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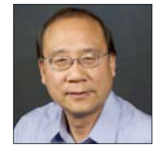

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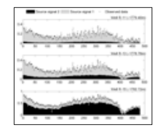

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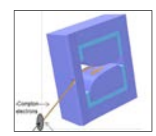

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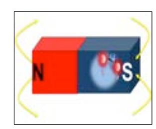


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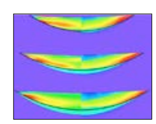

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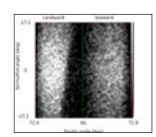

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LALP 14-001

# SCIENCE HIGHLIGHTS November 12, 2014

## AWARDS AND RECOGNITIONS

### Dee Magnoni honored with SLA Special Recognition Award

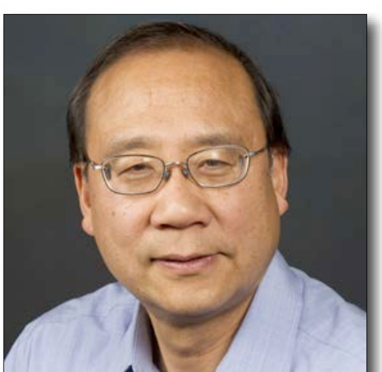
The SLA has selected Dee Magnoni (Research Library, SRO-RL) to receive the SLA New England Chapter's 2014 Special Recognition Award. The award is given to a longstanding chapter member who has made a tremendous impact at the chapter and association levels. Magnoni has held leadership positions across SLA, serving on the Board of Directors and as President of the New England and Rhode Island Chapters; chairing the Leadership & Management Division, the Engineering and Information Technology Divisions, and the 2014 Conference in Vancouver, B.C. She has been involved with local and international mentoring programs and competency initiatives.

Magnoni has a master's degree in library science from the State University of New York – Albany. She served as the first library director at Olin College of Engineering in Needham, MA. Magnoni developed many of their library services to integrate library services into institutional practices and make library resources accessible to users. She joined LANL in January 2014 as the Research Library director. Magnoni oversees the Lab's work in applied information science research and the development of digital library applications.

Magnoni is a Fellow of the SLA (Special Library Association). Other awards include the SLA Rose Vormelker Award for mentoring and the SLA Factiva Leadership Award for work on Competencies for Information Professionals.

SLA is a nonprofit international organization for information professionals and their strategic partners. SLA serves information professionals in more than 60 countries and in a range of working environments, including business, academia and government agencies. Technical contact: *Dee Magnoni*

### Michael Hamada gives plenary talk accepting Gerald J. Hahn Award



Michael Hamada (Statistical Sciences, CCS-6) gave one of two plenary talks at the 58th Fall Technical Conference in Richmond, VA as the first recipient of the Gerald J. Hahn Quality and Productivity Achievement Award from the American Statistical Association (ASA). The Quality and Productivity Section of the ASA presents the award to recognize an individual who has demonstrated outstanding and sustained achievement and leadership in developing, promoting and successfully improving the quality and productivity of products and organizational performance using statistical concepts and methods over a period of 20 or more years.

His talk titled “The Elegance of Statistics for Analyzing Data in a Complex World” presents how statistics, as a science, provides theory (and thinking) and methods for analyzing complex data. Statistics can be used properly to account for the form of the data and how they were collected in analyzing them. Five examples based on Hamada’s publications illustrated the elegance and flexibility of statistics for analyzing complex data that combine multiple information sources, account for measurement error, and handle biases arising from the collection process.

Hamada presented the examples in the context of a general work process that he has developed over a career since earning his Ph.D. at the University of Wisconsin-Madison in 1987 and has honed since joining LANL in 1998. He works in the NNSA Core Surveillance Program at LANL where such scientific challenges arise in analyzing data collected by this program. Hamada conducts uncertainty quantification for many applications across LANL. NNSA Directed Stockpile Work sponsored his research, which supports the Lab’s Nuclear Deterrence mission area and the Information, Science, and Technology science pillar.

Recent publications:

- “The Analysis of Misclassified Ordinal Data from Designed Experiments,” ***Quality and Reliability Engineering International*** (2014); doi: 10.1002/qre.1743. Authors are M. S. Hamada (CCS-6) and K. J. Ryan (West Virginia University).
- “Analyzing Deficient Response Summaries from Designed Experiments,” ***Quality Engineering*** *26*, 440 (2014). Researchers include M. S. Hamada (CCS-6) and R. L. Warr (Air Force Institute of Technology).
- “Accounting for Nonrandom Sampling in Nonlinear Regression,” ***Quality Engineering***, in press (2014). Authors are Richard P. Picard, M. S. Hamada, and Geralyn M. Hemphill (CCS-6); and Robert E. Hackenberg (Metallurgy, MST-6).

The American Statistical Association is the world’s largest community of statisticians. Its members serve in industry, government and academia in more than 90 countries, advancing research and promoting sound statistical practice to inform public policy and improve human welfare. Technical contact: *Michael Hamada*

## CHEMISTRY

### Development of rubidium-metal targets for enhanced production of strontium-82

LANL regularly produces strontium-82 ($^{82}$Sr) under the direction of DOE Office of Science – Office of Nuclear Physics and the National Isotope Development Center (NIDC) to generate the Positron Emission Tomography (PET) isotope rubidium-82 ($^{82}$Rb). This isotope is used in myocardial perfusion studies for cardiac imaging via a $^{82}$Sr/$^{82}$Rb generator. Tens of thousands of patients have this procedure each month. Several potential nuclear routes for producing $^{82}$Sr are possible, as shown in Table 1.

**Table 1. Possible Target Materials, Reactions, and Energy Ranges for Sr-82 Production**

| **Reaction** | **Target** | **Projectile Energy (MeV)** |
|---|---|---|
| Y(p, spallation) | Y-oxide | 60-240 |
| Mo(p, spallation) | Mo-metal | 500, 800 |
| Rb(p,xn) | RbCl or Rb-metal | 40-90 |
| Kr($\alpha$, pxn) | Kr gas | 20-120 |

The Mo(p,spall) and Rb(p,xn) routes have been used for large scale production with recent focus on the $^{nat}$Rb(p,xn)$^{82}$Sr reaction at the LANL Isotope Production Facility (IPF) and at the Brookhaven National Laboratory LINAC Isotope Producer (BLIP) by taking advantage of the intermediate energy proton beams at each site. Since the IPF's commissioning in 2004, rubidium chloride (RbCl) has been the target material of choice due to its availability as a very high purity salt and its ease of handling relative to Rb-metal (which reacts violently with water). However, several facilities including the Institute of Nuclear Research (INR, Russia), iThemba (South Africa) and TRIUMF (Canada) have safely irradiated Rb-metal targets for the purpose of $^{82}$Sr production for decades.

