INDEX of SCIENCE HIGHLIGHTS   May 12, 2010

PADSTE HIGHLIGHTS May 12, 2010

ASSOCIATE DIRECTORATE - ENGINEERING & ENGINEERING SCIENCES

W. Scott Gibbs and Kevin W. Jones present keynote addresses

W. Scott Gibbs (Associate Directorate for Engineering and Engineering Sciences, ADE) and Kevin W. Jones (Accelerator Operations and Technology, AOT) gave keynote talks at the Beam Instrumentation Workshop sponsored by LANL in Santa Fe, New Mexico. The international workshop is dedicated to beam diagnostics and instrumentation for charged particle accelerators and beam transport lines.

Gibbs' presentation provided an overview of the rich history of LANL's contributions to the field of accelerator technology, including the early-generation low-energy proton and electron accelerators: (1) Cockroft-Walton and Tandem proton and light ion machines for nuclear physics measurements, and (2) PHERMEX (Pulsed High Energy Radiation Machine Emitting X-Rays) for dense object radiography. Additional contributions include the invention of the side-coupled cavity room temperature radio-frequency accelerating structure that led to the design and construction of LANSCE (Los Alamos Neutron Science Center) – the world's first 1MW-class accelerator that has accelerated almost 1.4 moles of protons, and the development of Proton Storage Ring technology for pulse compression to generate intense neutron pulses. LANSCE provides uniquely flexible time-structured beams from 100 to 800 MeV to serve over twenty active experimental stations. LANL and Argonne National Laboratory jointly established the EPICS (Experimental Physics and Industrial Control System) collaborative community. The Lab performed the first lasing using a compressed electron beam, made the first measurements of longitudinal and transverse wakefields and their effects on lasing, and invented the Free Electron Laser photoinjector. LANL developed the DARHT (Dual Axis Radiographic Hydrotest Facility) with two orthogonal high-intensity pulsed electron beam induction accelerators for dense object radiography. Gibbs also described current initiatives in accelerator science and technology, including the LANSCE Life Extension Project to revitalize core accelerator systems.

Photos. LANL accelerators: (*left*) LANSCE and (*right*) DARHT.

Kevin Jones presented "Looking Beyond LANSCE: MaRIE" (Matter-Radiation Interactions in Extremes Facility), noting that the transition from "observation and validation" to "prediction and control" is the central mission challenge and the frontier of materials research. MaRIE's goals are to achieve transformational materials performance and predictive multi-scale understanding of materials. Experimental tools with unprecedented capabilities are needed to validate and test the limits of modeling and simulation. Future research capabilities must enable bridging atomic scale/molecular dynamics studies and continuum models/integrated tests. MaRIE is LANL's vision for a facility to study dynamic materials by combining proton microscopy and coherent light sources with extreme environments. MaRIE is being designed to provide international user resources to solve important extreme matter challenges. The planned facility will include a fission and fusion materials facility, a multi-probe diagnostic hall, and the M4 facility dedicated to making, measuring, and modeling materials.

