rev. Sci. Instrum.* **81**, 10D314. LLNL-CONF-423472.

Shepherd, R., in press. "Ionization balance and proton energy loss in high-density plasmas." *High Energy Density Phys.* LNL-CONF-423472.

Improved Spectral Line-Shape Models for Opacity Calculations—Carlos Iglesias (09-ERD-004)

Abstract

Opacity, or the measure of impenetrability to electromagnetic or other radiation in a medium, is important for energy-transport simulations used in the design and analysis of Laboratory applications such as inertial-confinement fusion. However, theoretical opacities vary by as much as a factor of two because of uncertainties in models of spectral line shape. Our main goal is to improve line-shape models in the opacity codes by applying line-broadening theory to complex electronic configurations that have been heretofore neglected by the scientific community, but which are essential for opacity calculations. The results will be extended to the super-configuration array concept, which is vital for calculations involving myriad configurations. Finally, we will synthesize this gained knowledge into a suite of routines for incorporation into opacity codes.

The project will produce improved opacity codes by addressing three uncertain aspects of line-shape models: line-width calculation using approximate

formulas, far-wing behavior, and line broadening in complex multi-electron ions. We will produce fast computer subroutines that parameterize these complex processes and incorporate those subroutines into opacity codes. These achievements will result in improved theoretical opacities, which will in turn resolve uncertainties in many LLNL applications that depend on the accurate simulation of energy-transport mechanisms.

Mission Relevance

This project supports the Laboratory's missions in national and energy security by addressing an important knowledge gap in advanced physical models for predictive capabilities for nuclear physics, astrophysics, and high-energy-density science.

FY10 Accomplishments and Results

In FY10 we (1) investigated the essential physics describing line shapes, taking into consideration excited spectator electrons; (2) developed a new multi-electron line-shape model for opacity that accounts for the effects of excited spectator electrons in spectral line shapes and also takes advantage of new language capabilities and improved numerical techniques for greater computational speed; and (3) determined that the new model has wide applicability in plasma characterization through spectroscopy. For example, the model was shown to significantly impact inferred free-electron densities using dielectronic satellite lines and may well impact spectral analysis in fusion energy experiments.

Proposed Work for FY11

In FY11 we will apply our multi-electron line-shape approach, implemented as fast algorithms, to opacity models to mimic the essential features of line broadening.

Publications

Iglesias, C. A., 2010. "Excited spectator electron effects on spectral lines." *High Energ. Density Phys.* **6**, 318. LLNL-JRNL-418104.

First-Principles Planetary Science— Kyle Caspersen (09-ERD-012)

Abstract

The objective of this project is to provide a first-principles understanding of the interiors of the four gas giants in our solar system—Jupiter, Saturn, Uranus, and Neptune. The lack of experimental data on the interior of these four planets leads to uncertainty and unanswered questions about their formation, current structure, and how they will evolve. We will address these questions using the predictive capability of first-principles calculations. In particular, we will calculate planetary isentropes (lines of constant entropy) to predict the pressures and temperatures in these gas giants and transport properties along the isentropes to provide insight into the planetary dynamics.

We intend to construct thermodynamically consistent isentropes that are free from most current assumptions. We will also calculate transport properties along these isentropes. This will be the first time that planetary isentropes and their corresponding transport properties have been calculated completely with first-principles calculations. The unequaled precision and predictive power of these calculations have, and will, allow us to address fundamental questions in the field of planetary science and in the more general field of high-energy-density science. This project will also directly benefit many ongoing efforts at LLNL, including equation-of-state table development, the generation of mixing and plasma models, and dynamic compression experiments.

Mission Relevance

This project supports LLNL's national security mission by developing predictive modes for examining the properties of materials under extreme conditions. Such techniques, if successful, will have direct application to equation-of-state models for materials of interest for stockpile stewardship and other Laboratory missions.

FY10 Accomplishments and Results

In FY10 we (1) continued the calculation of isentropes by constructing a free-energy grid appropriate for the relevant phase (pressure vs. temperature); (2) calculated viscosities for hydrogen at conditions relevant to planets and electrical and thermal conductivities for mixtures similar to the composition of Uranus and Neptune; (3) started investigation of the kinetics of helium condensation by focusing on how it affects transport properties, with a focus on electrical conductivity; and (4) performed simulations of hydrogen–argon mixtures.

Proposed Work for FY11

In FY11 we will (1) complete the calculation of the free-energy grid for constructing any isentrope for hydrogen–helium planets and publish the results; (2) continue calculation of transport properties, with a focus on thermal conductivity; and (3) continue to study the kinetics of helium condensation and how those kinetics might affect our proposed experiments.

Publications

Morales, M. A., et al., 2009. "Phase separation in hydrogen–helium mixtures at Mbar pressures." *Proc. Natl. Acad. Sci. USA* **106**, 1324. LLNL-JRNL-411757.

Imaging X-Ray Line-Shape Diagnostic for Burning Plasmas—Peter Beiersdorfer (09-ERD-016)

Abstract

We intend to investigate the suitability of neon-like tungsten as a tracer ion for measuring ion temperature and velocity in a hot, ignited plasma. Such measurements are crucial for achieving fusion ignition and burn. We will build a new type of imaging spectrometer, which will operate in a vacuum and use a spherically bent crystal in its Johann geometry.

We will also test key aspects of a tungsten-based spectrometer, including throughput issues, window design, performance over a large temperature range, and power dissipation of the detector in a vacuum. We will utilize LLNL's Electron Beam Ion Trap facility, which is uniquely suited to produce the relevant radiation.

If successful, we will produce novel atomic data and perform world-class science experiments such as measurements of excitation-rate coefficients, ultrafast radiative lifetimes, and dielectronic-rate coefficients, which have never before been measured for such high-atomic-number systems but are needed to determine ion temperature and motion. We will also provide the scientific and technological basis for choosing a tungsten-based instrument design and create a prototype instrument for hot plasmas with which we will assess the technological hurdles of measuring radiation from an ignited plasma.

Mission Relevance

This project supports the Laboratory's missions in energy security by developing groundbreaking technologies for achieving fusion-driven energy sources. This project will also help attract top talent to the Laboratory in this topical, cutting-edge field.

FY10 Accomplishments and Results

We (1) finished the design of a high-resolution imaging spectrometer based on a spherical crystal and a novel x-ray detector; (2) acquired both quartz and germanium crystals and tested them for use in the new instrument and found only the quartz suitable; (3) procured and tested the new detector and began taking first data with the new instrument, but were not yet able to acquire spectral data because the quartz crystal was found to have a very low reflectivity; and (4) continued analyzing our FY09 measurements, which were published in several key papers, including one that defines key instrumental parameters for a future line-shape diagnostic for temperature measurements of a burning plasma.

Proposed Work for FY11

In FY11 we will (1) use our new high-resolution imaging spectrometer for measuring tungsten L-shell lines with very high resolution, (2) use these measurements to determine the wavelength of salient features of the tungsten spectrum and to assess blends that may affect the line shapes that can serve as burning plasma diagnostics, and (3) attempt to use the instrument to determine the natural line shape of the resonance line of neon-like tungsten, from which we will determine the associated radiative transition probability. If successful, this will be the highest resolution x-ray line-shape measurement ever achieved and will validate the scientific and technical concepts of the new instrument.

Publications

Beiersdorfer, P., et al., 2010. "The ITER core imaging x-ray spectrometer." *J. Phys. B: Atom. Mol. Opt. Phys.* **43**, 144008. LLNL-JRNL-416157.

Beiersdorfer, P., et al., 2010. "The ITER core imaging x-ray spectrometer: X-ray calorimeter performance." *Rev. Sci. Instrum.* **81**, 10E323. LLNL-JRNL-432594.

Bitter, M., et al., 2010. "Imaging with spherically bent crystals or reflectors." *J. Phys. B: Atom. Mol. Opt. Phys.* **43**, 144011. LLNL-JRNL-461839.

Clementson, J., and P. Beiersdorfer, 2010. "Wavelength measurement of $n = 3$ to $n = 3$ transitions in highly charged tungsten ions." *Phys. Rev. A* **81**, 052509. LLNL-JRNL-425770.

Clementson, J., P. Beiersdorfer, and M. F. Gu, 2010. "X-ray spectroscopy of E2 and M3 transitions in Ni-like W." *Phys. Rev. A* **81**, 012505. LLNL-JRNL-419970.

Clementson, J., et al., 2010. "Spectroscopy of M-shell x-ray transitions in Zn-like through Co-like W." *Phys. Scripta* **81**, 015301. LLNL-JRNL-414669.

Clementson, J., et al., 2010. "Tungsten spectroscopy relevant to the diagnostics development of ITER divertor plasmas." *J. Phys. B: Atom. Mol. Opt. Phys.* **43**, 144009. LLNL-JRNL-420920.

Clementson, J., et al., 2010. *Tungsten spectroscopy at the Livermore electron beam ion trap facility.* LLNL-JRNL-458474.

Hill, K. W., et al., 2010. "Development of spatially resolving x-ray crystal spectrometer (SCS) for measurement of ion-temperature (Ti) and rotation-velocity (v) profiles in ITER." *Rev. Sci. Instrum.* **81**, 10E322. LLNL-JRNL-43352.

Podpaly, Y., et al., 2009. "High-resolution spectroscopy of $2s_{1/2}$ – $2p_{3/2}$ transitions in W^{65+} through W^{71+} ." *Phys. Rev. A.* **80**(5), 052504. LLNL-JRNL-416158.

Podpaly, Y., et al., 2010. *Tungsten measurement on Alcator C-Mod and EBIT for future fusion reactors.* LLNL-JRNL-438512.

Safronova, U. I., A. S. Safronova, and P. Beiersdorfer, 2010. *Dielectronic recombination and satellite line spectra of highly charged tungsten ions.* LLNL-JRNL-458494.

Safronova, U. I., A. S. Safronova, and P. Beiersdorfer, 2010. "Excitation energies, radiative and auto-ionization rates, dielectronic satellite lines, and dielectronic recombination rates for excited states of Na-like W from Ne-like W." *Atom. Data Nucl. Data* **95**(6), 751. LLNL-JRNL-407732.

Safronova, U. I., A. S. Safronova, and P. Beiersdorfer, 2010. "Excitation energies, radiative and auto-ionization rates, dielectronic satellite lines, and dielectronic recombination rates for excited states of Mg-like W from Na-like W." *J. Phys. B: Atom. Mol. Opt. Phys.* **42**, 165010. LLNL-JRNL-413406.

Safronova, U. I., et al., 2011. "Excitation energies, radiative and autoionization rates, dielectronic satellite lines, and dielectronic recombination rates for excited states of Ag-like W from Pd-like W." *J. Phys. B Atom. Mol. Opt. Phys.* **44**, 035005. LLNL-JRNL-455914.

Trabert, E., in press. "In pursuit of high precision atomic lifetime measurements of multiply charged ions." *J. Physics B: At. Mol. Opt. Phys.* **43**(7), 074034. LLNL-JRNL- 413576.

Wang, E., et al., 2010. "Calculation of the Johann error for spherically bent x-ray imaging crystal spectrometers." *Rev. Sci. Instrum.* **81**, 10E329. LLNL-JRNL-434556.

Ultrafast Nanoscale Dynamic Imaging Using X-Ray Free-Electron Lasers— Stefan Hau-Riege (09-ERD-023)

Abstract

By delivering ultrashort pulses of unprecedented brightness, x-ray free-electron lasers (fourth-generation light sources) will revolutionize x-ray science. Our goal is to take advantage of the timely coincidence of the advent of these lasers, such as the Linac Coherent Light Source (LCLS) at Stanford, and our team's recently gained experience at LCLS in molecular-resolution imaging with x-ray free-electron lasers to answer several questions concerning the properties and dynamics of high-energy-density matter of importance to NNSA programs. Experiments at LCLS will directly complement results obtained at the National Ignition Facility by providing a very high-fidelity probe for materials in only moderate high-energy-density states. Energy densities accessible at the National Ignition Facility will be substantially higher, but the probe is less suited for imaging.

Besides developing new capabilities for LLNL, such as a novel plasma probe with high penetration power and an ultrahigh-precision high-energy-density lattice and microstructure diagnostic, we will perform fundamental research in the field of x-ray and material interaction. This will benefit a wide variety of other areas, including ultrafast atomic molecular physics, cluster physics, and coherent x-ray imaging of nanometer-scale objects.

Mission Relevance

By exploiting an entirely new generation of x-ray sources, this project supports the Stockpile Stewardship Program, which is highly dependent on high-quality data describing the properties and processes of high-energy-density matter. National security and weapons science are served through the proposed study of dynamic systems with broad application to the investigation of material dynamics under extreme conditions. Novel imaging techniques are also at the cutting edge of photon science applications, which will be developed at LCLS.

FY10 Accomplishments and Results

Our outstanding accomplishments resulted in the publication of two articles in *Physical Review Letters* in FY10, and two articles for *Nature* in FY11. In FY10 we (1) performed x-ray Thomson scattering and Bragg reflection experiments at LCLS; (2) conducted x-ray and matter experiments at the LCLS on gases and solids, studying the collective effects of the interaction of LCLS radiation with gaseous matter using nitrogen fluorescence and, for solids, investigating damage thresholds and characterizing LCLS optics using imprints in solids; and (3) conducted massively parallel molecular dynamics simulations of the scattering experiments by pioneering a new method of interacting molecular dynamics simulations.