RbCl salt targets display poor thermal conductivity (RbCl thermal conductivity is 7.6 $Wm^{-1}K^{-1}$), which limits the amount of proton beam power that can be deposited in the metal-clad production target. Until recently, this thermal performance limitation did not present an issue from a $^{82}$Sr supply perspective. However, a steady increase in demand for $^{82}$Sr has encouraged the re-evaluation of Rb-metal as a target material for its enhanced thermal performance (Rb metal thermal conductivity is 58.2 $Wm^{-1}K^{-1}$) and for its anticipated enhanced $^{82}$Sr yield potential.

Therefore, IPF staff performed yield calculations using the International Atomic Energy Agency (IAEA) recommended nuclear cross sections and Andersen and Ziegler stopping formalisms for RbCl and Rb-metal target materials in a proton energy window of 92-44 MeV. These initial calculations suggested that a practical yield multiplier (independent of beam power) of ~ 1.4 could be realized upon switching to Rb-metal. This promising, preliminary analysis led to proof of concept target production aimed at establishing target design, target fabrication methods, safety protocols, and validation of $^{82}$Sr production yields. Researchers irradiated two prototype targets in January 2014 to build practical experience with these new target designs. The team performed radiochemical separation of one target to yield finished $^{82}$Sr product. Final batch analysis validated the projected increase in yield compared with that obtained from RbCl targets and provided product of sufficient quality to warrant additional effort aimed at production scale-up. Several "proto-production" runs are tentatively scheduled for the 2014-2015 IPF production period.

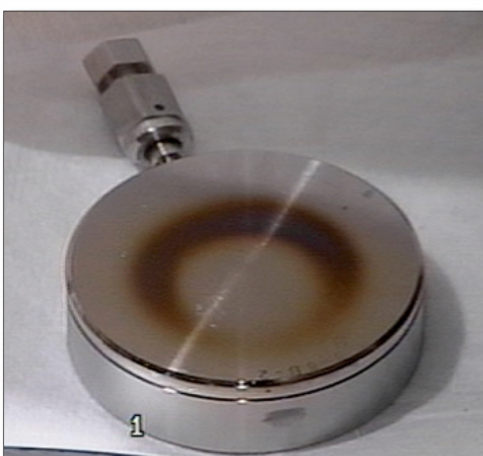



Photo. Prototype Rb-metal target irradiated at 230 microAmps. The impact of the IPF proton beam caused the dark ring. Rastering the beam in a circle on the target distributes the energy from the protons into a greater target area. Successful irradiation at IPF suggests that even higher beam currents could be used with this design to enhance yield.

Los Alamos Isotope Production staff performed the research (Meiring Nortier, team leader and Eva Birnbaum, program manager). The DOE Office of Science – Office of Nuclear Physics funded the work, which supports the Lab's Energy Security and Global Security mission areas and the Nuclear and Particle Futures and Materials for the Future science pillars. Technical contact: *Meiring Nortier*

## EARTH AND ENVIRONMENTAL SCIENCES

### Identification of physical source separation for groundwater pressure analysis

The identification of the physical sources causing spatial and temporal fluctuations of aquifer water levels is a challenging, yet a very important hydrogeological task. Variations in natural and anthropogenic sources cause the fluctuations. The source identification can be crucial for conceptualization of the hydrogeological conditions and characterization of aquifer properties. Boian Alexandrov (Physics and Chemistry of Materials, T-1) and Velimir Vesselinov (Computational Earth Science, EES-16) developed a new computational framework for model-free inverse analysis of pressure transients. The journal ***Water Resources Research*** published the research.

The framework is based on a Non-negative Matrix Factorization (NMF) method for Blind Source Separation (BSS) coupled with k-means clustering algorithm, called NMFk. The NMFk algorithm can distinguish a set of unique sources from a set of experimentally measured mixed signals without any information about the sources, their transients, and the physical mechanisms and properties controlling the signal propagation through the subsurface flow medium. The NMFk analysis only requires information about pressure transients at a number of observation points, m, where $m \geq r$, and r is the number of unknown unique sources causing the observed fluctuations. This new method identifies the physical sources causing spatial and temporal fluctuations in state variables.


The authors demonstrated an NMFk analysis on a water-level dataset from the Los Alamos National Laboratory site. They analyzed water-level data collected at four monitoring wells within the regional aquifer beneath LANL. Water-supply pumping wells surround these monitoring wells. The NMFk methodology determined the influence of water supply pumping on the observed pressures at the wells (Figure 2). The methodology also extracted the barometric pressure effects on the observed water levels (Figure 3).

Figure 1. Yellow dots represent the four regional wells that were analyzed in this study. Green dots depict surrounding/nearby monitoring wells.

The possible applications of the NMFk algorithm are not limited to hydrogeology problems. A classical Blind Source Separation conundrum is the so-called "cocktail-party" problem where several microphones are recording all the sounds in a room (e.g., music, conversations, noise, etc.). Each of the microphones records a mixture of the available sounds, and each sound is recorded with a different amplitude that depends on many factors including the distance from the sound source to the microphones. To be able to "unmix" and reconstruct the original sound sources (melodies, voices, etc.) from the records, a BSS algorithm is needed to obtain the best possible extraction of the original source signals from the mixtures. As a result, the Blind Source Separation algorithms as NMFk reveal hidden features and dependencies in large sets of observed data. Based on these features, the method can build a representation of the data that could contribute to understanding the physical mechanisms behind these data. NMFk can be applied to any problem where temporal system behavior is observed at multiple locations and an unknown number of physical sources cause these fluctuations. Such problems can be related to important aspects of national security including energy and water production, carbon capture and sequestration, waste disposition and storage, and restoration of contaminated sites.