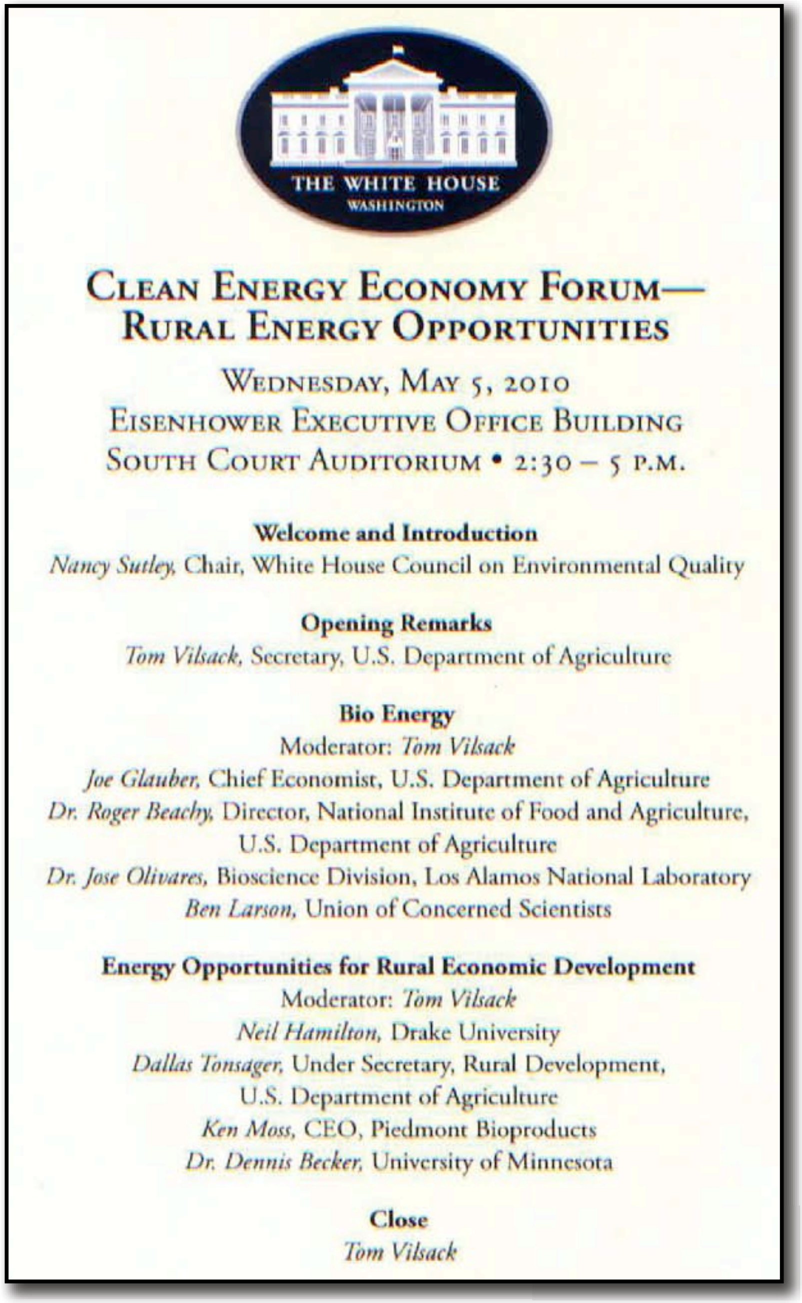
Figure 1. The MaRIE conceptual design incorporates a new XFEL and a LANSCE proton beam power upgrade.

BIOSCIENCE

José Olivares gives talk for Clean Energy Economy Forum at the White House

On May 5, Biofuels Program Manager José Olivares (Biosciences, B-DO) participated in a Clean Energy Economy Forum at the White House. As part of a series of Clean Energy Forums, the objective of this forum was to promote renewable energy (especially its benefits for rural America and agriculture) and to mark the one-year anniversary of President Obama’s Biofuels Directive. U.S. Department of Agriculture (USDA) Secretary Tom Vilsack invited Olivares and other panelists to participate in the forum. The goal was to engage the audience in discussion and to educate them about the environmental and economic benefits of renewable biofuels. The audience included more than 100 energy executives, developers, bankers, lawyers, rural stakeholders, and others at the Eisenhower Executive Office Building. The group discussed renewable energy opportunities for rural communities and the Obama Administration’s efforts to help rural America build a clean energy economy that creates jobs, reduces our dependence on foreign oil, and enhances our position in the global economy. The Administration officials also had the opportunity to hear from farmers, ranchers, and energy producers about their experiences in the emerging clean energy economy. The day after the Clean Energy Forum, the USDA announced new funding opportunities for biofuels research.

As a representative of the Southwest Region, Olivares spoke about the need for further collaboration between the USDA and DOE, the value of job training and education in the biofuels arena, and the contributions that are being made by research institutions and companies in the Southwest. He specifically spoke about the land-grant universities in the area that can be used to train a biofuels industry-ready workforce if the resources are allocated appropriately. A USDA press release also quoted Olivares as recommending new incentives for nascent technology and more collaboration among federal agencies.



THE WHITE HOUSE
WASHINGTON

CLEAN ENERGY ECONOMY FORUM—
RURAL ENERGY OPPORTUNITIES

WEDNESDAY, MAY 5, 2010
EISENHOWER EXECUTIVE OFFICE BUILDING
SOUTH COURT AUDITORIUM • 2:30 – 5 P.M.