Proposed Work for FY11

In FY11 we will (1) evaluate the diffraction data obtained in FY10 through further semiclassical molecular dynamics simulations, (2) evaluate new schemes to simulate the interaction of LCLS radiation with matter, (3) perform a time-resolved x-ray Thomson scattering experiment and compare the

results to simulations, and (4) perform laser-driven experiments. This work will constitute the first set of high-energy-density state experiments at LCLS and will lay the groundwork for experimentation with the Matter in Extreme Conditions instrument at LCLS.

Publications

Bogan, M. J., et al., 2010. "Aerosol imaging with a soft x-ray free-electron laser." *Aerosol Sci. Tech.* **44**(3), i. LLNL-JRNL-464094.

Bogan, M. J., et al., 2010. "Single-shot femtosecond x-ray diffraction from randomly oriented ellipsoidal nanoparticles." *Phys. Rev. ST Accel. Beams* **13**, 094701. LLNL-JRNL-463908.

Chapman, H., et al., 2011. "Femtosecond x-ray protein nanocrystallography." *Nature* **470**, 73. LLNL-JRNL-434309.

Hau-Riege, S. P., et al., 2010. "Interaction of low-Z inorganic solids with short x-ray pulses at the LCLS free-electron laser." *Optic. Express* **18**, 23933. LLNL-JRNL-460592.

Hau-Riege, S. P., et al., 2010. "Near-ultraviolet luminescence of N₂ irradiated by short x-ray pulses." *Phys. Rev. Lett.* **105**, 043003. LLNL-JRNL-448991.

Hau-Riege, S. P., et al., 2010. "Sacrificial tamper slows down sample explosion in FLASH diffraction experiments." *Phys. Rev. Lett.* **104**, 064801. LLNL-JRNL-411959.

Khorsand, A. R., et al., 2010. "Single-shot damage mechanism of Mo-Si multilayer optics under intense, pulsed extreme-ultraviolet exposure." *Optic. Express* **18**, 700. LLNL-JRNL-463951.

Seibert, M. M., et al., 2010. "Femtosecond diffractive imaging of biological cells." *J. Phys. B* **43**, 194015. LLNL-JRNL-463923.

Seibert, M. M., et al., 2011. "Single mimivirus particles intercepted and imaged with an x-ray laser." *Nature* **470**, 78. LLNL-JRNL-448874.

Scrape-Off-Layer Flow Studies in Tokamaks—Thomas Rognlien (09-ERD-025)

Abstract

We propose to develop new techniques to measure boundary-plasma flows in tokamak reactors and assess and implement new physics and computational methods in the UEDGE code to understand and predict the flows, which are presently unexplained. Boundary flows play a critical role in tritium accumulation via co-deposition in devices using carbon, such as the ITER international tokamak fusion reactor project, which will operate with a strict tritium-inventory limit. We will design an optical imaging system that permits measurements in high-power plasmas to be tested in the DIII-D tokamak in San Diego. To make reliable predictions of boundary flows with UEDGE, we will implement and validate new algorithms and physics such as kinetic effects distilled from our kinetic TEMPEST code.

We expect to deliver a prototype optical system for the DIII-D tokamak that can reliably measure plasma flows in at least one poloidal segment of the scrape-off layer, the outer layer of a tokamak plasma that is affected (scraped off) by a divertor or limiter. In addition, other suitable diagnostic techniques may be identified. The upgraded version of UEDGE will be implemented and comprehensive validation performed to determine physics of the measured flows that can be applied to optimize device operation and future design. Synergy of experimental and theoretical and simulation work will lead to major advancement of boundary-plasma physics, positioning LLNL as a leader in efforts for an anticipated new device design. Results will be published in journals relevant to magnetic-confinement fusion.

Mission Relevance

Development of a new diagnostic system and its use to validate advanced simulations of the boundary plasma in magnetically confined fusion devices supports the Laboratory's mission in energy security through development of fusion energy in tokamaks. The project will help to establish fusion as an abundant, reliable, and clean energy source. In addition,

our research supports the Laboratory's science and technology plan of research in high-energy-density and burning plasmas, as well as efforts in high-fidelity simulations.

FY10 Accomplishments and Results

In FY10, we (1) implemented the Rozhansky algorithm for cross-magnetic-field ion and electron drifts in the UEDGE plasma transport code and found it to be slightly more robust but less accurate than our improved gradient-B-drift method, after which we clarified the role of numerical diffusion and developed techniques to reduce it; (2) positioned the new Fourier transform spectrometer diagnostic in the divertor region of the DIII-D tokamak and used it to obtain measurements of edge-plasma flow for ionized carbon impurity by imaging, in collaboration with the Australian National University, emission of the 465-nm CIII spectral line; (3) obtained and set up a new camera for improved signal resolution; (4) simulated experimental results using UEDGE and found similar two-dimensional carbon flow patterns, including reversal with B-field direction; and (5) presented our results at two international and two national conferences.

Proposed Work for FY11

In FY11 we will (1) extend simulation capability for edge-plasma flow to include long-mean-free-path kinetic effects by utilizing the kinetic codes TEMPEST and COGENT to parameterize a reduced model for the fluid UEDGE code; (2) develop the capability for the Fourier transform spectrometer to measure higher charge states of carbon, making the diagnostic applicable to high-temperature edge plasmas such as in ITER; (3) continue detailed comparisons between experimental flow measurements and UEDGE to validate the transport model; (4) develop a more detailed data analysis package to analyze flow data obtained in FY10; and (5) plan a proposed extended flow diagnostic for DIII-D, ITER, or both.

Publications

Nam, S. K., and T. D. Rognlien, 2009. *Comparison of cross-magnetic-field drift algorithms in UEDGE*. 51st

Ann. Mtg. APS Division of Plasma Phys., Atlanta, GA, Nov. 2–6, 2009. LLNL-ABS-414790.

Nam, S. K., and T. D. Rognlien, 2010. *Cross-magnetic-field drift algorithms and results for edge-plasma transport*. Intl. Conf. Plasma Surface Interactions, San Diego, CA, May 24–28, 2010. LLNL-CONF-432901.

Nam, S. K., et al., 2010. *High-resolution numerical schemes for cross-magnetic-field drift in UEDGE and comparison with impurity measurements*. 52nd Ann. Mtg. APS Division of Plasma Physics, Chicago, IL, Nov. 8–12, 2010. LLNL-ABS-443194.

Rognlien, T. D., et al., 2010. *Advances in understanding tokamak edge/scrape-off layer transport*. IAEA Fusion Energy Conference, Daejeon, Korea, Oct. 11–16, 2010. LLNL-CONF-457153.

Understanding the Initiation of High-Voltage Vacuum Insulator Flashover—Timothy Houck (09-ERD-028)

Abstract

Advanced, high-performance pulsed-power systems are used in applications related to national security. Repetitive pulsed power technologies and x-ray and energetic beam sources are used in high-energy-density physics research, nuclear survivability and hardness testing, measurement of material properties, and scientific studies in areas such as radiation hydrodynamics. The vacuum insulator is a critical component of such systems, limiting performance. If designed incorrectly, the insulator can lead to failure of the entire system. Scientific knowledge developed from simple experiments provides an understanding of an insulator's performance, but has proven insufficient to provide a reliable basis for predicting operational performance. In this project, we will develop a computer model of electrical breakdown (known as vacuum insulator flashover) at a dielectric–vacuum interface, for use in designing

vacuum insulators for advanced, high-performance pulsed-power systems. We will leverage LLNL's advances in computational resources to bridge the gap between knowledge and application.

If successful, we will produce an important computational tool for designing pulsed-power systems. We also expect to demonstrate computationally that a few basic physics phenomena are responsible for the initiation of electrical breakdown across the dielectric–vacuum interface. We will show how different initiation mechanisms evolve by varying the geometry, materials, and environment used in simulations. This tool will make it possible to study complex insulator designs in realistic operational applications and predict performance. We will also deliver a proposed insulator design for the next generation of coaxial flux-compression generators, including expected performance.

Mission Relevance

This project supports LLNL's national security mission by providing an important tool for developing capabilities in high-energy-density physics and nuclear weapons science. Our computational model will allow LLNL to become a world-class center for high-voltage vacuum insulator design and testing, thus helping the Laboratory attract top talent.

FY10 Accomplishments and Results

We developed a sophisticated computational model of vacuum insulator flashover that mimics observed flashover behavior for positive angle insulators, the orientation considered most difficult to model. To achieve this capability, we (1) began with the commercial code VORPAL and improved the algorithms related to electromagnetic fields and secondary electron emission, (2) added a simplified static gas layer to the insulator surface using published data from insulator experiments and the Paschen curve to estimate layer thickness and density, (3) further improved this model by adding elastic and inelastic scatterings to the gas ionization collision algorithm, and (4) developed a dynamic gas algorithm where electron impact causes desorption

of the neutral gas. While developing the gas model, we studied the power flow channel of magnetic-flux compression generators, including ultralow-inductance channels. We found from our simulations that a combination of electron scattering from gas molecules and electrodes, surface charging, and geometrical field enhancements lead to localized electric fields near the insulator surface that promotes electron avalanche and flashover. In summary, we developed a very powerful computational tool that includes sophisticated secondary electron yield, neutral gas desorption, and gas ionization models for designing vacuum insulators. The Phoenix Project, being pursued by LLNL at the Nevada Test Site to examine the properties of materials at extreme pressures, will utilize our model for the design of insulators in the power flow region of their magnetic-flux compression generators. In addition, we are working with another Laboratory project to use VORPAL to study sputtering of thin films using magnetrons.

Publications

Perkins, M. P., et al., 2010. *FDTD-PIC modeling for initiation of vacuum insulator flashover*. 37th IEEE Intl. Conf. Plasma Science, Norfolk, VA, June 20–24, 2010. LLNL-POST-432933.

Perkins, M. P., et al., 2009. *Progress on simulating the initiation of vacuum insulator flashover*. 17th IEEE Intl. Pulsed Power Conf., Washington, DC, June 29–July 2, 2009. LLNL-PROC-414298.

Perkins, M. P., et al., 2010. *Progress on simulating vacuum insulator flashover*. University of California at Berkeley Plasma Theory Group Seminar, Berkeley, CA, Sept. 9, 2010. LLNL-ABS-454055.

Perkins, M. P., et al., 2010. *Simulations for initiation of vacuum insulator*. 29th IEEE Intl. Power Modulator and High Voltage Conf., Atlanta, GA, May 23–27, 2010. LLNL-PROC-433487.

Critical Enabling Issues for Burning-Plasma Diagnostics—Steven Allen (09-ERD-030)

Abstract

This project will study and define two diagnostic techniques for tokamak burning plasmas: a motional Stark effect technique to measure current profile and an infrared radiation fast-scanning technique to measure plasma wall temperature. For the motional Stark effect technique, we will address several important issues of measurement including a polarization-preserving vacuum window, techniques to minimize double refraction caused by vacuum forces and temperature gradients, and whole-spectrum measurement of the Stark spectrum. For the infrared technique, we will investigate the feasibility of developing a fast, two-color scanning diagnostic for conducting measurements in burning plasma experiments such as the ITER international tokamak fusion reactor project.

In collaboration with the University of Arizona, we will pursue motional Stark effect polarization engineering and develop a polarization-preserving vacuum window. Measurements of the whole Stark spectrum will be used to compare an alternate measurement technique with motional Stark effect and to evaluate the effects of different plasma conditions on spectrum details. We will implement and test a novel data-acquisition scheme that will allow real-time monitoring of both plasma instabilities and optical properties of the polarimeter. Lastly, we plan to develop a prototype fast two-color infrared radiation line scanner (two colors make the measurements less susceptible to changes in surface emissivity) for the measurement of tokamak wall temperatures.

Mission Relevance

This project supports LLNL's mission in energy security by making important contributions to the study of the physics of magnetic-fusion burning plasmas, such as those in the ITER project, and by applying cutting-edge tools to the development of

fusion energy as an abundant, reliable, and clean energy source.

FY10 Accomplishments and Results

In FY10 we (1) successfully demonstrated operation of a new digital data-acquisition system, along with detection of magnetohydrodynamic signals from the plasma, showing that an edge magnetohydrodynamic mode can interfere with pitch-angle measurements of the motional Stark effect; (2) developed an analysis plan for the large set of data obtained; (3) began scoping materials for design of the new polarization-preserving vacuum window; and (4) identified prototypical positive and negative Verdet (Faraday rotation) glasses.

Proposed Work for FY11

We will (1) analyze our large dataset with the new digital data-acquisition system; (2) model the effect of magnetohydrodynamic fluctuations in the plasma and their effect on the motional Stark effect pitch-angle measurements; (3) attempt a Mueller matrix calibration of the four motional Stark effect systems at the General Atomics DIII-D fusion facility; (4) continue to develop the concept of a polarization-preserving vacuum window and, if successful, build, test, and install a prototype on the tokamak; and (5) conduct a preliminary scoping of a fast far-infrared system.