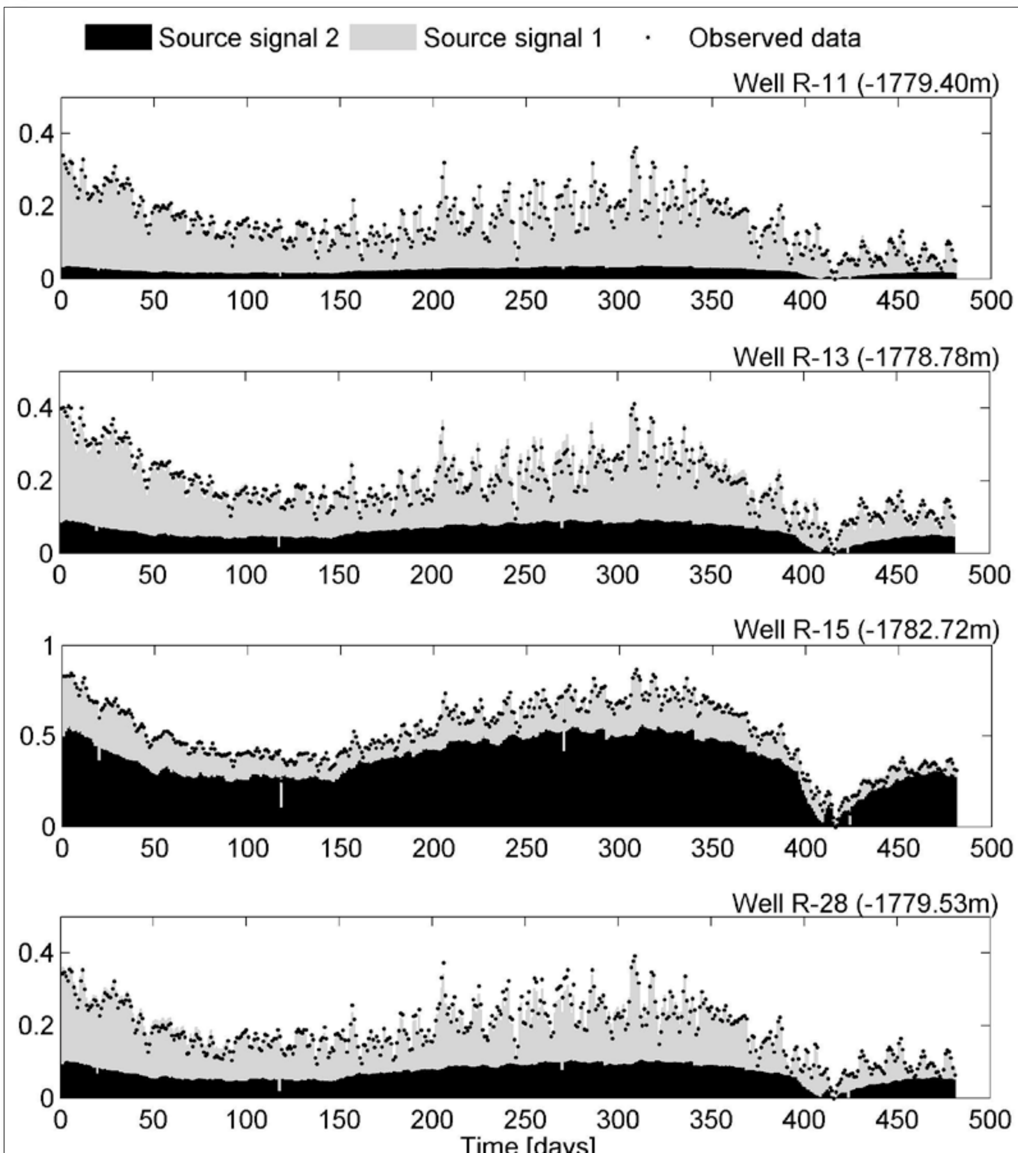



Figure 2. Reconstruction of the observed pressure transients by the two identified source signals.

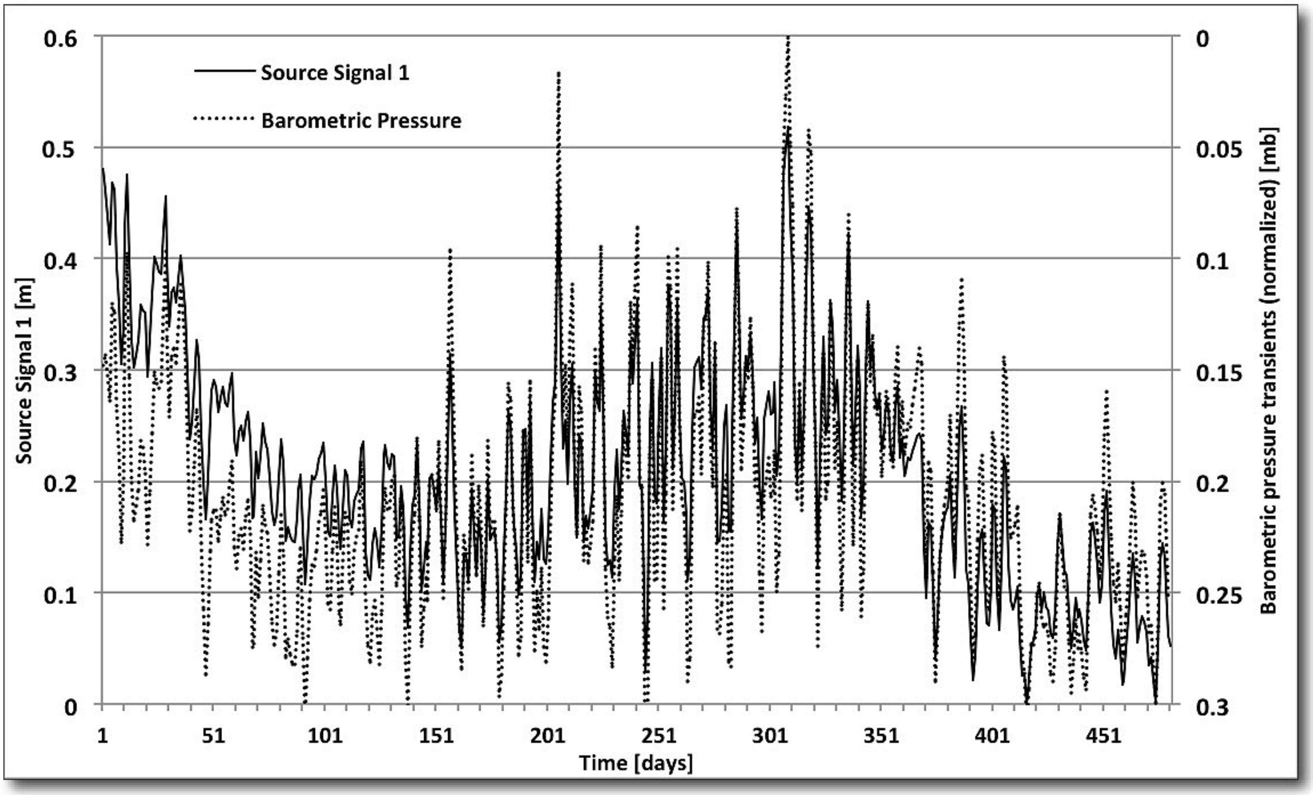



Figure 3. Comparison between the first reconstructed source signal and measured barometric pressure fluctuations at the LANL site (note that the right axis is reversed).

Reference: "Blind Source Separation for Groundwater Pressure Analysis Based on Nonnegative Matrix Factorization," ***Water Resources Research*** *50*, 7332 (2014); doi: 10.1002/2013WR015037. Authors include Boian S. Alexandrov (Physics and Chemistry of Materials, T-1) and Velimir V. Vesselinov (Computational Earth Science, EES-16).