Welcome and Introduction
Nancy Sutley, Chair, White House Council on Environmental Quality

Opening Remarks
Tom Vilsack, Secretary, U.S. Department of Agriculture

Bio Energy
Moderator: *Tom Vilsack*
Joe Glauber, Chief Economist, U.S. Department of Agriculture
Dr. Roger Beachy, Director, National Institute of Food and Agriculture, U.S. Department of Agriculture
Dr. Jose Olivares, Bioscience Division, Los Alamos National Laboratory
Ben Larson, Union of Concerned Scientists

Energy Opportunities for Rural Economic Development
Moderator: *Tom Vilsack*
Neil Hamilton, Drake University
Dallas Tonsager, Under Secretary, Rural Development, U.S. Department of Agriculture
Ken Moss, CEO, Piedmont Bioproducts
Dr. Dennis Becker, University of Minnesota

Close
Tom Vilsack

CHEMISTRY

Actinide Analytical Chemistry Group (C-AAC) supports Mixed Oxide Fuel Program milestone
LANL was placed on the Approved Suppliers list for Shaw Areva MOX Services, LLC, following an extensive audit of all supporting organizations' implementation of ANSI/ASME Standard NQA-1 "Quality Assurance Requirements for Nuclear Facility Applications". Approved Supplier status allows LANL to supply plutonium oxide (PuO_2) material recovered from nuclear weapons dismantlement to MOX Services, for fabrication into mixed-oxide fuel to be burned in commercial nuclear reactors. As part of the US agreement with the Russian Federation to jointly eliminate 68 tons of weapons-grade plutonium that are no longer needed for defense purposes, LANL will deliver approximately 2000 kg of plutonium oxide by 2018. C-AAC will support the program with chemical and radiochemical analyses of 15-25 lots of plutonium oxide per year, including the initial 50 kg of PuO_2 that are scheduled to be

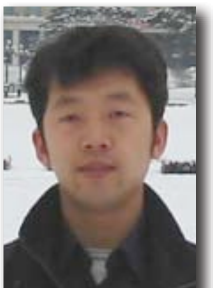
 

prepared and packaged in FY10. The Associate Directorate for Stockpile Manufacturing and Support (ADSMS), Process Automation and Control (AET-5), Quality Assurance-Institutional Quality (QA-IQ), and Safeguards Science and Technology (N-1) support the MOX Program. Jim Ostic is the LANL Program Manager. Technical contact: *Donivan Porterfield*

Photos: Plutonium oxide product resulting from direct metal oxidation, before (*left*) and after (*right*) milling.

EARTH AND ENVIRONMENTAL SCIENCES

Moran Wang joins editorial boards



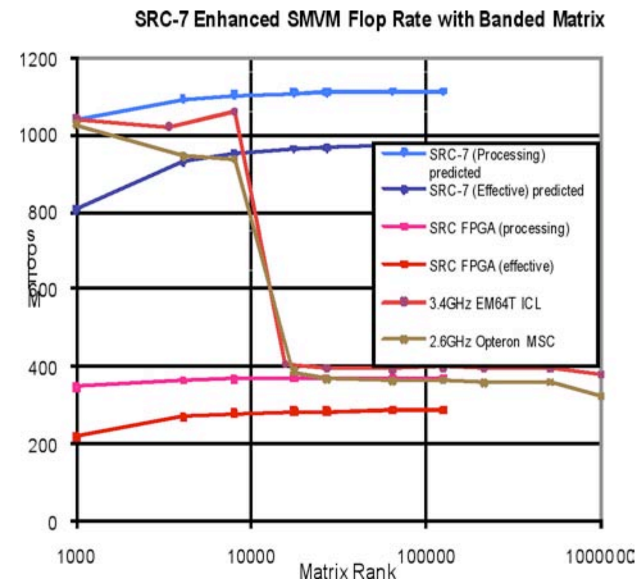
The ***Journal of Porous Media*** and ***Special Topics and Reviews in Porous Media*** invited Moran Wang (Computational Earth Science, EES-16) to join their editorial boards. The ***Journal of Porous Media*** publishes porous media research, including mathematical modeling, numerical and experimental techniques, industrial and environmental heat and mass transfer, conduction, convection, radiation, particle transport and capillary effects, reactive flows, deformable porous media, biomedical applications, and mechanics of the porous substrate. ***Special Topics & Reviews in Porous Media*** presents research on special topics and reviews covering a wide range of fields related to porous media.