Publications

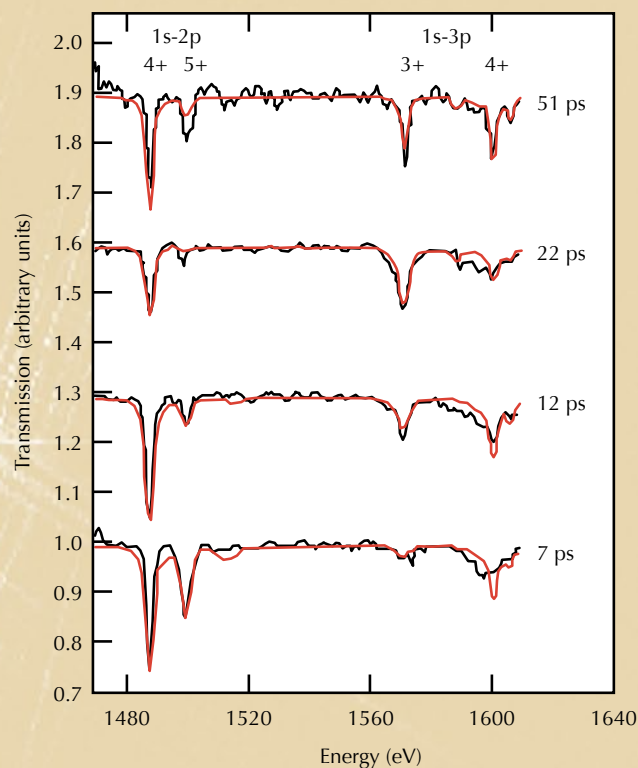
King, J. D., et al., in press. "A digital lock-in upgrade of the motional Stark effect diagnostic on DIII-D." *Rev. Sci. Instrum.* LLNL-POST-443181.

King, J. D., et al., in press. "MHD interference with the edge pedestal motional Stark effect diagnostic due to intensity and sideband fluctuations on DIII-D." *Rev. Sci. Instrum.* LLNL-JRNL-443180.

Experimental Determination of Dense Plasma Effects on Bound States in Extreme States of Matter—Ronnie Shepherd (09-ERD-032)

Abstract

We propose a series of experiments coupled with calculations and simulations to study the bound states of a well-characterized, dense plasma to determine the conditions in which the outer electrons are no longer bound to the ionic core in a dense plasma. We will measure K-shell absorption spectra while varying electron density with the use of aerogels and shock-compressing solids. In addition to absorption, we will measure target temperature to account for ionization. The measurements will test the effects of continuum lowering and pressure ionization in



Our experimental data (black line) of aluminum absorption (in relative units) at about 20 eV temperature and 0.1 g/cm^3 (7 ps) to 0.01 g/cm^3 (51 ps) matches well with theory (red line). As the laser-produced plasma density increases, the 1s to 3p spectral lines (between 1560 and 1600 eV) begin to merge into the continuum.

dense plasma—conditions that occur in stellar interiors and nuclear explosions.

We expect to provide detailed data on the average occupation number for outer bound states in plasmas ranging from weak to strong coupling regimes. We expect these data to benchmark pressure ionization and continuum-lowering models. This groundbreaking work is expected to appear in high-profile journals and set a new standard in plasma physics experiments.

Mission Relevance

This project supports LLNL's national and energy security missions by improving advanced physical models and enabling critical calculations for weapons physics and inertial-confinement fusion.

FY10 Accomplishments and Results

In FY10 we (1) finished analyzing data from experiments at the Jupiter laser facility—a multiplatform laser-target irradiation facility for high-energy-density research at Livermore—and began modeling the data, (2) acquired transmission gratings, (3) built a spectrometer with Kilpatrick–Baez collection optics, (4) began experiments with decompressed targets to gather low-density data, (5) successfully fabricated aerogel targets with densities from 0.01 to 0.5, and (6) designed a plan for experiments to complete the sub-solid-density data set.

Proposed Work for FY11

In FY11 we will (1) complete the sub-solid-to-solid data-gathering experiments at the Jupiter laser facility, using aerogel targets rather than allowing the target to decompress to achieve sub-solid density; (2) analyze the data; (3) conduct compressed-matter experiments, focusing on the density effects on bound states at densities greater than solid as well as fielding our transmission-grating x-ray pyrometer; and (4) analyze the full dataset and compare the results to predictions generated with the Purgatorio equation-of-state and Opal opacity computer codes.

Publications

Cone, K. V., et al., 2010. *Development of a time-resolved soft x-ray spectrometer for laser produced plasma experiments*. 18th Topical Conf. High-Temperature Plasma Diagnostics, Wildwood, NJ, May 16–20, 2010. LLNL-CONF-431867.

Uses of Ignition at the National Ignition Facility—L. John Perkins (09-ERD-036)

Abstract

This research seeks to address one of the most important scientific questions facing the Laboratory: How will achievement of ignition and thermonuclear yield at the National Ignition Facility (NIF) be utilized to provide unique weapons physics data for the Stockpile Stewardship Program? Accordingly, we propose to establish the technical basis of new target concepts that operate in the nuclear (high-energy-density) regime and provide stockpile stewardship data unattainable at any other facility outside of an underground nuclear test. We will focus on target designs that have the potential to provide data for the most pressing perceived needs in primary design physics and emphasize a very-near-term target variant that could be fielded before, or in parallel with, the NIF ignition campaign.

We expect to produce significant progress in target design to answer the question of how NIF could be best utilized for stockpile stewardship once ignition is achieved. Livermore Advanced Simulation and Computing weapons simulation codes are the basis for high-consequence stockpile decisions, but they must be validated against real data in the nuclear regime. Accordingly, the results from this study will position the Laboratory to take full advantage of NIF ignition with technically credible proposals for advanced, stockpile-relevant targets that make full use of the high-energy densities stemming from ignition and thermonuclear burn.

Mission Relevance

This work supports the Laboratory's mission in national security by furthering the development of advanced experimental platforms for NIF, advanced physical models for predictive capability, and advanced weapons physics simulation capabilities and by supporting high-energy-density burning-plasma science and beyond state-of-the-art diagnostics for stockpile science.

FY10 Accomplishments and Results

We (1) selected the most promising target design scoped in 2009 as the potential first NIF ignition platform after determining that it offers simple target fabrication, modest laser requirements, good prospects of near-term deployment without the need for cryogenics, and the ability to provide unique data of direct relevance to our principal design codes; (2) optimized one-dimensional fusion yield performance and assessed initial two-dimensional symmetry and stability; (3) determined an optimum configuration for NIF polar drive in terms of pointing, focusing, and power phasing of the laser beams; (4) modeled target performance in two of our principal design codes together with assessments of its

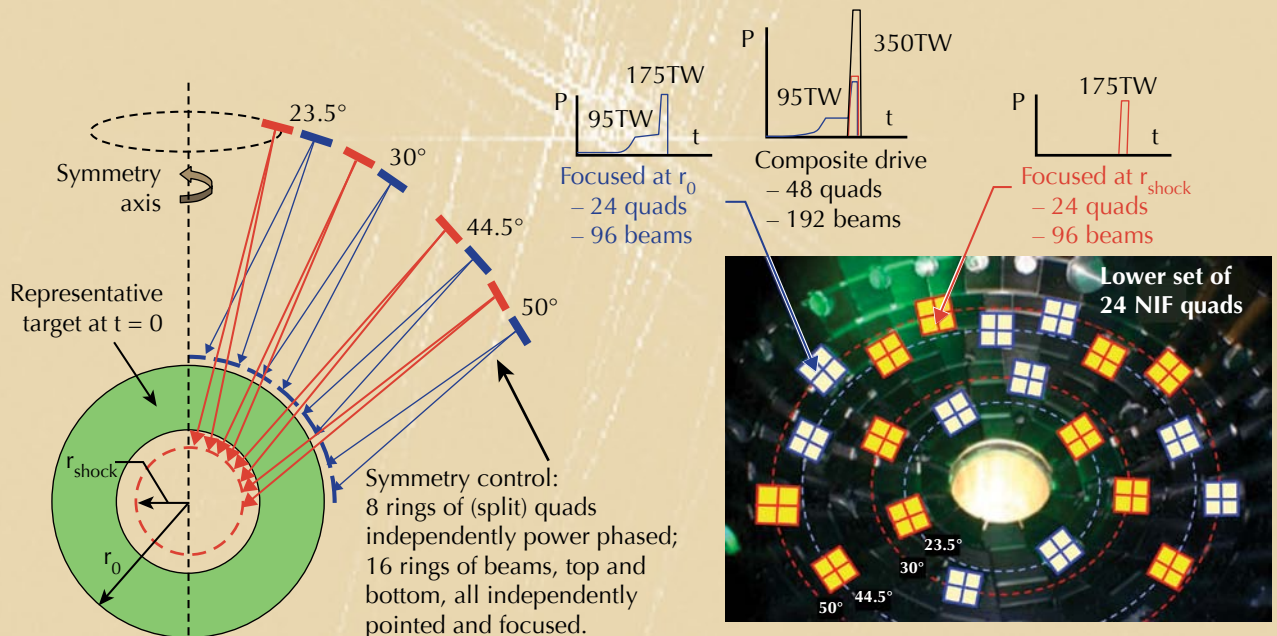
potential to provide specific benchmarking data; and (5) performed experimental planning for deployment of a NIF proof-of-principle surrogate target including specification of NIF laser requirements and diagnostic needs.

Proposed Work for FY11

We propose to (1) complete the final target design and finish assessing symmetry, stability, and laser-plasma interactions; (2) complete comparisons of target performance between two of our principal weapon design codes; (3) scope the deployment plan for NIF experiments, including assessment of the required shot schedule through 2013 and define the required NIF diagnostic suite, including needs for late-time nuclear performance; and (4) characterize proposed NIF experiments to be performed with this target to provide data central to the National Boost Initiative and validation of our primary design codes.

Publications

Perkins, L. J., et al., 2010. *Development of a polar drive shock ignition platform on the National Ignition Facility*. UCRL-TR-432811.



Candidate laser geometry for the National Ignition Facility to achieve polar direct drive, a technique that potentially can produce higher energy gain and more energy output, at a high target-convergence ratio.

Perkins, L. J., et al., 2010. *On the fielding of a high gain shock-ignited target on the National Ignition Facility in the near term.* UCRL-TR-428513.

Perkins, L. J., et al., 2009. "Shock ignition: A new approach to high gain inertial confinement fusion on the National Ignition Facility." *Phys. Rev. Lett.* **103**, 045004. LLNL-POST-416611.

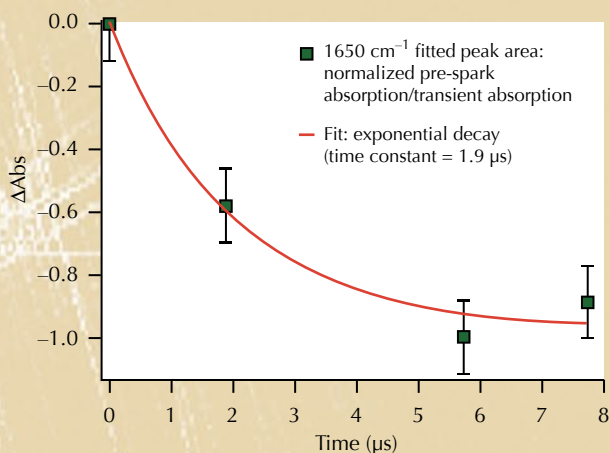
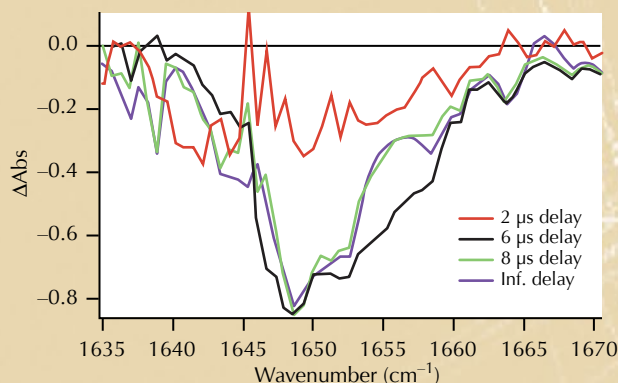
Arc Initiation of High Explosives— James McCarrick (09-ERD-042)

Abstract

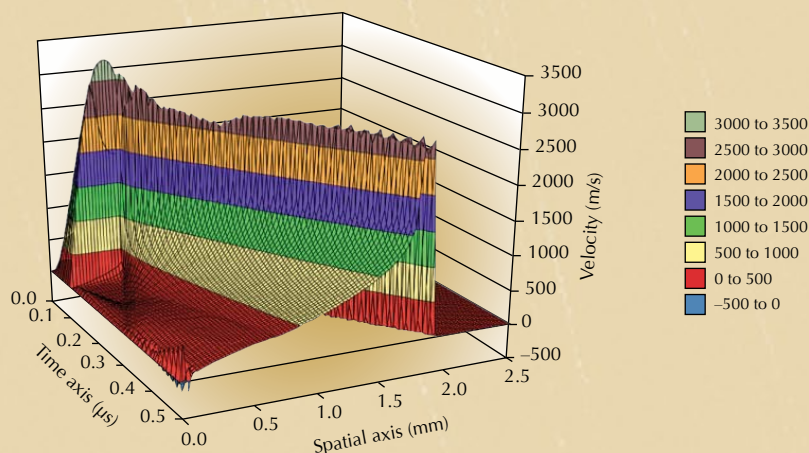
Recent experiments have shown unique aspects of arc initiation in high explosives that cannot be predicted or reproduced with existing computational models, such as those with low thresholds that scale inversely with input power. These issues pose significant implications for the safety and surety of existing and future weapon systems. Our objective is to develop a fundamental understanding of the physical mechanism of arc initiation in high explosives. To

this end, we will perform experiments required to support the physical model for specific explosives. We will also develop a rigorous, nonempirical physical model appropriate to the unique combinations of plasma-energy transport and high-temperature, high-explosives kinetics. Time-resolved infrared spectroscopy and microcalorimetry will supply data to support the model.