DOE Environmental Management and LANL Environmental Programs sponsored the work, which supports the Lab's mission areas and the Information, Science, and Technology science pillars. Technical contact: *Velimir V. Vesselinov*

## ENHANCED CAPABILITIES

**First nuclear material operations at the Radiological Laboratory Utility Office Building**

The TA-55 Radiological Laboratory Utility Office Building (RLUOB) received its first-ever shipment of nuclear material and distributed it to analytical chemistry laboratories on August 28, 2014. This shipment, a result of cooperation between the Actinide Analytical Chemistry Group (C-AAC), TA-55 Facility Operations, and Hazardous Materials Management (NPI-7), marked the formal commencement of Radiological Operations in the recently constructed RLUOB. On September 3, workers extended the nuclear material transfer capabilities further with the first demonstration of a small-sample hand-carry procedure between the PF-4 Plutonium Facility and the RLUOB laboratories. The Nuclear Materials Science Group (MST-16) assisted in the development of this hand-carry process for dissolved chemistry samples originating in PF-4. The hand-carry

process will be crucial for implementing the future analytical chemistry workflow that spans the two facilities.

Photo. Andres Borrego (C-AAC) verifies nuclear material in a RULOB laboratory.

Once fully outfitted, RLUOB is a radiological facility that will replace most of the capabilities for analytical chemistry and materials characterization that have historically been located in the aging Chemistry and Metallurgy Research (CMR) nuclear facility. Currently, RLUOB houses three C-AAC core technical capabilities: radiochemistry, trace element analysis, and mass spectrometry for actinides and gases. The implementation of Radiological Operations mode will allow the chemists to fully validate their sample preparation and instrumental analysis methods for determining chemical and isotopic compositions of nuclear materials, such as plutonium and uranium metals and oxides, for a diverse suite of Weapons Program and Global Security sponsors. More information: http://www.lanl.gov/about/_assets/docs/fact-sheets/RLUOB1.pdf

The NNSA Defense Programs Plutonium Strategy Initiative (Brian Colby, LANL program manager) funded the startup of RLUOB laboratories. The capability supports the Lab's Nuclear Deterrence and Global Security mission areas and the Science of Signatures and Materials for the Future science pillars. Technical contact: *Alice Slemmons*

**Gamma-detection instrument yields better fusion energy measurements**
Plasma Physics (P-24) staff designed, engineered, and fabricated core parts of the newest gas Cherenkov detector (GCD-3). The detector records gamma reaction history measurements during inertial confinement fusion implosions (ICF) – important details for understanding the fusion process. The researchers successfully fielded the GCD-3 on the Omega laser at the University of Rochester in New York. They operated the detector at 400 psia of carbon dioxide (3 MeV threshold) to measure the 5.5-MeV gamma rays resulting from proton + deuteron (H + D) fusion as part of the nuclear-astrophysics collaboration with the Massachusetts Institute of Technology. This fusion reaction, which produces helium-3, is the second step in the solar proton-proton fusion chain, and is of significance in brown dwarfs and proto-stars as well as models of Big Bang Nucleosynthesis.

The Cherenkov response is consistent with computer simulation predictions using Monte Carlo methods in the (Geant4) GEometry And Tracking platform (Mike Rubery, Atomic Weapons Establishment). This result indicates that the instrument has a higher-sensitivity, lower-energy-threshold gamma ray detection than expected, opening a new window for gamma ray spectroscopy to investigate inertial confinement fusion.

The heart of the new detector system, also known as the "SUPER GCD," is an American Society of Mechanical Engineers (ASME) code-stamped pressure vessel designed by the P-24 Diagnostic and Systems Engineering Team and fabricated and tested per the requirements of the ASME Boiler and Pressure Vessel Code, Section VIII, Division 1 by Meyer Tool & Manufacturing Inc.

The internal light collection components mimic the design of a Cassegrain telescope. P-24's years of experience fielding previous Cherenkov detectors have enabled the researchers to optimize the detector. The system also contains a pressure distribution system to supply pressure to three detector systems and one Gamma Reaction History system simultaneously. The P-24 team and SwageLok Southwest of Albuquerque, NM designed the LaCave manifold panel and target bay portable manifolds.


Photos. (Left): GCD-3 pressure vessel prior to insertion in an OMEGA Ten Inch Manipulator for diagnostic insertion into the OMEGA target chamber. (Right): Gas panel manifold mounted in the diagnostics basement under the target chamber (LaCave) to enable remote pressurization of the detector and the Gamma Ray History system. The new gas detector is can be pressurized to 400 psia, providing Cherenkov thresholds as low as 1.8 MeV. The vessel is approximately 1 meter long. (Photos courtesy of Eugene Kowaluk, University of Rochester)

For the Omega laser experiments, the detector acquired fusion gamma signals, backed up by control implosions of molecular deuterium ($D_2$) and molecular hydrogen ($H_2$) and simultaneous detector measurements at 6.3 MeV threshold. These measurements demonstrated that the scientists are observing 5.5 MeV H + D fusion gammas. Alex Zylstra (Massachusetts Institute of Technology), the principal investigator for these experiments, obtained excellent quality data to support the Stellar and Big Bang Nucleosynthesis portion of his Ph.D. thesis.

Further qualifications will be required to allow operation with hexafluoroethane ($C_2F_6$), which will enable thresholds down to approximately 1.8 MeV. An investigation of $^{13}$C(n,n'g) vs $^{12}$C(n,n'g) using carbon-powder-pucks near deuterium-tritium implosions will be conducted as a feasibility study for possible "dark mix" studies at the National Ignition Facility (NIF) at Lawrence Livermore National Laboratory. This investigation will allow fusion researchers to see a deleterious mix of plastic or diamond ablator material into the hot spot of ignition capsules that cannot be diagnosed by other techniques that rely on such mix to heat the carbon, which radiates x-rays. These new results bode well for those experiments.

The newest gas Cherenkov detector has been a two-year project led by principal investigator Hans Herrmann and project manager John Oertel. The P-24 Diagnostic and Systems Engineering Team consisted of electrical/mechanical technicians Tom Archuleta, Robert Aragonez and Tom Sedillo, mechanical design engineer Valerie Fatherley, electrical engineer Albert Hsu, and pressure safety officer/mechanical engineering supervisor Frank Lopez.

The NNSA Inertial Confinement Fusion program (Campaign 10, Steve Batha, LANL program manager) funded the project. The work supports the Lab's Nuclear Deterrence and Energy Security mission areas and High Energy Density Physics and Fluid Dynamics (HEDPF) within the Nuclear and Particle Futures and the Science of Signatures science pillars. Technical contact: *Hans Herrmann*

**Compton spectrometer determines x-ray spectra of radiographic sources**

Flash radiography is a useful diagnostic, and other diagnostics are needed to characterize the energy spectra of the x-rays produced by flash radiographic sources. Researchers have proposed a Compton spectrometer to conduct these measurements at the Dual-Axis Radiographic Hydrodynamic Test Facility (DARHT) at LANL and the Radiographic Integrated Test Stand (RITS-6) at Sandia National Laboratories, among other locations. The device could aid in the analysis of images produced and the underlying physics of intense bursts of x-rays with doses of several hundred rad at 1 m. Los Alamos physicists and engineers, with National Security Technologies, re-commissioned a Compton spectrometer and conducted calibration experiments. ***Proceedings of the Society of Photo-Optical Instrumentation Engineers*** published the work.