Wang joined LANL in 2008 as an Oppenheimer Fellow. He studies multiscale multiphase and multiphysiochemical transport in porous materials, interfacial and electrokinetic transport in microfluidics and nanofluidics, and renewable energy and thermophysics. His computational capabilities include Molecular Dynamics (MD), Monte Carlo (MC), Lattice Boltzmann method (LBM), and various continuum scale simulation methods. Wang has authored more than 80 publications.

HIGH PERFORMANCE COMPUTING

Sparse Matrix-Vector Multiplication on a reconfigurable supercomputer

Sparse Matrix-Vector Multiplication (SMVM) is a critical computational kernel used in iterative solvers for systems of sparse linear equations. The poor data locality exhibited by sparse matrices along with the high memory bandwidth requirements of SMVM result in poor performance on general-purpose processors. Field Programmable Gate Arrays (FPGAs) offer a possible alternative with their customizable and application-targeted memory sub-system and processing elements. High Performance Computing Systems Integration (HPC-5) researchers David DuBois, Andrew DuBois, Mike Boorman, and Carolyn Connor; and collaborator Steve Poole (Oak Ridge National Laboratory) investigated two separate implementations of the SMVM on an SRC-6 MAPStation workstation. They revealed the potential of a co-design approach. The first implementation investigated peak performance capability, while the second balanced the amount of instantiated logic with the available sustained bandwidth of the FPGA subsystem. Both implementations yield the same sustained performance, and the second produces a much more efficient solution. The scientists demonstrated a fully implemented non-preconditioned Conjugate Gradient Algorithm utilizing the second SMVM design. The results show that large (high matrix rank) SMVM problems can be computed effectively on FPGA devices and that the projected



improvements in clock rate and bandwidth provided by the next generation SRC-7 have potential for significant performance improvement (Figure 2). An FPGA-based system can perform on par with today's processors despite running over 30 times slower (i.e., 100 MHz vs. 3.4 GHz). The FPGA-enhanced system enables designs that more optimally match the computational units to available memory bandwidth, providing a more balanced system. Reference: "Sparse Matrix-Vector Multiplication on a Reconfigurable Supercomputer with Application", ***Association for Computing Machinery (ACM) Transactions on Reconfigurable Technology and Systems 3***, No. 1, Article 2, published January 2010: doi: 10.1145/1661438.1661440.

Figure 2. Performance comparison for Sparse Matrix-Vector Multiplication on a banded matrix implemented across a variety of architectures, including standard processor technology (2.6 GHz Opteron Dual Socket, Single Core, MSC compiler and 3.4 GHz Xeon EM64T, Intel C++ 8.1 compiler), an SRC FPGA-based reconfigurable supercomputer, and an SRC-7 FPGA-based reconfigurable supercomputer (theoretical result based upon projected improvements in clock rate and bandwidth).

MATERIALS PHYSICS AND APPLICATIONS

Multipurpose acoustic sensor for downhole fluid monitoring of geothermal reservoirs

Cristian Pantea, Dipen Sinha, and Blake Sturtevant (Sensors and Electrochemical Devices Group, MPA-11) gave a presentation on their geothermal project for the New Mexico Office of Recovery and Reinvestment leaders visiting LANL. The scientists explained the concept behind an American Recovery and Reinvestment Act (AARA) project that could improve Enhanced Geothermal Systems (EGS). In this new type of geothermal power technology, high pressure cold water is pumped down an injection well into rock. The injection increases the fluid pressure in the naturally fractured rock, enhancing the permeability of the fracture system. Water travels through fractures in the rock, capturing the heat of the rock until it is forced out of a second borehole as very hot water, which can be used to generate electricity. The water, now cooled, is injected back into the ground to heat again in a closed loop (Figure 3). The technology could produce power 24 hours a day, as does a fossil fuel power plant.