This project will result in a fundamental understanding of (1) the processes governing energy transport in confined high-power arcs, (2) the kinetics of high explosives in the unique limit of temperatures of the same order as activation energies, and (3) the transition process from a static volume of overdriven reactive material to a propagating detonation. This combination of knowledge will yield a physical model that will provide a previously nonexistent predictive capability for safety analysis and future engineered applications. We expect publications in peer-reviewed journals and patent opportunities relating to the use of high explosives for mining operations.



Time-gated absorption spectra of pentaerythritol tetranitrate explosive, showing rapid depletion with time following a spark (top). A pumped convective burn model of a spark-driven burn wave in a low-density high explosive is shown at bottom.



Mission Relevance

This work supports the Laboratory's mission in national security by achieving better understanding of the safety of the existing nuclear stockpile and by improving basic high-explosives science, which in turn enables improved safety of the future designs that will ultimately be necessary for a more efficient weapons complex. In general, this work provides a strong head start in the Laboratory becoming a high-explosives center of excellence as part of NNSA's nuclear weapons complex transformation.

FY10 Accomplishments and Results

In FY10 we (1) extended the temperature and density characterization of the high-power arc channel to tens of microseconds and compared the behavior of channels for energetic and inert materials; (2) redesigned and rebuilt the electrode configuration to increase shot throughput by increasing the electrode lifetime; (3) carried out the first-ever time-resolved infrared spectroscopy of sparked pentaerythritol tetranitrate—while the dataset will need to be vastly increased before one could draw definitive conclusions on kinetic timescales, it is interesting to note that the initial estimates are very different from simple extrapolations of current kinetic models, which are calibrated for much lower temperatures; and (4) began development of an energy transport model based on a novel “pumped” regime of convective burn. While this model is still quite preliminary, it is the first to predict arc initiation threshold values similar to those observed experimentally.

Proposed Work for FY11

We plan to modify the existing standard time-resolved infrared spectroscopy snapshot methodology with a truly time-resolved capability by exploiting the high-channel-density, fast-voltage digitizers that have recently become available to provide temporal response. A successful modification will allow us to greatly increase the amount of kinetic data obtained for pentaerythritol tetranitrate and possibly for other energetic materials by removing a substantial bottleneck in the shot rate. Following data reduction and extraction of rate parameters, kinetics models suitable for high temperatures will be finalized.

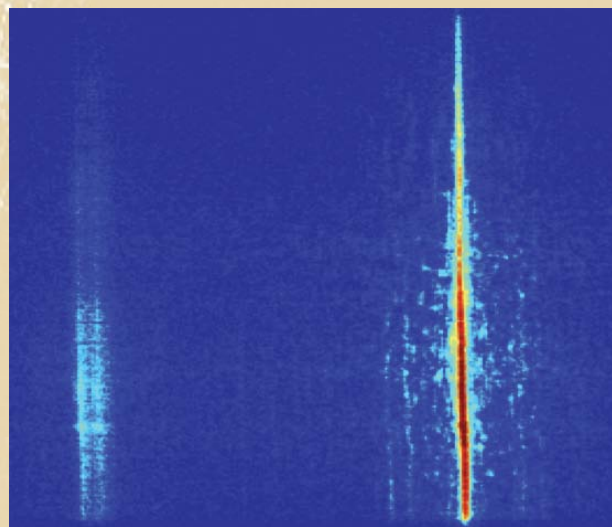
Publications

Grant, C., et al., 2010. “Initiation of pentaerythritol tetranitrate using a fast and high power arc source.” *Proc. 14th Intl. Detonation Symp.*, paper 76903. LLNL-CONF-425208.

An Atomic Inner-Shell X-Ray Laser Pumped by the Linac Coherent Light Source— Nina Rohringer (09-LW-044)

Abstract

We propose to develop a discretely tunable x-ray laser that will produce femtosecond pulses of nanometer wavelengths by using Stanford's Linac Coherent Light Source (LCLS) to pump an atomic inner-shell x-ray laser. In contrast to other methods, our inexpensive technique can be directly implemented in one of the LCLS user instruments. Methods such as x-ray photoelectron spectroscopy and diffraction would benefit from femtosecond time resolution. The new source would enable the study of nonlinear quantum optical effects in the x-ray regime for the first time, opening avenues to new basic science. We will assess the optimal pumping regime by numerically simulating the time-dependent gain, then field a first experiment at LCLS,



Raw charge-coupled device image of the spectrum created by the interaction of a focused Linac Coherent Light Source beam with neon gas. The line on the left corresponds to the transmitted beam pump at 960 eV. The created x-ray laser line with a central frequency of 850 eV is shown on the right.

demonstrating lasing at 1.4 nm in singly ionized neon gas.

We intend to demonstrate our proposed lasing scheme of inner-shell photoionization with LCLS on atomic neon to achieve x-ray pulses at nanometer wavelengths, pulse durations of a few femtoseconds, and intensities reaching 5×10^{17} W/cm². With our method, LCLS pulses will be transformed into x-ray pulses of shorter pulse duration and better longitudinal coherence. The increased time resolution would enable pump-probe studies of chemical reactions of an ensemble of molecules or phase transitions in solids. The longer coherence time and higher shot-to-shot spectral stability will make possible, for the first time ever, the direct study of nonlinear quantum optical effects in the x-ray regime.

Mission Relevance

The proposed work supports LLNL's mission in frontier science and advanced technology by developing a instrumental capability beyond the state of the art for studying ultrafast, nonlinear physics and the physics of interactions of high-intensity x rays and atoms.

FY10 Accomplishments and Results

In FY10 we (1) advanced our theoretical model to determine the self-consistent time-dependent gain and expected output parameters of our new x-ray laser source, including study of multicolor lasing schemes; (2) collaborated with Argonne National Laboratory to simulate the resonant and nonresonant interaction of the focused LCLS beam with neon gas; (3) developed a model to calculate the resonant Auger electron spectrum for high x-ray intensity; (4) manufactured an extendable high-pressure gas cell for the x-ray laser experiment; (5) successfully prepared and performed a proof-of-principle experiment at LCLS; and (6) demonstrated a photoionization atomic inner-shell x-ray laser scheme on the neon K-alpha transition.

Proposed Work for FY11

We will (1) evaluate and interpret data from the FY10 experimental campaign at LCLS, including analysis of the gain of the two x-ray lasing schemes (based on two different neon ions) as a

function of gas density and beam parameters such as photon energy, pulse duration, focus size, and pulse energy; (2) perform an experiment of resonant photon pumping in neon at the LCLS to demonstrate stimulated x-ray Raman scattering and alternatively stimulated resonance fluorescence in atomic neon; and (3) develop the underlying theory of generalized Bloch equations to determine density matrix of the ionic system and the created vacuum ultraviolet laser radiation, including calculating output of the amplified, down-converted vacuum ultraviolet light.

Publications

Dunn, J., et al., 2010. "Design and measurement of a Cu L-edge x-ray filter for FEL-pumped x-ray laser experiments." *Rev. Sci. Instrum.* **81**, 10E330. LLNL-JRNL-452611.

Goulielmakis, E., et al. 2010. "Real-time observation of valence electron motion." *Nature* **466**(7307), 739. LLNL-JRNL-417496.

Rohringer, N., 2009. "An atomic inner-shell laser pumped with an x-ray free-electron laser." *J. Phys.: Conf. Ser.* **194**, 012012. LLNL-CONF-415032.

Rohringer, N., 2010. *The need for an open quantum system approach to describe high-intensity x-ray interactions with matter*. Kavli Institute for Theoretical Physics (KITP) Program: X-Ray Frontiers, Fall 2010 Podcast, Santa Barbara, CA, Aug. 2–Sept. 10, 2010. LLNL-PRES-448504.

Rohringer, N., 2009. *Ultrashort non-linear interactions of x-rays with atoms*. DAMOP 2009, 40th Ann. Mtg. Division of Atomic, Molecular, and Optical Physics, Charlottesville, VA, May 19–23, 2009. LLNL-ABS-410509.

Rohringer, N., and R. London, 2009. "Atomic inner-shell x-ray laser pumped by an x-ray free-electron laser." *Phys. Rev. A* **80**, 013809. LLNL-JRNL-410667.

Rohringer, N., and R. London, 2009. "Pumping a photoionization atomic inner-shell x-ray laser by x-ray free electron laser radiation." *Proc. SPIE* **7451**, 74510C. LLNL-CONF-414918.

Rohringer, N., and R. Santra, 2009. "Multichannel coherence in strong-field ionization." *Phys. Rev. A* **79**, 053402. LLNL-JRNL-410943.

Varma, H. R., et al., 2009. "Above-threshold ionization in the x-ray regime." *Phys. Rev. A* **80**, 053424. LLNL-JRNL-413508.

Young, L., et al., 2010. "Femtosecond electronic response of atoms to ultra-intense x-rays." *Nature* **466**, 091777. LLNL-JRNL-423408.

Direct Search for Decay of the Thorium-229 Nuclear Isomer— Jason Burke (09-LW-061)

Abstract

The main objective of our proposal is measurement of the thorium-229 isomer half-life to determine the transition linewidth. Using an ultraviolet grating spectrometer, we will attempt to observe the ultraviolet light that would be emitted by the nucleus directly if the isomeric transition is not strongly internally converted. Observation of this transition would allow direct excitation of the nucleus for applications such as nuclear clocks, precision tests of fundamental constants, and, potentially, quantum computer bits.



Deonte Thomas, a summer student who assisted with the project, is shown assembling part of the electrostatic reflector used for the thorium-229 research. Deonte won first prize in the physics division of the Laboratory's 2010 Summer Student Poster Symposium for his work on this project.

We intend to measure the half-life of the thorium-229 isomer and will attempt to directly measure the wavelength of light emitted in the decay. Knowledge of these properties are required to enable direct manipulation of the nuclear state. We expect that laser manipulation of the thorium-229 nucleus could lead to unprecedented studies of the interplay between atomic and nuclear systems, provide a new frequency standard, enable a quantum bit for quantum computing with extremely long de-coherence times, and improve the search for time variation of fundamental physical constants by as many as six orders of magnitude.

Mission Relevance

Our research supports the Laboratory's commitment to pursuing frontier science and technology and developing new capabilities that advance scientific discovery and enable future missions. Potential applications include the areas of photon science, high-performance computing, and global security. The low-lying nuclear level in thorium-229 has attracted the attention of scientists all over the world and has been the subject of much experimental and theoretical interest. A successful determination of the half-life, and therefore natural linewidth, of the thorium-229 isomer would position Livermore as an eminent facility for the pursuit of fundamental issues in nuclear physics.

FY10 Accomplishments and Results

We (1) investigated the effect of numerous semiconductor and dielectric materials on the decay of the uranium-235 isomer, discovering that by electrically polarizing dielectric materials, we can increase internal conversion detection sensitivity by a factor of approximately seven; (2) performed experiments to detect photons from thorium-229 gamma decay and bound internal conversion decay in the wavelength range of 110 to 600 nm and timescales covering microseconds to seconds; (3) performed experiments to directly detect internal conversion electrons from thorium-229 isomer decay using our very-low-background multichannel plate detector, ruling out multiple half-life ranges with photon searching and ruling out half-lives greater than 1 s with internal

conversion electron searching; and (4) conducted a new type of experiment using a time-of-flight arrangement to examine nanosecond and microsecond timescales. This project has expanded our research capabilities in the area of nuclear-atomic coupling and high-energy-density physics, and it has contributed to the start of new research in excited-state physics.

Publications

Burke, J. T., et al., 2010. *^{229}Th —the bridge between nuclear and atomic interactions*. LLNL-TR-463538.

Burke, J. T., et al., 2009. "Determination of the ^{229}Th isomer half-life." *Bull. Am. Phys. Soc.* **54**, 10. LLNL-ABS-414414.

Swanberg, E., et al., 2010. "Measuring the half life of $^{229\text{m}}\text{Th}$." *Bull. Am. Phys. Soc.* **55**, 14. LLNL-ABS-463656.

Investigation of Short-Pulse Laser-Pumped Gamma-Ray Lasers—Ronnie Shepherd (09-LW-080)

Abstract

Since lasers were first developed, researchers have speculated about the possibility of lasing nuclear transitions. The promise of coherent, directional, and energetic photons would have applications in basic science, technology, medicine, and defense. The goal of this project is to create a gamma-ray laser pumped by one of two possible drive mechanisms—synchrotron radiation or hot electrons generated by a short-pulse laser. We will determine the laser coupling efficiency to synchrotron radiation and hot electrons as a function of laser input energy. After determining the drive characteristics, we will choose from a list of possible inversion nuclei (both isomeric and non-isomeric) and attempt to measure gain.

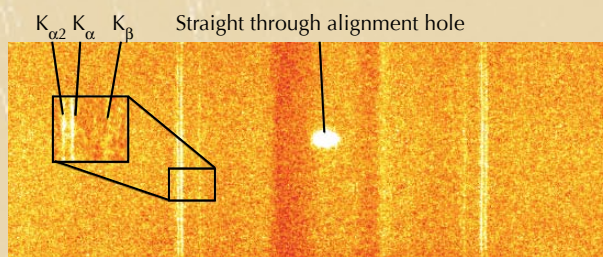
If successful, this project will achieve the first-ever gamma-ray laser, which would have potential impact in both scientific and industrial applications. At the very least, we will produce an accurate study of the requirements for such a system to succeed.

Mission Relevance

This technology could find eventual application to the national security mission by enabling the efficient delivery of large amounts of energy to a target. This project also supports LLNL's efforts in breakthrough science and technology by pursuing new and unique applications of ultrashort-pulse laser technology, which if successful, will advance research in the areas of chemistry, materials science, and life sciences.