The researchers used a Compton spectrometer, a 300-kg neodymium-iron magnet that Los Alamos scientists designed and constructed to measure spectra in the less than 1MeV to 20 MeV range. Compton spectrometer collimates the x-rays from a radiographic source into a narrow beam directed on a converter foil. The forward-selected Compton electrons that are ejected from the foil enter the magnetic field region of the spectrometer. The electrons are imaged on a focal plane, with their position determined as a function of their energy. Scientists then reconstruct the x-ray spectrum.

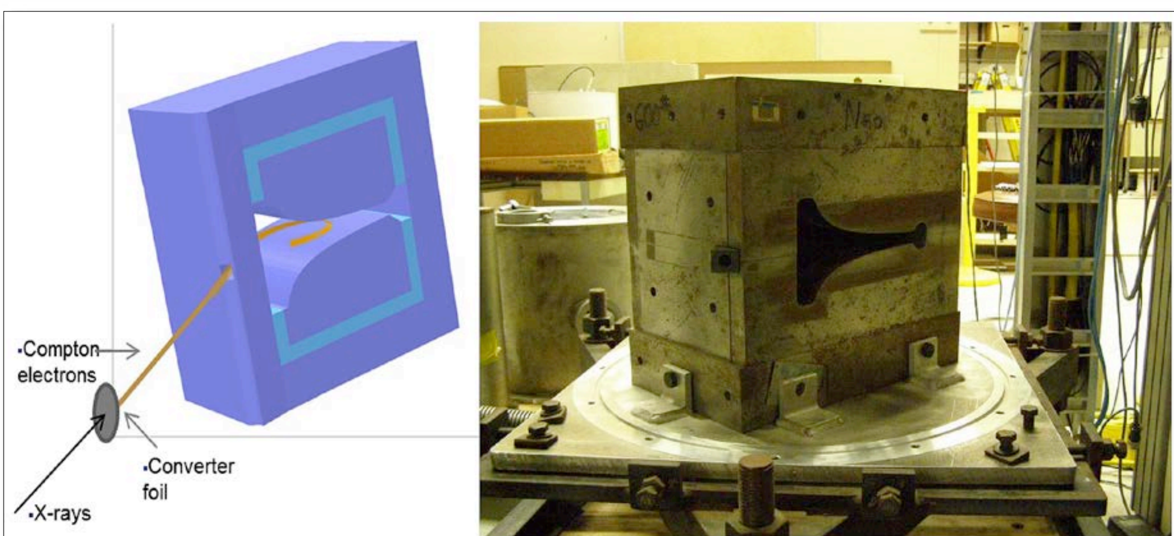



Figure 4. (*Left*): A schematic of the Compton spectrometer with x-ray and electron trajectories. (*Right*): A photograph of the Compton spectrometer.

The team made the first source measurements at the Microtron, a bremsstrahlung source at LANL that accelerates a continuous beam of electrons to 6, 10, 15, or 20 MeV. The electrons impinge upon a rotating target. The researchers plan more experiments at both DARHT and RITS-6. They are developing two detector systems: a time-integrated system that will consist of scintillator segments along the focal plane, and a time-resolved system with a target resolution of less than 2 ns.

Reference: "Determining X-ray Spectra of Radiographic Sources with a Compton Spectrometer," ***Proceedings of the Society of Photo-Optical Instrumentation Engineers*** (SPIE) 9215, Radiation Detectors: Systems and Applications XV, 921508 (September 4, 2014); doi:10.1117/12.2065588. Authors are Amanda E. Gehring, Todd J. Haines, Nick S. P. King, Frank E. Merrill, and George L. Morgan (Neutron Science and Technology, P-23); James F. Hunter (Applied Engineering Technology-6, AET-6); Michelle A. Espy, Robert Sedillo, Algis V. Urbaitis, and Petr Volegov (Applied Modern Physics, P-21); Manuel J. Manard and Rusty Trainham (National Security Technologies). David Barlow (RF Engineering, AOT-RFE) mapped the magnetic field of the spectrometer; John Stearns (AET-6) operated the Microtron; Samuel Gonzales and Timothy Dugan (Advanced Nuclear Technology, NEN-2) provided controlled the cobalt-60 (Co-60) source.

NNSA Campaign 3: Advanced Radiography and Transformational Technologies (Robert Reinovsky, LANL program manager) funded the work, which supports the Lab's Nuclear Deterrence mission area and the Nuclear and Particle Futures and Science of Signatures science pillars. Technical contact: *Amanda E. Gehring*

## MATERIALS PHYSICS AND APPLICATIONS: Road to MaRIE

### Materials-by-design effort aids search for abundant sources of non-rare-earth magnets

Magnets play a central role in a range of applications – from wind turbines to zero emission vehicles – at the heart of modern technology. Permanent magnetic materials are needed for power generation and energy conversion. Due to the scarcity of heavy, rare-earth elements that currently fill that demand, scientists are seeking plentiful, non-rare-earth replacements. To guide this search, scientists must develop theoretical methods that can estimate the magnetocrystalline anisotropy energy (MAE) of 3d, 4d, and 5d transition metals, which are the natural candidates to replace rare-earth elements. Researchers from Los Alamos and Argonne National Laboratory's Advanced Photon Source have combined theory and experiment to demonstrate a promising theoretical method for predicting an essential prerequisite to direct the search for these new materials. ***Physical Review X*** published the research.

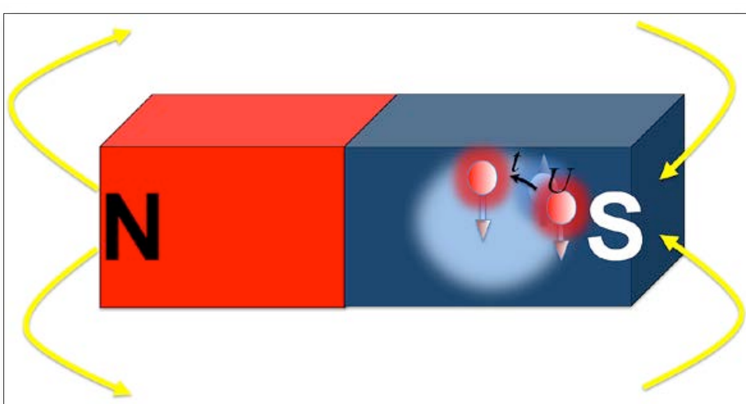



Figure 5. Schematic of a strong magnet. Alignment of electron magnetic moments produces ferromagnetism. The strong coercivity (resistance of a magnetic material to changes in magnetization) prevents the magnet from being easily

demagnetized. This property determines permanent magnets with north (N) and south (S) pole magnetic field lines. U is Coloumb interaction. As a measure of the coercivity, the magneto-crystalline anisotropy energy arises from the electron spin-orbit coupling. Electronic correlation also plays an important role.