The high pressures and temperatures in Enhanced Geothermal Systems reservoirs require specialized materials for the down-hole sensor package, starting from the active part of the sensor and ending with communication cables. The team plans to use sound waves as the basis for a sensor package that could operate at very high temperatures and pressures to provide real-time data about temperature, pressure, flow rate, salinity, and other properties of fluids within geothermal reservoirs. This information could help determine the best locations for potential geothermal reservoirs or how to maximize heat production from them for increased efficiency and cost effectiveness. The researchers are developing a multipurpose acoustic sensor to use at depths of several thousand feet, pressures up to 220 bar, temperatures up to 374ºC, and in a very corrosive environment.

Science Highlights (042110)

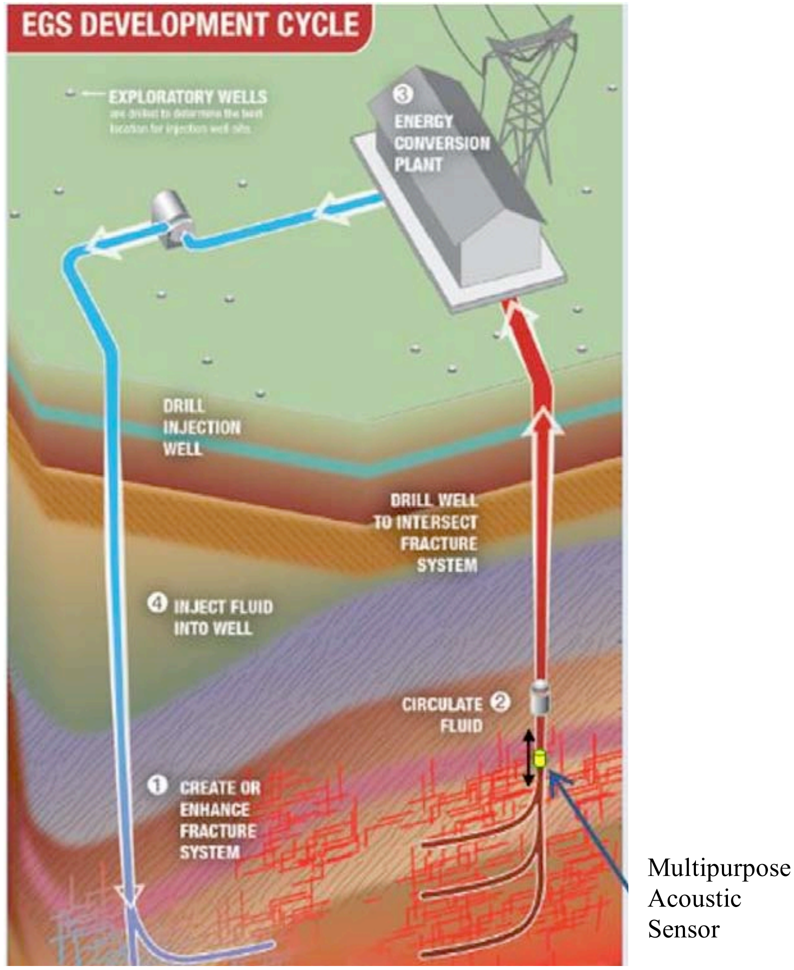


Figure 3. Schematic representation of an Enhanced Geothermal System.

The scientists used the resonance of a piezoelectric crystal for a novel solution to the problem of accurate, repeatable down-hole temperature determination. They found that lower vibrational modes of the crystal provide a reliable temperature determination. The team obtained very good sensitivity of frequency variation as a function of temperature of 83 ppm/deg in the crystal (Figure 4). There is no hysteresis between the heating and cooling cycle. With appropriate calibration, the temperature of the reservoir can be precisely determined. This new approach can be used for an inexpensive and reliable temperature sensor for harsh environments in general and down-hole measurements in particular. The American Recovery and Reinvestment Act funds the DOE Energy Efficiency and Renewable Energy project. Technical contacts: *Cristian Pantea and Dipen Sinha*