FY10 Accomplishments and Results

In FY10 we (1) developed the required experimental targets, (2) purchased a spectrometer to measure and characterize transition energies, and (3) performed energy measurements at the University of Michigan HERCULES laser because laser time at the Livermore Titan laser facility was not available. The HERCULES laser could only provide 15 J maximum on target, which was well below the threshold to produce the necessary hot electron population to create a sufficient concentration of hole states where there is a relative abundance of neutrons rather than protons. Preliminary results suggest no lasing occurred at this laser energy. Overall, this project has provided the hardware and foundation to test short-pulse laser-driven nuclear transitions in the plasma state. As a result, we have established a working collaboration with the University of Michigan on this subject and are hopeful that will continue with future campaigns. In addition, we intend to elicit support for future research from the DOE or Defense Threat Reduction Agency.



Gold K-shell spectrum generated by hot electrons from short-pulse laser–solid interaction. The gold spectrum is used to characterize the hot electron pump for the gamma-ray laser.

Publications

Zulick, C., et al., 2010. "K-Shell spectroscopy of Au plasma generated with a short pulse laser." *Bull. Am. Phys. Soc.* **55**(15), BAPS.2010.DPP.JP9.125. LLNL-JRNL-464312.

Science and Technology of Unconventional Fiber Waveguides for Emerging Laser Missions—Jay Dawson (10-SI-006)

Abstract

Fiber lasers are a critical technology for 21st-century energy and defense missions. Fiber lasers have scaled in output power and pulse energy in the last 25 years and are reaching the output-power (~20-kW) and pulse-energy (~4-mJ) limits imposed by the physics of a technology that was developed for telecommunications systems. Livermore theoretical models show the physical reasons for the limits, which suggest that radical, new optical-fiber designs based upon rectangular ribbon cores are needed to enable fiber lasers with up to two orders of magnitude more pulse energy and output power. We propose to provide the research and development to enable these new waveguide designs with flexible, efficient transport of ultrahigh-power light from any laser source to the end application.

We expect to develop and demonstrate a breakthrough ribbon-fiber waveguide with the potential to achieve 100-kW to 1-MW continuous-wave laser powers from a single-fiber laser aperture. The ribbon fiber will enable higher-energy laser pulses

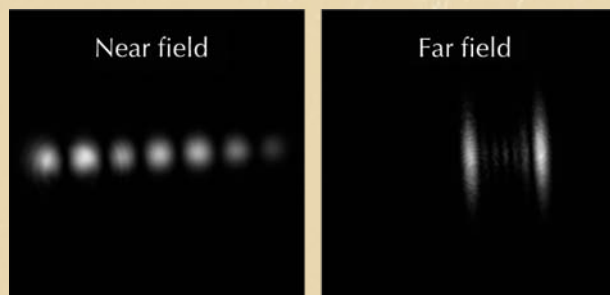
from fiber sources. A range of wavelengths will be explored from 900 to 2000 nm, and we will construct a comprehensive model of the waveguide and laser physics. We will (1) develop new optical fibers and new fabrication techniques; (2) model, fabricate, and test mode-conversion techniques; and (3) construct and test a pulsed system demonstrating all but the thermal physics for scaling fiber lasers beyond 10 kW. Numerous publications and patents are anticipated and the new technology will enable new missions.

Mission Relevance

Development of megawatt-power fiber lasers falls squarely within the advanced laser-optical systems and applications strategic mission thrust of the Laboratory. Fiber lasers are an important technology needed to produce efficient, high average power with good beam quality in a compact, robust form at a variety of wavelengths. Extending these lasers to higher pulse energies and average powers will be enabling for national missions as diverse as directed-energy laser weapons, laser range finders and remote sensors, generation of mono-energetic gamma rays, laser-based particle acceleration, K-alpha x-ray sources, extreme ultraviolet sources, and advanced machining.

FY10 Accomplishments and Results

We (1) investigated the power scaling of non-silica-based fibers, (2) identified a modulation instability issue at high peak power, (3) invented two new waveguide designs to overcome modulation instability (one record of invention was filed and a second one was begun), (4) began working with the U.S. Air Force Academy to generate supercomputer modeling codes of photonic crystal fiber, (5) developed new methods of characterization and characterized an existing ribbon fiber, (6) set up a fiber-geometry and spectral-measurement apparatus, (7) invented a 99.5%-efficient diffractive optical-element mode converter, (8) completed a theoretical analysis of the power scaling of ribbon fiber, (9) tested a new passive ribbon fiber, (10) completed initial modeling



Near- and far-field images from a 5- × 50-μm core ribbon fiber showing a 7-lobe mode excited with greater than 90% of total power.

codes and established a second collaboration with the University of Michigan, and (11) purchased, installed, and commissioned a Vytran glass working station for producing long-period gratings and optical fiber couplers.

Proposed Work for FY11

We plan to (1) incorporate thermal and laser gain effects in our photonic crystal-fiber supercomputer modeling codes, (2) begin fabricating ribbon fiber prototypes on the new LLNL fiber-drawing tower, (3) create a diffractive optical-element mode converter based upon the FY10 design, (4) begin developing long-period grating mode converters, (5) demonstrate laser amplification in a ribbon fiber, and (6) demonstrate both mode conversion and laser amplification in a ribbon fiber sample.

Publications

Dawson, J., et al., 2010. "Power scaling analysis of fiber lasers and amplifiers based on non-silica materials." *Laser Technology for Defense and Security VI, Proc. SPIE*, vol. 7686, p. 768611. SPIE, Bellingham, WA. LLNL-CONF-427009.

Dawson, J., et al., 2010. *Ultimate power limits of optical fibers*. Optical Fiber Communication Conf. and Expo. and National Fiber Optic Engineers Conf. (OFC/NFOEC 2010), San Diego, CA, Mar. 22–25, 2010. LLNL-PRES-426108.

Heebner, J., et al., 2010. "High brightness, quantum defect limited conversion efficiency in cladding-pumped Raman fiber amplifiers and oscillators." *Optic. Express* **18**, 14705. LLNL-JRNL-426353.

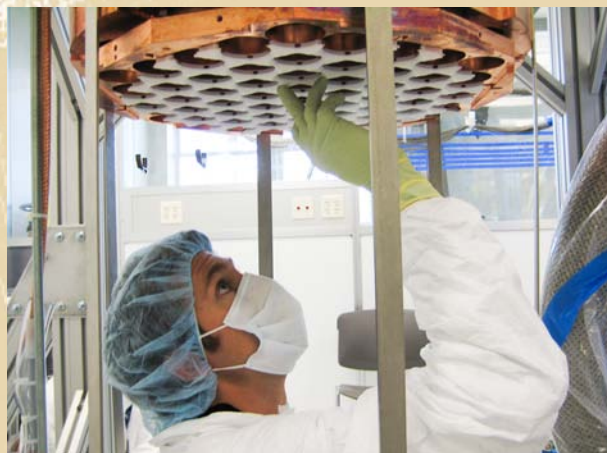
Rubenchik, A., et al., 2010. *Solar pumped laser microthruster*. 2010 Intl. High-Power Laser Ablation Conf., Santa Fe, NM, Apr. 18–22, 2010. LLNL-CONF-423782.

Advanced Rare-Event Detectors for Nuclear Science and Security— Adam Bernstein (10-SI-015)

Abstract

Remote nuclear reactor monitoring using anti-neutrino detectors could revolutionize global nonproliferation efforts by providing continuous and near-real-time monitoring of plutonium production at its source. We propose to lay the foundation for a program to develop ultrasensitive rare-event neutral particle detectors for global nuclear security. We will collaborate on five international, next-generation physics experiments to enable reactor monitoring at hundreds of kilometers and fissile material detection at a standoff of hundreds of meters. We hope to provide neutral-particle detector capabilities with dramatically improved standoff distance, energy spectroscopy, directionality, particle identification, cost effectiveness, and robustness.

We expect to transform two core global nuclear security missions that require breakthrough research and development in rare-event detection: stand-off monitoring of nuclear reactors and detection of noncritical special nuclear materials. We will apply transformative capabilities from fundamental science and establish Livermore as a world center for rare-event detection. We intend to demonstrate the



Livermore postdoctoral researcher and collaborator Peter Sorensen installs mounting fixtures for photomultiplier tubes in the Large Underground Xenon Dark Matter Experiment detector.

technology for standoff detection of nuclear reactors with antineutrino detectors, which will enable discovery of operating reactors across borders, as well as provide reactor safeguards. In addition, we will develop technologies for fissile material search and monitoring by addressing essential needs for practically deployed systems, including neutron and gamma-particle identification, directionality, nano-second-scale timing resolution, low-cost large-solid-angle coverage, and spectroscopy.

Mission Relevance

Detection of rare gamma rays, neutrons, and antineutrinos emitted by nuclear materials and reactors directly supports Laboratory efforts in non-proliferation and homeland and national security. This project integrates the high-profile fundamental science of dark matter and neutrino physics with the very practical research required to achieve breakthroughs in reducing the global nuclear threat. In addition, it will provide Laboratory access to cutting-edge technology, expertise, and top-notch researchers as potential hires.

FY10 Accomplishments and Results

We (1) tested and deployed a 350-kg dual-phase xenon detector as part of the Large Underground Xenon (LUX) Dark Matter Experiment in South Dakota; (2) tested our x-ray imaging optics at Switzerland's Axion Solar Telescope in the search for axions, a technology which is also applicable to spent-fuel imaging for nuclear safeguard applications; (3) performed reactor simulations to predict the neutrino energy spectrum emitted by the reactors of the Double Chooz Experiment, which is expected to achieve the major physics result of measuring neutrino oscillation angle θ_{1-3} , and which also relates to our ongoing nonproliferation work using antineutrino detectors for reactor safeguards; and (4) recruited, to participate in these experiments, three postdoctoral researchers and three graduate students from top schools, including the Massachusetts Institute of Technology and University of California at Berkeley. Sponsors in nonproliferation are already expressing interest in spinoff technology from our xenon detector, and DOE's Office of Nonproliferation Research and Development has

already launched a project based on x-ray imaging optics capabilities we have developed in this project.

Proposed Work for FY11

In FY11 we will continue all five of the fundamental physics experiments begun in FY10. Specifically, we will (1) deploy the neutrino mass detector at the Enriched Xenon Observatory or the Neutrino Experiment with a Xenon Time Projection Chamber Experiment in Spain, (2) measure the final neutrino mixing angle at the Double Chooz reactor in France, (3) search for axionic dark matter using x-ray imaging optics at the Axion Solar Telescope, (4) search for weakly interacting massive particle as evidence of dark matter at the LUX facility, and (5) measure sea-level cosmic rays as part of an ongoing study at LLNL of space and time correlations in cosmic rays at the Earth's surface.

Publications

Bernstein, A., et al., 2010. "Nuclear security applications of antineutrino detectors: Current capabilities and future prospects." *Sci. Global Secur.* **18**, 127. LLNL-JRNL-416517.

Bulaevskaya, V., and A. Bernstein, in press. "Detection of anomalous reactor activity using antineutrino count evolution over the course of a reactor cycle." *J. Appl. Phys.* LLNL-JRNL-452551.

Sorensen, P., 2010. "A coherent understanding of low-energy nuclear recoils in liquid xenon." *J. Cosmol. Astropart. P.* **9**, 033. LLNL-JRNL-454331.

Sorensen, P., et al., 2010. "Lowering the low-energy threshold of xenon detectors." *Proc. 8th Intl. Workshop on the Identification of Dark Matter (IDM2010)*. LLNL-PROC-463991.

Mix at the Atomic Scale—Paul Miller (10-ERD-004)

Abstract

The need to compute the effects of mixing in a dynamical system is central to a wide variety of mission-relevant work at LLNL. Mixing involves

diffusion and is dependent on processes occurring at the atomic scale. Approximations are employed in continuum simulations of mixing that simplify or ignore complications and subtleties of diffusion and transport coefficients. We aim to formulate better mixing models by employing both continuum hydrodynamics and molecular dynamics codes—both LLNL strengths. We will develop metrics and a framework for the interchange of information between the two approaches, use molecular dynamics methodology to uncover atomic-level transport properties, and use a continuum hydrodynamics code to define limitations of the continuum approach and explore strategies for improving models.

We will develop a transport theory with the aid of molecular dynamics and continuum simulations. Large-scale simulation problems will be used for discovery and exploration, to gauge the adequacy of the methods, and to assess model improvements. Through an analysis of these simulations, we will begin developing a more complete, atomistically informed model of mixing for use in continuum calculations. By the end of this project, we expect to have made significant improvements in our ability to model complex mixing processes at both atomistic and continuum levels of resolution, resulting in substantial advancements in our understanding of diffusion and mixing.

Mission Relevance

By improving our ability to simulate mixing phenomena related to nuclear weapons more accurately, this work supports the Laboratory's mission in stockpile stewardship.

FY10 Accomplishments and Results

In FY10 we obtained a first set of results for stable diffusion systems. Specifically, we (1) analyzed two- and three-dimensional molecular dynamics and continuum simulations for transport in mixed plasmas; (2) used the results of molecular dynamics simulations to adjust our continuum models; (3) developed and tested metrics for comparison between the molecular dynamics and continuum hydrodynamics simulations—specifically, the power spectrum of

kinetic energy of the evolving shear layer, the persistence length for features at the mixing interface, and vorticity profiles versus time; and (4) implemented a first-generation formulation of Yukawa potentials for mixed plasmas and performed the first set of atomically informed diffusion simulations.