In a first-time demonstration using the yttrium-cobalt compound $YCo_5$ as a prototype, the researchers proved that electronic correlations provide a significant role in determining the magnetocrystalline anisotropy of transition metals. Magnetocrystalline anisotropy is a key property that determines the performance of a permanent magnet. It locks the orientation of the magnetization (the axis that connects the north and south poles of a magnet) along a specific crystalline direction of the material. The magnet becomes "hard" when the magnetocrystalline anisotropy is high. The direction of magnetization remains unchanged when manipulated by external electromagnetic fields, which is critical for use in electric motors or generators.

The authors concluded that incorporating the local effects of electronic correlations through dynamical mean-field theory into the conventional band structure theory [local density approximation plus dynamical mean field theory (LDA+DMFT)] is key to enhanced predictive power. This new approach leads to reliable estimates of the orbital moment, out of which magnetic anisotropy arises. The researchers confirmed this calculation via x-ray circular magnetic dichroism (XMCD) measurements at the Advanced Photon Source. Their theoretical methods can estimate the electronic correlations and the magnetocrystalline anisotropy of materials containing 3d, 4d, and 5d transition metals, which are candidates to replace rare-earth elements in permanent magnets.

Reference: "LDA+DMFT Approach to Magnetocrystalline Anisotropy of Strong Magnets," ***Physical Review X*** *4*, 021027 (2014); doi: 10.1103/PhysRevX.4.021027. Authors include Jian-Xin Zhu and Cristian Batista (Physics of Condensed Matter and Complex Systems, T-4), Marc Janoschek, Filip Ronning, J.D. Thompson, Michael Torrez, and Eric Bauer (Condensed Matter and Magnet Science, MPA-CMMS), and Richard Rosenberg (Argonne National Laboratory).

This materials-by-design effort in support of discovering non-rare earth magnets aligns with grand challenges outlined by the DOE Office of Basic Energy Sciences and the Laboratory's Materials for the Future science pillar. This research is an example of science on the roadmap to MaRIE (Matter-Radiation Interactions in Extremes), LANL's proposed experimental facility that could be used to discover advanced materials needed to meet 21st century national security and energy security challenges. Using MaRIE's advanced capabilities, similar theory and experiment studies could further refine materials-by-design techniques such as the search for non-rare-earth magnets.

The Laboratory Directed Research and Development (LDRD) program funded the Los Alamos portion of the work, with some theoretical calculations performed at a Linux cluster in LANL's Center for Integrated Nanotechnologies (CINT), a DOE Office of Science, Basic Energy Sciences user facility. The research supports the Lab's Energy Security mission area and Materials for the Future science pillar. Technical contact: *Jianxin Zhu* (theory) and *Marc Janoschek* (experiment)

## MATERIALS SCIENCE AND TECHNOLOGY: Road to MaRIE

### Dynamic density field measurements of an explosively driven phase transition in iron

Iron is an important element because it is the major constituent in steel and in the Earth's core. Los Alamos researchers completed a novel experiment providing quantitative density and kinetic data for comparison with advanced physical/computational treatments, either existing or in development, of a first-order shock-induced phase transformation in iron. The ***Journal of Applied Physics*** published the findings.

Most studies of the α-ε phase transition have employed uniaxial shock wave loading. For a given material subjected to a uniaxial shock (plane, one-dimensional shock wave), the shear stress throughout both any elastic precursor and the plastic wave are uniquely related to the amplitude. This phase transition in iron has been well studied.

In this new work, Los Alamos researchers determined density distributions, dynamically measured at five times using the Dual Axis Radiographic Hydrodynamic Test Facility (DARHT) at LANL, of an iron sample undergoing the α-ε phase transition from loading induced by a detonation wave sweeping along one surface. This loading path differs from one-dimensional shock wave loading because there are regions of shear developed in the sample that are an evolving function of the obliquity with which the detonation wave interacts with the sample, and consequent shock and elastic wave reflections from the free surface of the iron.

The researchers measured shocked regions and boundaries, as well as regions and boundaries of elevated density (presumed to be the ε-phase iron). The experiments captured the formation and dynamics of these regions and made the data available for comparisons with material descriptions. The researchers also applied 16 photon Doppler velocimetry (PDV) probes to examine the free surface velocity along a discrete set of radially distributed points to compare and correlate the density measurements with previous shock wave studies. The velocimetry data are in nearly exact agreement with previous shock wave studies of the α-ε phase transition. The density distributions, while generally in agreement with expectations evolved from the shock wave studies, show for the first time quantitatively that the epsilon phase is generated in regions of high shear stress but at hydrostatic stresses below the typically quoted 13 GPa value. The density field measurements are particularly useful for observing the effects of the forward and reverse transformation kinetics, as well as the reverse transformation hysteresis that is not predicted in current multi-phase equation of states descriptions of iron.

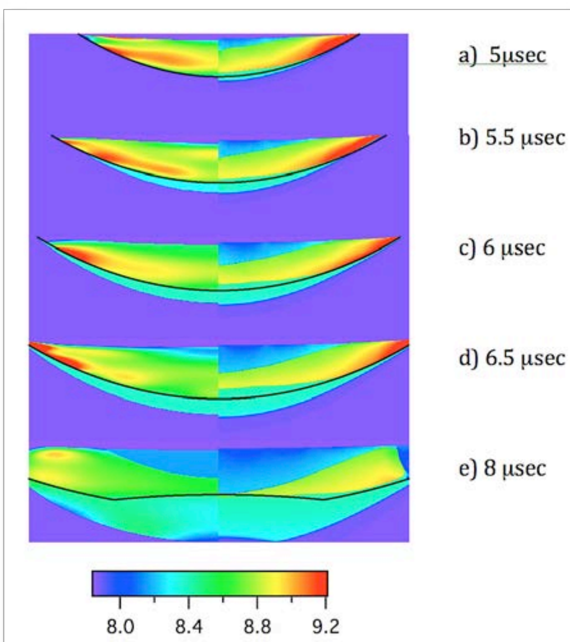



Figure 6. (*Left half*): The measured density data (g/cm$^3$) distributions at times relative to initiation of the explosive PBX 9501. (*Right half*): The calculated data.

Future facilities, such as MaRIE (Matter-Radiation Interactions in Extremes), could take this research into phase transition kinetics and the importance of stress-state on shock-induced transitions even further by facilitating direct coupling of the shock-induced transition microstructure with the initial starting material microstructure.