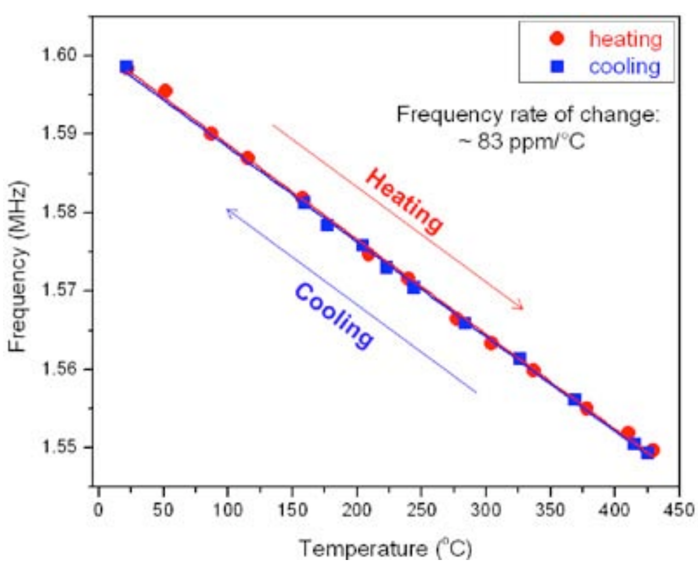


Figure 4. Temperature determination from a lower frequency vibrational mode (1.6 MHz).

MATERIALS SCIENCE AND TECHNOLOGY

Advanced strain diagnostics applied to PBX 9501 high explosive

Digital Image Correlation (DIC) is a high fidelity, non-contact strain measurement technique that relies on a computer vision approach to extract whole-field displacement data (both 2D and 3D) by comparing features in a pair of digital images of the specimen surface before and after deformation. It is a surface diagnostic constrained by surface conditions and camera/optical capabilities. Researchers used the digital image correlation technique for simultaneous measurements with embedded strain sensors during uniaxial tension and compression of PBX 9501 high explosives. The purpose of these tests was to determine the impact of embedded fiber-optic strain sensors on structural integrity under various testing conditions and the fidelity and uncertainties of these measurements compared to DIC and conventional extensometer displacement gages.

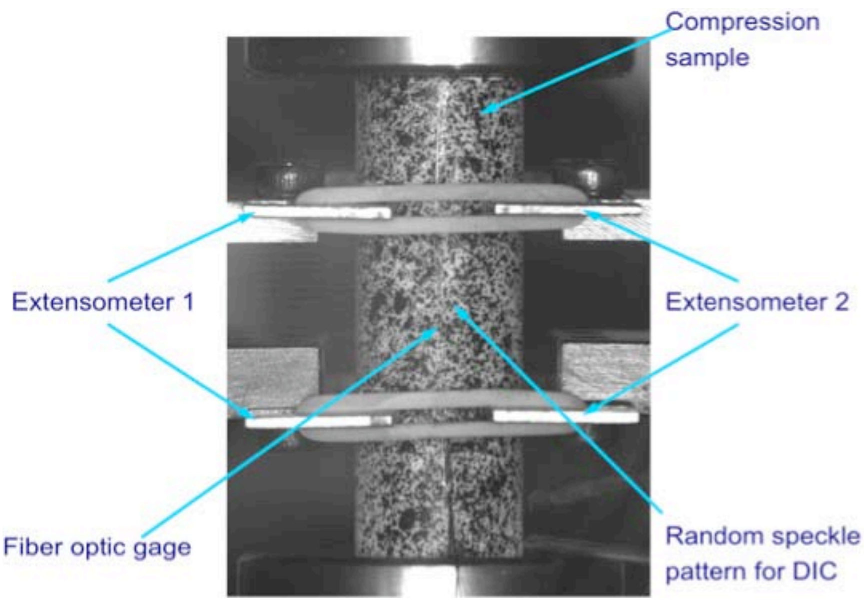


Figure 5. Compression sample of PBX 9501 showing the fiber-optic sensor along the loading axis and the random speckle pattern for DIC measurement. Conventional extensometers are used for comparison.

Fiber-optic strain and displacement sensors are state-of-the-art fiber-based devices designed to sense mechanical strain, displacement, and temperature. The general principle of such devices is that light from a laser is sent through an optical fiber, experiences subtle parameter changes either in the fiber or in one or several fiber Bragg gratings, and then reaches a detector arrangement that measures these changes. Fiber-optic sensors are embedded in structures to remotely monitor the health and integrity of the structure over long periods of time in harsh environments and extreme applications, such as high explosives. Cheng Liu and Manuel Lovato (Structure/Property Relations, MST-8), Anthony Puckett (Advanced Engineering Analysis, W-13), Darla Thompson and Racci DeLuca (High Explosive Science and Technology, DE-1) performed the work for the High Explosive Assembly Stress State Characterization project. Campaign 6, the Enhanced Surveillance Campaign, and the DOE/DoD Joint Munitions Program funded the work. Technical contact: *Cheng Liu*