Proposed Work for FY11

We will continue to focus on stable diffusion systems in FY11, extending the work begun in FY10 to more fully explore and understand the physics of mixing by diffusion. Specifically, we will (1) further develop the Yukawa potentials and incorporate an improved model into the continuum hydrodynamics code, (2) calculate selected transport coefficients and run validation simulations with the improved model, (3) further test the metrics for comparing atomistic and continuum models and identify transport issues, and (4) conduct a large-scale integrated simulation for mixed plasmas, which will be further improved and analyzed in FY12.

Publications

Rudd, R. E., et al., 2010. *Self-diffusivity and inter-diffusivity of molten aluminum-copper alloys from molecular dynamics*. LLNL-JRNL-455401.

High-Gradient Inverse Free-Electron Laser Accelerator—Scott Anderson (10-ERD-026)

Abstract

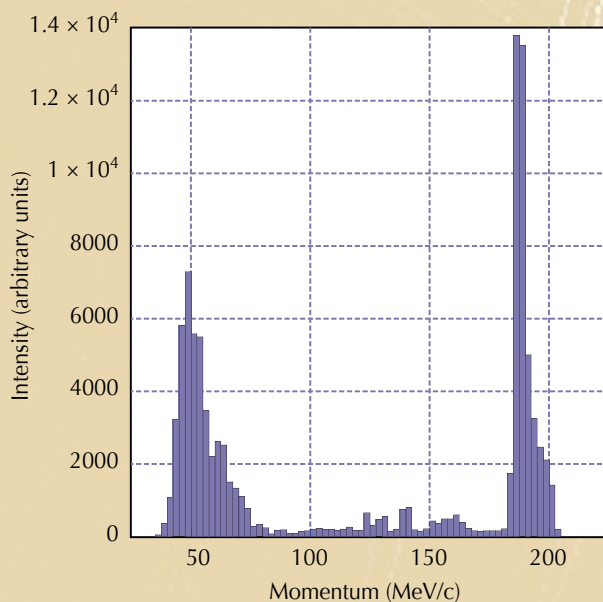
We will employ the inverse free-electron laser (IFEL) advanced acceleration technique to prove the feasibility of its use to create compact light sources. The IFEL is a leading contender to demonstrate high-gradient, high-quality acceleration at medium-energy ranges, and scales naturally to megahertz repetition rate with advancing laser technology. The technology has the potential to be the acceleration mechanism in deployable, compact light sources for special nuclear materials detection, or provide tabletop, gigaelectronvolt-class accelerators for academia and industry. Our IFEL will capture a 50-MeV beam and accelerate it to 125 MeV through a 50-cm

undulator installed at Livermore's high-brightness electron facility.

A successful IFEL demonstration will change future accelerator design for applications needing from 50 MeV to a few gigaelectronvolts. The tabletop footprint of our IFEL opens the door for academia and industrial applications needing compact, high-quality, low-emittance gigaelectronvolt beams not currently available. Compared to conventional acceleration, this IFEL will enable a reduction in size by a factor of 20 and cost by a factor 10. Meter-scale IFEL accelerators have the potential to produce greater than 350-MeV high-brightness electron beams with repetition rates driven by ever-advancing laser technology. As such, IFELs are attractive for future gamma-ray sources. Our IFEL will lead the advanced accelerator community, demonstrating compact, high-quality, high-gradient acceleration.

Mission Relevance

The accelerator technology developed in this project supports the Laboratory's mission to reduce or counter threats to national and global security. Our project specifically impacts Livermore's strategic



Simulation of the momentum spectrum of the 50-MeV electron beam after acceleration in the inverse free-electron laser experiment. Up to 40% of the electrons are accelerated at a gradient of 300-MeV/m to 200 MeV/c momentum.

mission thrust of nuclear threat elimination, with its capability for standoff detection. In addition, it supports efforts in cutting-edge science—specifically, energy manipulation to reduce accelerator footprints by three orders of magnitude at fixed energy. The LLNL strategic thrust of advanced laser optical systems and applications will be supported through the potential to upgrade the Laboratory's mono-energetic gamma-ray source for nuclear resonance fluorescence science and applications.

FY10 Accomplishments and Results

For FY10 we accomplished all of our proposed goals. Specifically, we (1) acquired the undulator and vacuum chamber and mapped the undulator magnetic field in three dimensions for use in simulations and to verify the field profile; (2) designed the 500-mJ, 100-fs titanium-sapphire drive laser and the matching and focusing optical system; (3) procured the “front end” of the laser system, including oscillator, stretcher, regenerative amplifier, and low-energy compressor and frequency conversion optics to drive the photocathode; (4) designed the IFEL beam line and made preparations for its installation at the linear accelerator facility; and (5) completed thorough theoretical and numerical analysis of the IFEL experiment, including the very important effects of slippage in the regime of short laser pulses.

Proposed Work for FY11

For FY11 we will (1) construct the IFEL beam line, including installation of the undulator, electron focusing optics and spectrometer, and laser-coupling mirrors; (2) complete the design and begin construction of the IFEL high-power laser transport and compressor vacuum systems; (3) install the front end of the IFEL laser system; (4) continue procuring needed IFEL laser system components, including a high-power amplifier; (5) perform initial propagation of the electron beam through the IFEL undulator and subsequent beam diagnostic line; and (6) communicate our research at conferences and in publications in collaboration with the University of California at Los Angeles.

Modeling and Measuring Quark–Gluon Plasma Shock Waves—Ron Soltz (10-ERD-029)

Abstract

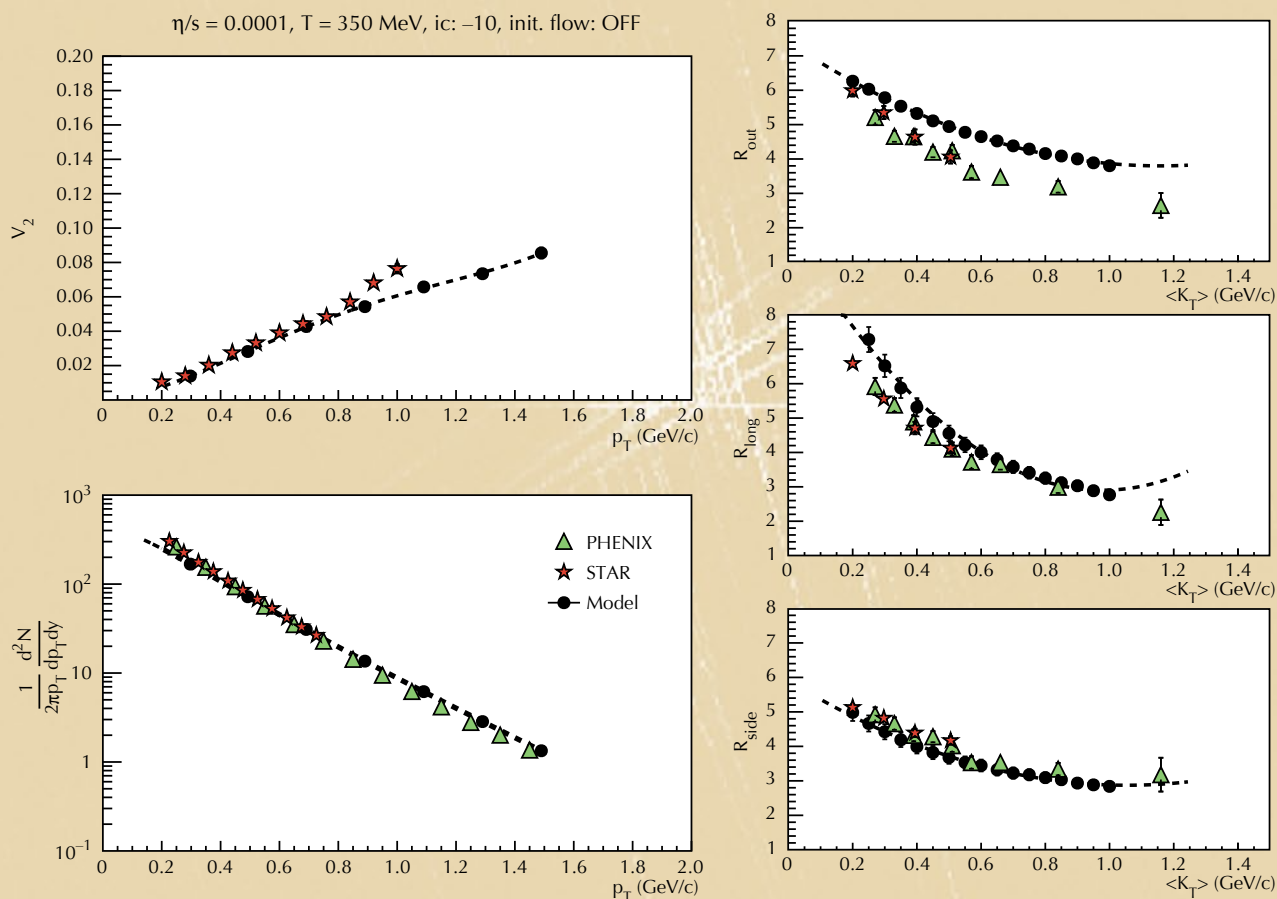
The possibility of developing shock waves in heavy-ion collisions was first suggested as a consequence of the compression of nuclear matter during initial stages of collision. The discovery of jet suppression has renewed interest in the possibility that high-energy partons—quark or gluons—generated by hard scatterings early in the collision process might induce shock waves in the surrounding medium. We propose to collaborate with theorists to model the jet energy loss and medium response with sufficient accuracy to determine whether measurable signatures exist. This project leverages an LLNL-developed capability that has already been successfully used

to identify non-Gaussian, long-range components in the space–time emission of pions and kaons in heavy-ion collisions.

This proposal will use hydrodynamic models to predict the space–time signatures of shock waves in heavy-ion collisions, and to measure these signatures at the ALICE (A Large Ion Collider Experiment) detector facility during lead–ion collision runs at the Large Hadron Collider near Geneva. This project leverages the Laboratory’s high-performance computing capabilities and will bring new talent to LLNL by hiring a postdoctoral researcher to run hydrodynamic models.

Mission Relevance

Heavy-ion collisions, which elucidate some of the most fundamental physics of matter, are studied with some of the most complex detectors and



Comparison indicates our model’s excellent agreement for pion spectra, flow, and femtoscopy data obtained with the PHENIX (Pioneering High Energy Nuclear Interaction Experiment) and STAR (Solenoidal Tracker at RHIC) detectors at Brookhaven National Laboratory.

models ever developed. By advancing capabilities in modeling heavy-ion collisions, this project extends the capability for modeling transport of particles and photons in matter, which is a required capability for radiation detection systems for national security and many other applications. This project also extends capabilities in high-energy-density science and very large data manipulation tools, in support of the Laboratory's national security mission.

FY10 Accomplishments and Results

In FY10 we (1) assembled a multistage collision model (Chimera) by inserting the lattice quantum chromodynamics equation of state and pre-equilibrium flow into a viscous, two-dimensional hydrodynamics model with a cascade afterburner; (2) developed a computer code to perform statistical hypothesis test comparisons and obtained good agreement with published data; and (3) adapted a fitting method that allows us to make chi-squared comparisons to data in a way that naturally incorporates systematic errors. Chimera is the first two-dimensional hydrodynamics model to incorporate all of the essential ingredients required to describe the physics of a heavy-ion collision—initial state fluctuations in eccentricity, pre-equilibrium flow, viscosity, a full quantum chromodynamics equation of state, freeze-out to hadrons, and a cascade afterburner.

Proposed Work for FY11

In FY11 we will (1) extend our multistage model by inserting an energy-loss mechanism into the hydrodynamics model to predict the medium response of plasma to high-energy jets, (2) collect our first heavy-ion data sets from the Large Hadron Collider by participating in ALICE, and (3) perform data analysis with the PHENIX (Pioneering High Energy Nuclear Interaction Experiment) at the Relativistic Heavy Ion Collider at Brookhaven National Laboratory in the event that the ALICE detector facility takes longer than expected to achieve collisions with heavy-ion beams at the Large Hadron Collider.

Publications

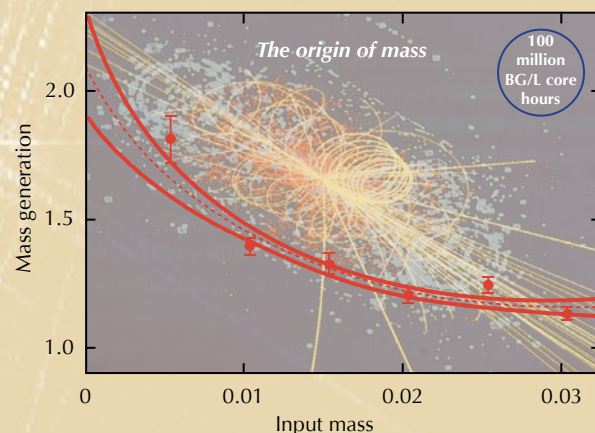
Garishvili, I., 2010. *Modeling hydrodynamic properties of the QGP at RHIC. 2010 Fall Mtg.* APS Division of Nuclear Physics, Santa Fe, NM, Nov. 2–6, 2010. LLNL-CONF-461619.

Soltz, R., 2010. *Quantifying properties of the QGP.* Institute for Nuclear Theory Workshop: Quantifying the Properties of Hot QCD Matter, Chicago, IL, June 14, 2010. LLNL-PRES-418133.