Reference: "Dynamic Density Field Measurements of an Explosively Driven $\alpha$-$\varepsilon$ Phase Transition in Iron," ***Journal of Applied Physics*** *116*, 043504 (2014). Authors include Larry Hull (Focused Experiments, WX-3), George T. (Rusty) Gray III (Materials Science in Radiation and Dynamics Extremes, MST-8), and Barry J. Warthen (DARHT Experiments and Diagnostics, WX-4).

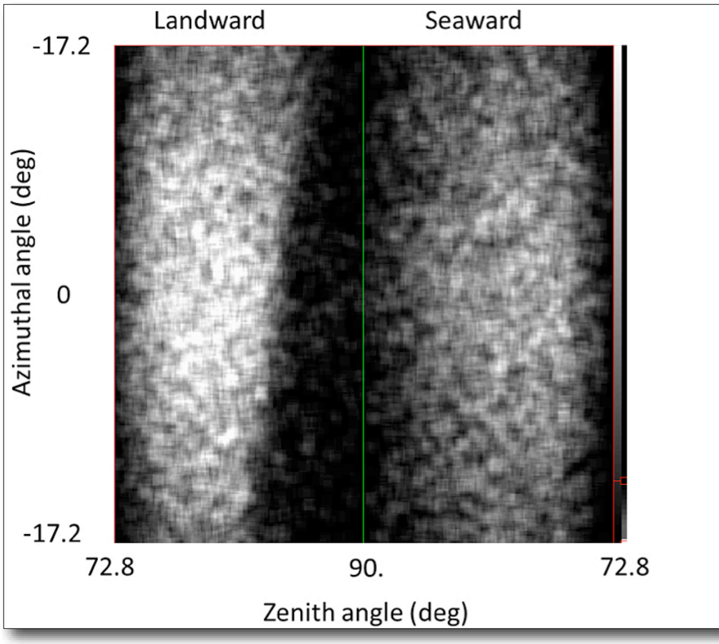
The execution of an experiment at a large facility such as DARHT necessarily involves large numbers of people and often their predecessors. Various funding sources are also involved. The researchers give special recognition to the accelerator and operations teams, the gamma ray camera team, the PDV team, and the mechanical design team, because each fine-tuned its respective contributions to make this particular experiment so successful. NNSA Science Campaign 2 (Rick Martineau, LANL program manager) and DoD/DOE Joint Munitions Program (Thomas Mason, LANL program manager) funded the work, which supports the Lab's Nuclear Deterrence and Global Security mission areas and the Materials for the Future and Science of Signatures science pillars.
Technical contacts: *Larry Hull* and *George T. (Rusty) Gray III*

## PHYSICS

### Toshiba Project measures cosmic ray muons at a seacoast

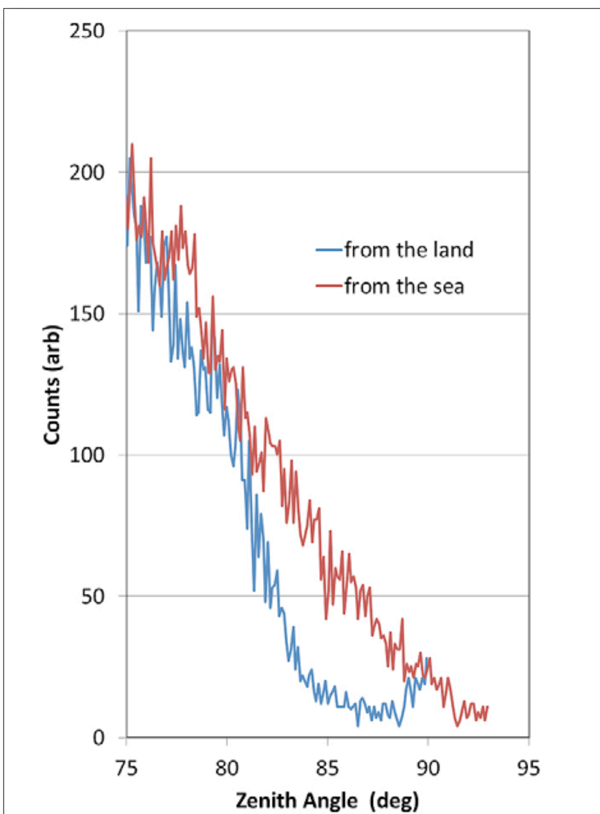
The Threat Reduction Team of Subatomic Physics (P-25) is helping Toshiba Corporation image Japan's damaged Fukushima reactor by using cosmic ray muons that pass through the reactor. Muon radiography (also called cosmic-ray radiography) utilizes secondary particles generated when cosmic rays collide with upper regions of Earth's atmosphere to create images of the objects that the particles, called muons, penetrate. The process is analogous to an x-ray image, except muons are produced naturally and do not damage the materials they contact. By placing "supermodule" sensing detectors on either side of the reactor core, the interaction of muons with the core material will be measured and the 3-dimensional makeup of the core inferred. To obtain the highest resolution image, it is important to know the energy spectrum and the flux of cosmic muons coming into the Fukushima core, which resides at the seacoast. A team of P-25 scientists and technologists traveled to San Diego to measure this seacoast spectrum. Lead experimenters are Chris Morris, Elena Guardincerri, Jeff Bacon, John Perry, and Matt Durham; and students Joseph Fabritius, Dan Poulson, Shelby Fellows, Kenie Plaud-Ramos, and Joey Elmblad.

The Mini Muon Tracker (MMT) is a tracking detector for muon radiography based on straw tubes, built by the P-25 Threat Reduction Team. Researchers transported it to California for five days of data collection of the near horizontal cosmic ray flux. The scientists mounted the detector to face in a near east-west direction. The ocean surface dominated the view to the west, and a north-south sloping ridge dominated the eastern view.




The team collected a total of 93 hours of data: 34 hours with no target in the tracker, 35 hours with 1382 gm /cm$^2$ of lead covering about half of the acceptance, and 24 hours with 691 g/cm$^2$ of lead. Figure 7 depicts a "cosmic radiograph" of the surroundings made by plotting a two dimensional histogram of counting rate versus the azimuthal and zenith angle. The horizon is marked with the green line and the west (seaward) and east (landward) directions are separated as positive and negative angles. The ridge looking landward is visible. The ridge shadows muons from the east that are near the horizon, allowing a clear view of muons from the ocean side below the horizon.

Figure 7. Grey scale image shown cosmic ray counts as a function of zenith and azimuthal angles. A green line marks the horizon.