PHYSICS

Gamma-ray physics studies at Duke University

The Gamma Reaction History Team had a highly successful, 2-week run characterizing their Inertial Confinement Fusion (ICF) gamma-ray detectors and exploring relevant gamma-ray physics at Duke University's High Intensity Gamma Ray Source (HIgS). The HIgS provided a well characterized, 1 cm diameter pencil beam of gamma rays at flux levels of several 10^7 gammas/sec and three different beam energies (4.4, 10.0, and 16.8 MeV). The scientists chose the upper beam energy to match the primary line of the deuterium-tritium (DT) fusion reaction at 16.75 MeV. A well-calibrated detector response at this energy will enable more accurate DT yield measurements than was previously possible. The lower beam energy will help diagnose implosion efficiency, and an intermediate energy of 10 MeV will further characterize the detector from which to validate codes. Recent upgrades to the facility have made it possible to run two detectors simultaneously – the NIF Gamma Reaction History diagnostic (GRH-6m) and the OMEGA Gas Cherenkov Detector (GCD-1). The scientists performed scans in beam position and Cherenkov threshold energy (i.e., gas pressure) for sulfur hexafluoride and carbon dioxide gases and various shielding configurations.

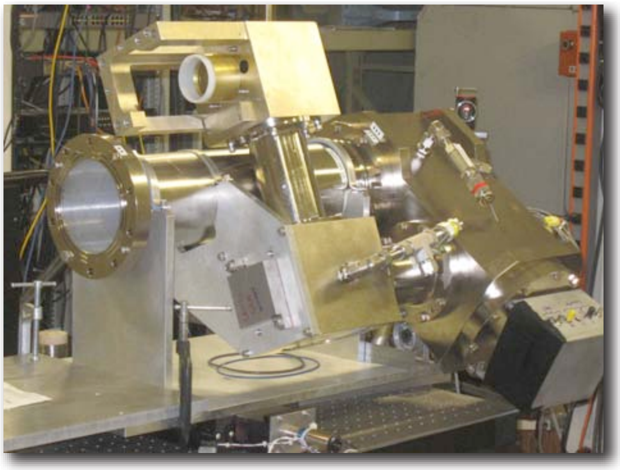


Photo: GRH-6m installed in the upper target room.

The researchers conducted measurements for the first time in a temporally-resolved, single-photon counting mode. This enabled them to characterize detector performance to unprecedented levels. The information will shed light on physics issues, such as below-threshold detector response, and will enable evaluation of interference from scattered radiation. Counting will enable separate measurements of the individual conversion efficiencies for gamma-to-electron and electron-to-photon conversions for a better assessment of shot noise statistics. The scientists collected previously unmeasured band parameters, such as temporal bunch width. The on-site, multi-institutional team consisted of Hans Herrmann (Principal Associate Directorate Weapons Programs, PADWP), Joe Mack, Yongho Kim, Carl Young, Steve Caldwell, Aaron McEvoy, Scott Evans, and Tom Sedillo (Plasma Physics, P-24); Wolfgang Stoeffl (Lawrence Livermore National Laboratory); and Elliot Grafil (Colorado School of the Mines).

THEORETICAL

Initial growth rate of HIV during primary infection

Early HIV infection can be seen as a race between the immune system and the virus. Understanding the kinetics of primary infection and its effect on the establishment of chronic infection is important for understanding the early pathogenesis of HIV and developing an effective vaccine. However, there are little data on the very earliest stages of disease before symptoms appear.