Unlocking the Universe with High-Performance Computing—Pavlos Vranas (10-ERD-033)

Abstract

We propose to use large-scale numerical simulations on LLNL's BlueGene supercomputers to unravel the inner workings of the universe—from the physics beyond the standard model of elementary particles created a trillionth of a second after the Big Bang, to the quark–gluon plasma created a millionth of a second after the Big Bang, to the stable nuclear



A strongly interacting theory known as “Technicolor” could explain the origin of mass. In this plot, mass is generated even with zero input mass. This project will compare and contrast its simulations of the related phenomena, performed using BlueGene/L (BG/L) and other LLNL high-performance computation resources, with experimentation at the Large Hadron Collider near Geneva, Switzerland.

matter that comprises most of the visible universe today. We will compare and contrast our simulation results with current and upcoming experiments at the Large Hadron Collider (LHC) near Geneva, Switzerland. We also intend to study the underlying theories of quantum chromodynamics and the Yang–Mills theories, which can only be numerically simulated using models consisting of a discretized space–time lattice mapped onto the nodes of massively parallel supercomputers.

We expect to develop a theoretical understanding of the inner workings of nature spanning three layers of physical phenomena: (1) the physics of mass generation of elementary particles, (2) the quark–gluon plasma and its transition to nuclei, and (3) the interactions of nuclei and the emergence of nuclear physics. The overall deliverable is the prediction, using the most fundamental scientific starting point, of particles and phenomena that will be observed in extremely high-energy ion collisions. Our work will help understand and guide the largest and highest-energy experiments of our time—those performed at the LHC. No other groups in the world are pursuing this type of research at this scale.

Mission Relevance

The use and development of high-performance computing underlies all aspects of this proposal and impacts multiple LLNL missions. For example, methods and algorithms we develop will be relevant to the new multicore architectures on which the most advanced stockpile stewardship simulations are now run. In addition, first-principles calculations of the nuclear force at the quantum chromodynamics level are directly relevant to light-ion reaction cross sections in fusion energy. By establishing LLNL as a world leader in this cutting-edge area of physical theory, this project will also attract leading postdoctoral researchers.

FY10 Accomplishments and Results

In FY10 we (1) completed simulations of two variations of the Yang–Mills field theory on the lattice,

compared our results with the expected phenomenology of six versus two flavors, and found significant condensate enhancement, which indicates mass generation; (2) performed simulations with quantum chromodynamics—controlling chiral symmetry (important for explaining the low-energy hadronic spectrum)—to determine the phase-transition temperature of the quark–gluon plasma and the equation of state; (3) incorporated the equation of state into hydrodynamic models and compared its results with experimental results from the Relativistic Heavy Ion Collider at Brookhaven National Laboratory; and (4) performed high-statistics measurements of baryon–baryon particle interactions.

Proposed Work for FY11

In FY11 we will (1) measure the spectrum and scattering parameters for the Yang–Mills lattice configurations calculated in FY10; (2) begin simulations of lattice configurations relevant to pion physics; (3) investigate the thermal transition region of quantum chromodynamics using a hypothetical pion mass of approximately 200 MeV; (4) begin measuring the equation of state for this region using chirally improved, staggered quark-lattice fermions; and (5) perform finite-volume, many-body calculations that will help integrate our lattice quantum chromodynamics results with *ab initio* many-body methods.

Publications

Appelquist, T., et al., 2010. “Toward TeV conformality.” *Phys. Rev. Lett.* **104**, 071601. LLNL-JRNL-420851.

Beane, S. R., et al., 2010. “High-statistics analysis using anisotropic clover lattices: (III) baryon–baryon interactions.” *Phys. Rev. D* **81**, 054505. LLNL-JRNL-424175.

Cheng, M., et al., 2010. “The finite temperature QCD using 2+1 flavors of domain wall fermions at $N_t = 8$.” *Phys. Rev. D* **81**, 054510. LLNL-JRNL-420858.

Discovery and Synthesis of Materials for High-Energy-Density Science— Stanimir Bonev (10-ERD-038)

Abstract

We propose to develop a first-principles computational framework that will enable prediction of the phase stability of materials at finite temperature, thereby accelerating discovery and synthesis of high-energy-density materials. Specifically, we will study nitrogen- and carbon-rich molecular compounds that, under the application of pressure, transform from weakly bound molecular crystals to covalent solids. Large amounts of energy can be released when a transformation is induced from a covalent crystal, a metastable high-energy state at low pressure, to the stable low-energy molecular phase. The potential use of such materials for practical applications is based on the ability to produce significant amounts of the high-energy-density state and to preserve the attained modifications when the materials are cooled to near-ambient conditions.

Successful project completion will result in development of a computational toolkit for examining similarities between low-atomic-number, high-pressure liquid and solid phases and for carrying out automated phase searches that are specifically designed to predict finite-temperature phase stability. We will apply these methods, in close collaboration with experiments, to examine the effect of impurities on phase transformations in nitrogen- and carbon-rich materials, which are good candidates for achieving metastable high-energy-density states of matter. The primary benefit of this work will be in the development of a first-principles-based approach that can be used to accelerate discovery and synthesis of novel materials for high-energy-density science.

Mission Relevance

The proposed project will result in new computational capabilities at LLNL that are directly applicable to the cross-cutting challenges to the Laboratory's science, technology, and engineering foundation. In particular, by combining sophisticated methods for automatic phase exploration with

first-principles simulation methods, we will develop an integrated approach that will enable a detailed understanding of high-energy-density matter and will accelerate the discovery of new materials, relevant to LLNL's mission of ensuring the safety, security, and reliability of the U.S. nuclear deterrent. In addition, continued development and application of predictive simulation capabilities will make full use of the Laboratory's investments in high-performance computing and simulation.

FY10 Accomplishments and Results

In FY10 we (1) developed a preconditioned random search algorithm by using structural information from simulations of liquids to seed the search for novel solid structures at finite temperatures and applied it to nitrogen, resulting in the discovery of a novel high-temperature and high-pressure crystalline phase; (2) developed tools for analyzing the structure of heterogeneous liquids and methods for computing Gibbs free energies of liquids and anharmonic solids, which were applied to nitrogen, liquid alloys, and solid calcium; (3) performed molecular dynamics simulations of nitrogen with various impurities, including all elements from rows I to III of the periodic table, over the range of 10 to 100 GPa and different impurity concentrations; (4) determined, based on these simulations, the elements that have the strongest effect on the polymerization of nitrogen; (5) made good progress in mapping the phase diagram of liquid carbon dioxide up to 100 GPa and 10,000 K; and (6) began studies of extended nitrogen solids with impurities.

Proposed Work for FY11

In FY11 we will (1) continue simulations of liquid mixtures rich in nitrogen and carbon dioxide as likely high-energy-density material candidates; (2) apply our new preconditioned random-search algorithm to these liquids to predict novel polymeric solids; and (3) begin developing an efficient phase search algorithm appropriate for finite temperatures using first-principles molecular dynamics combined with metadynamics.

Publications

Boates, B., and S. A. Bonev, 2010. *Metallic nitrogen at high pressure and temperature*. American Physical Society March Mtg., Portland, OR, Mar. 15–19, 2010. LLNL-ABS-420448.

Boates, B., and S. A. Bonev, 2010. *Metallic nitrogen*. Gordon Conf. Research at High Pressure, Holderness, NH, June 27–July 2, 2010. LLNL-POST-438642.

Boates, B., et al., 2010. “Structural and optical properties of liquid CO₂ up to 1 terapascal.” *Bull. Am. Phys. Soc.* **56**(2). LLNL-JRNL-458115.

Teweldeberhan, A. M., and S. A. Bonev, 2010. *Alkali and alkaline earth metal alloys at high-pressure*. American Physical Society March Mtg., Portland, OR, Mar. 15–19, 2010. LLNL-ABS-420450.

Teweldeberhan, A. M., and S. A. Bonev, 2010. “Comment on ‘Structural prediction and phase transformation mechanisms in calcium at high pressure’.” *Phys. Rev. Lett.* **104** 209610. LLNL-JRNL-421347.

Teweldeberhan, A. M., and S. A. Bonev, 2010. *Thermodynamic stability of alkali and alkaline earth metals at high-pressure*. Gordon Conf. Research at High Pressure, Holderness, NH, June 27–July 2, 2010. LLNL-POST-438596.

An Intense Laser-Based Positron Source— Scott Wilks (10-ERD-044)

Abstract

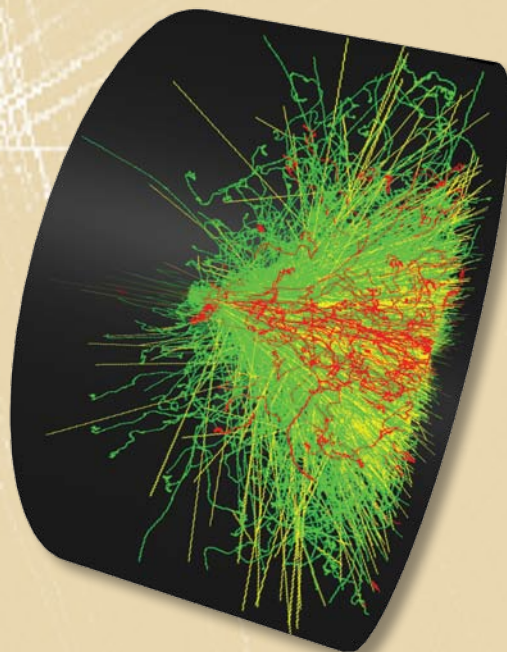
Our goal is to characterize and investigate a new high-brightness positron source based on ultra-intense laser–matter interactions. This work will allow us to understand the underlying science, assess potential applications, and result in the addition of a brand new class of positron sources. We will extend development of the world’s most advanced direct hot-electron diagnostic for high-energy-density physics research using experiment, theory, and simulation. We will use state-of-the-art

simulation codes to design experiments, execute several experimental campaigns on various high-intensity lasers around the world, and compare data with predictions.

We expect to lay the science foundation for a new class of intense positron sources. In particular, we will (1) develop an understanding of the detailed physics behind the laser-to-positron coupling, (2) investigate sheath physics behind the average positron beam energy, (3) measure beam emittance, (4) increase the accuracy with which laser-generated fast-electron distributions are measured, and (5) assess the possibility of generating gamma-ray radiation at 511 keV. Significantly, we will have determined the applicability of this source for researchers specializing in electron–positron jets, particle accelerators, gamma-ray generation, and noninvasive measurements of materials using positrons.

Mission Relevance

This project will lay the science foundation for a new and potentially powerful source of positrons, which may lead to new approaches for diagnosing experiments in plasma and atomic physics,



Electron (green), positron (red), and gamma-ray (yellow) shower initiated by laser-generated relativistic electrons with energies of 25 MeV.

fusion science, high-energy-density physics, accelerator and particle-beam science, nondestructive interrogation of materials, and astrophysics. These areas of science are foundational to the Stockpile Stewardship Program.

FY10 Accomplishments and Results

In FY10 we (1) completed a new set of experiments that measured emittance of the positron beam, as well as attempted to measure annihilation radiation in the target; (2) completed experimental campaigns on the University of Rochester's OMEGA and Livermore's Titan lasers—using advanced simulation capabilities to design targets for our experiments and the Electron Gamma Shower code to simulate gamma rays based on actual electron distributions from the Titan laser (as measured by our spectrometer, which we tested to ensure that the resolution was adequate to clearly detect annihilation radiation); and (3) held an international workshop on antimatter generation with lasers, where we presented our idea of using positrons to obtain detailed knowledge of sheath physics and hot-electron generation.

Proposed Work for FY11

In FY11 our work will culminate in experiments to create and diagnose a laser-generated gamma-ray burst, a first-ever scientific demonstration. Specifically, we will obtain a gamma-ray crystal spectrometer to investigate, at 511 keV, a gamma-ray burst caused by annihilation radiation of laser-generated positrons. The spectrometer will allow us to detect annihilation radiation at a resolution of approximately 10 keV.

Publications

Chen, H., and S. C. Wilks, et. al. 2009. "Making relativistic positrons using ultraintense short pulse lasers." *Phys. Plasma*. **16**, 122702. LLNL-JRNL-416496.

Chen, H., and S. C. Wilks, et. al., 2010. "Relativistic quasimonoenergetic positron jets from intense laser-solid interactions." *Phys. Rev. Lett.* **105**, 015003. LLNL-JRNL-418061.

Multiscale Polymer Flows and Drag Reduction—Todd Weisgraber (10-ERD-057)

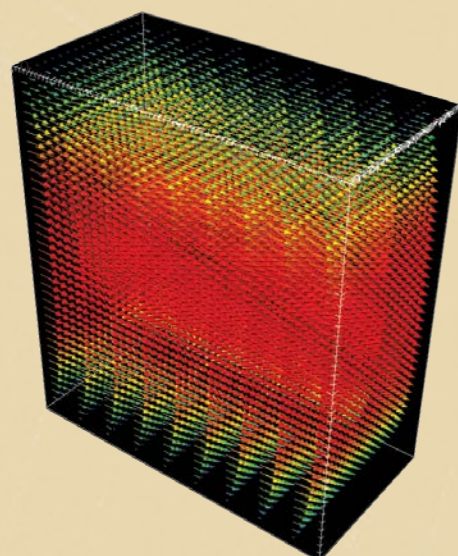
Abstract

The reduction in drag in bounded turbulent flows by addition of long-chain polymers is a well-established phenomenon. However, despite decades of research, the fundamental mechanisms underlying drag reduction are still poorly understood. We believe that a complete description of the coupled polymer and flow dynamics for drag reduction must incorporate wall roughness, a coarse-grained molecular representation of the polymer, and hydrodynamic fluctuations at the polymer length scale. We propose to develop new algorithms—including an unconditional, fluctuating lattice-Boltzmann solver coupled with molecular dynamics—to enable fully turbulent, multiscale simulations of drag reduction that will increase our understanding of the underlying physics.