The researchers integrated the angular distribution of cosmic rays over azimuthal angle and plotted it as a function of zenith. The shadow of the ridge to the east is clearly visible as a large difference between the two directions. There is a large excess of cosmic rays extending beyond 90° where most models predict zero cosmic-ray flux. Although this requires more modeling to verify, the team suggests that these events arise from muons that are scattered out of the ocean surface, resulting in a buildup of flux at 90°. Muons accumulate near the horizon because some scatter out of the ocean back into the air, but very few scatter from the air into the ocean because of the much lower density of air. If verified, this finding would improve the current knowledge of the horizontal muon flux at sea level. In addition to these activities, the team is developing two different tracking algorithms.

Figure 8. Cosmic-ray counting rate, integrated over azimuthal angle, as a function of zenith angle from the two directions.

The LANL team's efforts that will culminate in a measurement of the Fukushima core include: 1) analyze the data collected in California to extract the full energy spectrum of cosmic muons, 2) finish characterization of the tubes and detector setup that will be used at Fukushima (ongoing work at Los Alamos), and 3) travel to Japan to measure backgrounds in a reactor environment.

Toshiba and Decision Sciences fund the work, which supports the Lab's Energy Security and Global Security mission areas and the Science of Signatures pillar by using muons to aid nuclear reactor cleanup. Technical contact: *Chris Morris*

## THEORETICAL

### The effect of Greenland Ice Sheet's meltwater channels on ice movement

The Greenland Ice Sheet moves faster every summer as melt from the surface penetrates km-thick ice through moulins, vertical shafts melted through the ice. Water reaching the bed of the ice sheet lubricates the ice-bed interface, causing the ice sheet to accelerate each summer. Greater melt is predicted for Greenland in the future, but its impact on ice sheet flux and associated sea level rise is uncertain. Direct observations of the subglacial drainage system are lacking and its evolution over the melt season is poorly understood. Matthew Hoffman (Fluid Dynamics and Solid Mechanics, T-3) is part of an international team that made the first simultaneous measurements of moulin and borehole water pressure and ice velocity to investigate the ice sheet response to water-pressure changes within Greenland's subglacial hydrologic system. Their observations identified a previously unrecognized phenomenon controlling evolution of subglacial drainage during the summer. The journal ***Nature*** published their findings.

The team sought to understand how surface meltwater draining to the base of the ice sheet in summer causes the ice to accelerate in early summer and decelerate in late summer. The scientists drilled 13 boreholes through 700 meter-thick ice in west Greenland to perform the first combined analysis of ice velocity and water pressure in moulins and boreholes to the ice sheet bed.

Photos. (*Left*): Moulin in Greenland Ice Sheet. (*Right*): Researcher lowers Instruments down a 700 m deep borehole to the bed of the Greenland Ice Sheet at a remote field camp.

The team determined that moulin water pressure does not lower over the latter half of the melt season. The moulins connect to an efficient, channelized component of the subglacial drainage system, which exerts the primary control on diurnal and short-term multi-day changes in ice velocity. By mid summer, the channels stabilize and are unable to grow any larger. Boreholes in the study monitored a hydraulically-isolated component of the subglacial drainage system. The observations identified a previously unrecognized role of changes in hydraulically-isolated regions of the bed in controlling evolution of subglacial drainage over summer. The decreasing water pressure seen in some boreholes can explain the decreasing ice velocity seen over the melt season. The hydrologic changes that occur each summer may cause isolated pockets of pressurized water to drain out from under the ice sheet slowly, resulting in more friction and decreasing the movement of the ice sheet. The findings indicate that to understand the dynamic behavior of the ice sheet, it is essential to gain insight into the processes occurring in areas distal to the subglacial channels as well as in the channels themselves. Understanding this process will be crucial to predict the effect of increasing melt on summer acceleration and associated autumn deceleration of the ice sheet into the future.

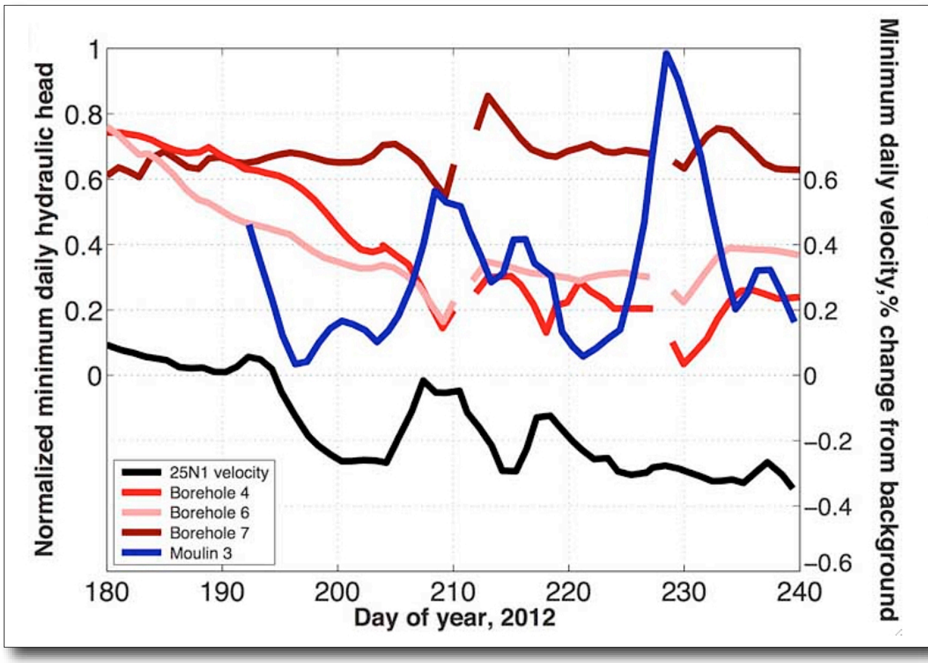



Figure 9. Normalized daily minimum hydraulic heads and ice velocity as a percentage of winter background for 2012. The measured late summer decrease in ice velocity (black) cannot be explained by water pressure in moulins (blue) that provide the external inputs to the basal system, but can be explained by lowering water pressure in hydraulically-isolated regions of the bed monitored by boreholes (red colors).

Reference: “Direct Observations of Evolving Subglacial Drainage beneath the Greenland Ice Sheet,” ***Nature*** *514*, 80 (2014): doi: 10.1038/nature13796. Authors include Lauren C. Andrews and Ginny A. Catania (University of Texas at Austin), Matthew J. Hoffman (Fluid Dynamics and Solid Mechanics, T-3), Jason D. Gulley (University of Texas at Austin and Michigan Technical University), Martin P. Lüthi (University of Zürich and the Swiss Federal Institute of Technology), Claudia Ryser (Swiss Federal Institute of Technology), Robert L. Hawley (Dartmouth College), and Thomas A. Neumann (NASA Goddard Space Flight Center).

NASA Cryospheric Sciences and climate modeling programs within the DOE, Office of Science funded different aspects of the Los Alamos research. The work supported the Lab’s Energy Security mission area and the Science of Signatures and Information, Science, and Technology science pillars. Technical contact: *Matthew Hoffman*