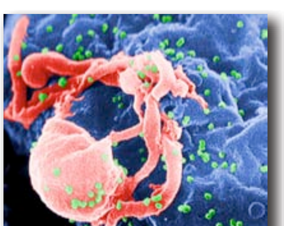
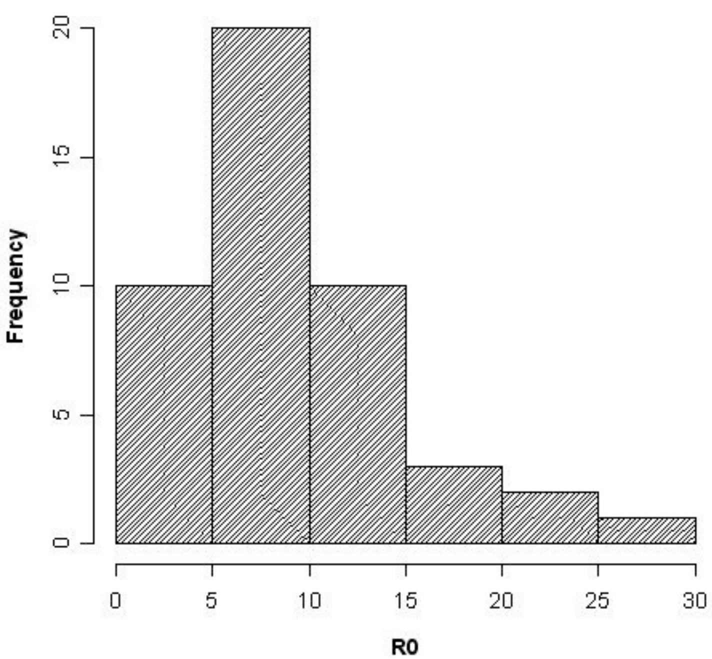


Photo. Scanning electron micrograph of HIV-1 (green) on the surface of a lymphocyte (T-cell/white blood cell). Round bumps on cell surface represent sites of assembly and budding of virions. Photo credit: CDC Public Health Image Library (C. Goldsmith, P. Feorino, E.L. Palmer, W.R. McManus)

Ruy Ribeiro, Leslie Chavez and Alan Perelson (Theoretical Biology and Biophysics group, T-6) and collaborators at the Statistical Center for HIV/AIDS Research and Prevention, Seattle, WA characterized the early events in infection and the pre-peak expansion of HIV-1 to better understand the biology of infection. The researchers studied a unique dataset of 47 subjects infected with HIV, who were identified through plasma donation screening. The subjects were frequent plasma donors who became HIV positive during the course of their plasma donations. These patients were identified very early in infection, and constitute the best set of patient data for the early events in infection.

From these data, the scientists measured the rate of viral expansion during primary HIV infection. The researchers calculated how fast the viral load increases and how variable this parameter is among individuals. They also estimated the basic reproductive ratio, *R*o, the number of new infected cells generated by an infectious cell at the start of infection when target cells are not limiting viral growth. Ro is a measure of whether a virus can establish infection. If *R*o is less than one, on average an infected cell infects less than one susceptible cell, and the infection will die out. If *R*o is greater than one, on average an infected cell infects more than one susceptible cell, and generally the infection will spread.



The researchers determined that the initial viral doubling time has a median of 0.65 days, leading to an estimated median basic reproductive ratio, *R*o, of 8.8. Their results also show how variable *R*o is in the human population (Figure 6). Seventy-five percent of the individuals in the sample had a value of *R*o less than 11, but a few individuals had a basic reproductive ratio larger than 20. These results indicate that a reduction in *R*o of 10 to 20-fold, such as by vaccine induced immunity, could drive *R*o below one and lead to prevention of HIV infection in a majority of HIV-exposed individuals. Thus, in order to prevent chronic infection in a majority of patients, an early infection intervention, such as a vaccine, must be about 90% effective in reducing viral growth.

Figure 6. Histogram of the distribution of *R*o found for 47 patients infected with HIV-1

These results characterize the early plasma viral dynamics in acute HIV infection better than had been possible previously. They also clarify the challenge that the immune response (or therapeutic intervention) must overcome to defeat HIV at this early stage before it becomes a chronic infection. This sets a standard for what any intervention (vaccine or treatment) must do to prevent spread of the virus within an infected person. The improved knowledge of the very early expansion of HIV-1 will be beneficial for our understanding of primary infection, and its effect in the establishment of chronic infection. Moreover, if the immune system primed by a vaccine could respond quickly enough to HIV, it might be possible to prevent infection. Reference: "Estimation of the Initial Viral Growth Rate and the Basic Reproductive Number during Acute HIV-1 Infection", published ahead of print in the ***Journal of Virology*** (31 March 2010); doi: 10.1128/JVI.00127-10. The National Institutes of Health supported the research.