We expect to perform a series of large-scale simulations to provide valuable insight into a fundamental hydrodynamics problem, including a more detailed understanding of the complex dynamics of polymers and turbulence. Additional knowledge of drag reduction could conceivably make it possible to

DB: lbpolymertest.plot.001000.3d.hdf5
Cycle: 1000 Time: 1000

Vector
Var: momentum
0.009972
0.007722
0.005472
0.003222
0.0009724
Max: 0.009972
Min: 0.0009724



A channel flow validation simulation using the lattice-Boltzmann solver within the Chombo adaptive mesh-refinement framework illustrates drag near the top and bottom walls.

optimize this effect in more practical applications. A modest decrease in drag would dramatically improve the efficiency of deploying naval vessels and reduce expenditures in the civilian sector. In addition to the fundamental science, we will also develop a high-performance computing capability applicable to biosecurity and Rayleigh–Taylor instability research.

Mission Relevance

Our research aligns well with high-performance computing and simulation, identified as an area of frontier science and technology where the Laboratory can develop new capabilities that advance scientific discovery and enable future missions. We will employ Livermore high-performance computing to address fundamental scientific questions in hydrodynamics. The interaction between flow and polymer physics is also relevant to development of the next generation of emerging pathogen detection and analysis systems, an important component for LLNL's biosecurity strategic mission thrust.

FY10 Accomplishments and Results

In FY10 we (1) completed algorithm development for the entropic lattice-Boltzmann solver with hydrodynamic fluctuations; (2) validated the algorithms by testing Reynolds number limits with channel-flow simulations; (3) developed adaptive mesh refinement in collaboration with Lawrence Berkeley National Laboratory, almost completing the refinements for the fluid phase; and (4) performed benchmarking simulations of the migration laminar flow of a single polymer in microchannels with various rough-wall configurations using the new entropic code.

Proposed Work for FY11

In FY11 we propose to (1) complete development of the adaptive mesh refinement; (2) begin Newtonian turbulent channel simulations with the adaptive mesh-refinement code; (3) continue laminar flow migration simulations with wall roughness; (4) begin the series of large-scale turbulent drag-reduction simulations; and (5) study how the size of roughness elements relative to coiled polymer radius—which we believe to be a critical parameter—affects flow stability, transition to turbulence, and magnitude of drag reduction.

Publications

Weisgraber, T., and B. Alder, 2010. *Polymer flows in channels with roughened walls*. 19th Intl. Conf. Discrete Simulation of Fluid Dynamics (DSFD 2010), July 5–9, 2010, Rome, Italy. LLNL-PRES-439178.

Fundamental Research in Advanced Quantum Simulation Algorithms— Jonathan DuBois (10-ERD-058)

Abstract

First-principles simulation of materials properties has played an essential role in Livermore's science and technology for the last half-century. Mission-critical applications range from quantum chemistry to plasma physics. Broadly, the most significant challenge for these simulations today is the ability to efficiently measure and controllably reduce systematic errors. While first-principles simulations continue to be applied, current shortcomings will ultimately limit their usefulness, regardless of available computing power. We propose a basic research program aimed at estimating and reducing systematic errors within the framework of ground-state and finite-temperature quantum Monte Carlo codes.

We intend to develop a robust tool set based on released-node quantum Monte Carlo for estimating the systematic error introduced by use of the fixed-node approximation for large systems, which is a robust method for obtaining an upper bound to the ground state energy by forcing the solution to have the same nodal structure as a trial wave function. Our techniques could increase the accuracy of state-of-the-art calculations by two orders of magnitude so that the typical error lies within the chemical accuracy bound. We will also develop a constant-pressure diffusion Monte Carlo algorithm in which the proton and electron degrees of freedom, along with the cell degrees of freedom, can adjust. Finally, we will implement several novel enhancements to the standard path-integral quantum Monte Carlo method using the knowledge garnered in ground-state quantum Monte Carlo calculations to extend the path-integral quantum method to lower temperatures.

Mission Relevance

Accurate first-principles simulations of materials are essential for current and future goals of LLNL for materials on demand, uncertainty quantification, and stockpile stewardship science, especially where experiments are not feasible. Currently available methods are unable to meet these demands with acceptable accuracy. Development of a high-accuracy first-principles simulation capability is therefore well aligned with the Laboratory's strategic missions.

FY10 Accomplishments and Results

In FY10 we (1) developed and tested existing and improved cancellation algorithms for random walkers in the released-node quantum Monte Carlo method, finding that cancellation did not significantly improve the efficiency of obtaining ground-state energies of many-body electronic systems relative to unconstrained (non-canceling) released-node calculations; (2) performed an initial investigation of the use of an exact stochastic sampling of Green's function; (3) performed maximum entropy and Lanczos diagonalization analysis of released-node imaginary time-correlation functions for first-row dimers, which allowed us to obtain the most accurate bounds to date on the ground-state energy of dimers ranging from lithium and fluorine; (4) developed and tested multiple trial wave functions and found consistent results (independent of trial function) for ground-state energies via statistical analysis of imaginary time-correlation functions; and (5) developed a finite-temperature Fermion path-integral quantum Monte Carlo (FPIMC) code capable of efficiently sampling permutation statistics within the grand ensemble.

Proposed Work for FY11

In FY11 we will (1) test our low-temperature FPIMC method by simulating low-temperature helium-3 and comparing our computed results for energy and specific heat with known experimental values; (2) implement the coulomb action within our FPIMC code and begin simulation of low-temperature (300–5000 K) compressed hydrogen; (3) introduce an enthalpy term in our FPIMC code along with the ability to use a trial function to enable study of the constant-pressure ground-state properties of solid hydrogen; (4) use the code to search for candidate structures for the solid hydrogen III phase

at pressures of about 150 GPa; and (5) begin exact released-node quantum Monte Carlo calculations of the ground-state properties of candidate structures for compressed hydrogen.

Publications

DuBois, J. L., D. Aberg, and V. Lordi, 2010. *Diffusion Monte Carlo calculations of formation energies of charged self interstitial defects in silicon*. American Physical Society March Mtg. 2010, Portland, OR, Mar. 15–19, 2010. LLNL-PRES-426109.

Tubman, N., et al., 2010. *Transient methods in quantum Monte Carlo calculations*. Quantum Monte Carlo in the Apuan Alps VI, Vallico Sotto, Tuscany, Italy, July 24–31, 2010. LLNL-PRES-444177.

Tubman, N., et al., 2010. *Transient quantum Monte Carlo investigations of few-electron systems*. American Physical Society March Mtg. 2010, Portland, OR, Mar. 15–19, 2010. LLNL-PRES-427939.

Feasibility of a Hybrid Rubidium Resonance and Exciplex Pump Laser—Raymond Beach (10-FS-002)

Abstract

We propose to examine a new concept for relaxing the tight wavelength tolerance on diode arrays used for excitation of alkali resonance lasers. This involves the use of a recently demonstrated excitation pathway in which the photo-association of an alkali metal atom and a polarizable buffer gas atom results in broad absorption-wing features on certain alkali spectral lines. These absorption features can easily accommodate the line widths of conventional laser diode arrays. The fundamental issue that must be addressed is pump irradiance required for efficient operation. We therefore propose to generate data and a companion laser model that permits us to reliably project laser system performance over a broad range of parameters.

We intend to evaluate the feasibility of a hybrid concept that uses the LLNL-developed hydrocarbon-free rubidium resonance laser scheme with a rubidium and rare-gas exciplex (excited-state complex) laser that can accommodate conventional

diode arrays for pump excitation. This is a high-risk, but if shown feasible, potentially very high-payoff investigation that could alter the landscape of high-average-power diode-pumped lasers envisioned for a broad range of defense activities, and already used in commercial material processing applications. This activity will contribute to maintaining LLNL's technical vitality and world dominance in the field of advanced diode-pumped laser development.

Mission Relevance

Our research supports the Laboratory's missions in advanced lasers and applications as well as national security. It is directly relevant to laser-based defense needs in addition to addressing future mission needs within the defense complex.

FY10 Accomplishments and Results

In FY10 we accomplished our experimental goals for exciplex lasers by developing a technique for measuring spectrally resolved absorption profiles using a weak white-light illumination source, and using this technique to obtain required absorption profiles with various buffer gas mixtures from samples characterized by large absorption cross sections—absorptions that are easily saturated. We used the collected data to support our generalized homogeneous line-width methodology and as input for development of our laser energetics model.

Proposed Work for FY11

In FY11 we propose to (1) develop a laser energetics model that can project laser system performance; (2) submit a patent covering the system concept, if our modeling results in a novel system; and (3) publish a document in a high-profile journal describing the projected performance of an exemplar system, along with power-scaling arguments.

Feasibility of Diode-Laser Array as Surrogate Source for Laser Lethality Studies— W. Howard Lowdermilk (10-FS-004)

Abstract

Our research objective is to establish the feasibility of using a compact, high-power diode-laser array at the High Explosives Applications Facility (HEAF) as a scientific surrogate for weapon-class lasers in

lethality experiments. In particular, we hope to demonstrate that sufficient power and beam uniformity can be delivered to produce laser lethality effects that are qualitatively identical to effects previously observed using high-power lasers developed for directed-energy weapon applications. Such simulations are needed for scenarios where the laser is incident upon targets containing energetic materials. The current inability to simulate these interactions leads to very costly field tests of military directed-energy systems. We intend to design and build systems to transport light from a diode-laser array to a target in a chamber at HEAF and conduct measurements on targets including pre-stressed material samples and pressurized cases. We will measure laser power and power distribution on the target using a laser power meter and spatially resolved calorimetry, as well as measure target interaction effects using thermocouples, thermal imaging, and high-speed photo and video cameras.

The project is expected to establish the feasibility of using a compact, diode-laser array as a low-cost surrogate for weapon-class experiments with energetic materials. This result will enable a means to benchmark advanced simulations of laser–target interactions for directed-energy systems.

Mission Relevance

This work is directly relevant to the Laboratory's core national security missions, and it builds upon Livermore's strategic capabilities to apply advanced diode-laser systems technology to energetic materials research.

FY10 Accomplishments and Results

In FY10 we (1) designed and built a diode-laser array light-transport system for target irradiation, (2) installed our system in the 1-kg firing tank at HEAF and verified the diode array was able to heat a target canister containing ammonium perchlorate solid rocket propellant to the cookoff temperature (where thermally induced explosion occurs) that was predicted by one-dimensional simulation, and (3) conducted a successful, integrated laser–target interaction experiment, including collection of all planned temperature, pressure, and high-speed video data. These data showed that fast laser cookoff produced explosive damage to the canister in a two-step process, resolving questions about the

key phenomena of such laser–target interactions. Preliminary two-dimensional simulations using the ALE (Arbitrary Lagrangian-Eulerian) code provided insight into the details of laser-induced deflagration. Successful completion of this project demonstrated the feasibility of using a diode-laser array as a compact, transportable, and low-cost surrogate weapon-class source for realistic experiments on laser lethality, including use of energetic materials. The Missile Defense Agency has expressed interest in supporting expansion of such a capability, including development of a full, predictive, laser-lethality simulation capability to support national directed-energy program objectives.

Suppressing Counterflow Turbulence with a Shear-Thickening Agent— Peter Beiersdorfer (10-FS-005)

Abstract

We propose an exploratory experiment for a novel way to improve the “top kill” approach that failed to stem the oil flow from the Macondo well in the Gulf of Mexico. We will conduct a simple experiment to investigate whether it is feasible to suppress the generally deleterious two-stream (Kelvin–Helmholtz) instability by adding a shear-thickening agent (cornstarch) to one of the fluids (drilling mud). If suppression of the oil flow can be demonstrated, this technique could make future top kill operations more successful.

This work is tremendously relevant to a current national need—stopping the oil flow from deep-sea wells. If shown to be successful, the method will provide a new tool not just for oil exploration but for energy exploration in general. In addition, successful suppression of Kelvin–Helmholtz instability using the proposed method and the proposed test setup would represent a first in experimental science.

Mission Relevance

This project addresses an important national need in energy exploration and thus has the potential to tremendously increase the nation’s energy security.

FY10 Accomplishments and Results

We conducted tests in which we introduced a dense fluid (water, as a surrogate for drilling mud) into the top of a column of less dense fluid (oil) that is immiscible with water and studied the water’s descent under the acceleration of gravity. We first showed that the water becomes turbulent and breaks up into droplets because of Kelvin–Helmholtz instability. We then investigated suppression of the instability by adding cornstarch to make the descending fluid act as a shear-thickening agent. We observed total suppression of Kelvin–Helmholtz turbulence once a certain shear-thickening threshold was reached, demonstrating the effectiveness of the approach. Thus, this project demonstrated the use of shear-thickening fluids as a means to suppress turbulence and droplet formation in gravity-driven counter-streaming fluids. These results can be applied to the formulation of drilling mud for the top kill of oil wells.

Publications

Beiersdorfer, P., et al., 2010. *Viscoelastic suppression of counterflow instability in “top kill” of flowing oil wells*. LLNL-JRNL-443633.



Stabilization of the turbulent breakup of descending water in oil (left) by cornstarch (middle), along with the descent of the same suspension at a slower speed (right).

INVESTING IN THE FUTURE
OF SCIENCE AND TECHNOLOGY



Laboratory Directed Research and Development
Lawrence Livermore National Laboratory
P.O. Box 808, L-19
Livermore, CA 94551

