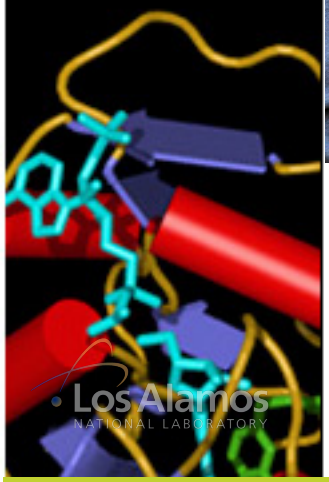
AOT & LANSCE The Pulse

July 2012

INSIDE



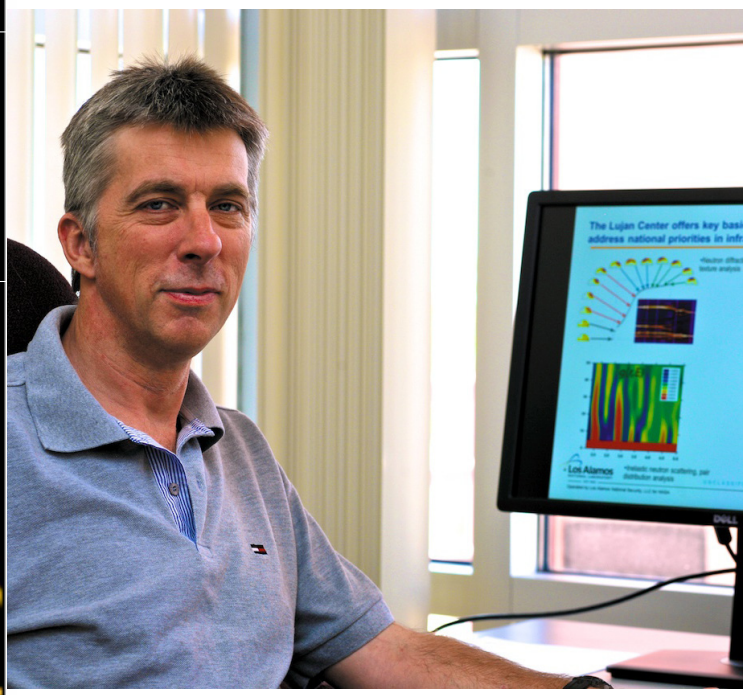
Mark Bourke

Queuing up new research possibilities at the Lujan Neutron Scattering Center

By Diana Del Mauro
ADEPS Communications

As Mark Bourke takes the reins as director of the Lujan Neutron Scattering Center, users can expect the same stellar service—and a commitment to new sample environments. In addition, senior staff scientists can expect more time for their own research, as well as encouragement to assume prominent roles in the neutron scattering community.

The combination, Bourke believes, will elevate the Lujan Center's presence at Los Alamos National Laboratory and around the globe, resulting in new research opportunities.



Visitors to Mark Bourke's office should be aware that he takes copious notes during meetings and is often fueled by multi-colored M&Ms.

In June, Bourke returned to the turquoise-and-pink-painted center where, in 1990, he began his Los Alamos career as an instrument scientist. In the United States, scientists can choose from 13 user facilities for their neutron scattering experiments. The Lujan Center, a vital part of the Los Alamos Neutron Science Center since 1985, was one of the first. Bourke's ambition is to make it even more competitive than it already is.

"There is a set of research and development that we do as well as anyone, given our talented instrument scientists and exclusive sample environments," Bourke said.

To assist him with that goal he has enlisted staff scientists Anna Llobet and Guenter Muhrer as acting science deputy center directors and Experimental Area Manager Charles Kelsey to oversee technical support.

continued on page 3

From Alex's Desk

Colleagues,

By the time this issue of *The Pulse* is out, assuming moving ahead as planned, we have started beam delivery to the Isotope Production Facility and probably some beam delivery to Weapons Neutron Research (WNR) facility, and Proton Radiography facility. The overall LANSCE user program is to resume August 23. This is once again a tremendous accomplishment by so many talented individuals involved that it's just impossible to list. It is clear, however, that there is a sense of a common goal here at TA-53 to deliver beam to our customers and users, which is an example to be followed and applauded. Thank you all for the hard work and dedication.

'It is clear, however, that there is a sense of a common goal here at TA-53 to deliver beam to our customers and users, which is an example to be followed and applauded.'

The construction of the new WNR building is complete (see photo at right). The building is approximately 4,000 square feet with a 5-ton crane capacity and houses two flight paths: 15-degrees right (15R) and 15-degrees left (15L). The 15L flight path is designed for the Chi Nu experiment and contains a 6x6x2 meter deep pit to reduce the background from scattered neutrons. The goal of the Chi Nu experiment is to measure the neutron output spectrum from fission, especially below 0.5 MeV and above 5 MeV where the existing data is sparse.

The building and the installation of the 15L flight path for Chi Nu opens up the 30-degree right flight path for semiconductor testing by industry and universities. Because the neutron spectrum at 30-degrees at WNR Target-4 mimics the cosmic-ray induced spectrum, there has been high demand for such a flight path to increase our capacity beyond what is presently available in the ICE House (30L). With the new 30-degree flight path we have doubled our capacity to accommodate industrial users.

Let me also take this opportunity to bring to your attention that new requirements have recently been put forward by DOE regarding conference attendance in general. Management is engaged and planning the next steps. It will be interesting.

LANSCE Deputy Division Leader Alex Lacerda

Bourke . . . Though relatively small compared to other national user facilities, the Lujan Center is highly productive, attracting more than 300 unique users and generating up to 150 scientific papers a year, including many by the center's 15 PhD instrument scientists.

"We have a very happy group of users," said outgoing Lujan Center Interim Director Jim Rhyne, citing recent survey results and positive reviews from the Office of Science.

The U.S. Department of Energy's Office of Science, Office of Basic Energy Sciences sponsors the lion's share of the Lujan Center's research and judges the center's success by the strength of its user program. The weapons program, industry, and DOE's Office of Nuclear Energy are important customers as well.

Key to Bourke's vision is a commitment to safety and security. He also wants the Lujan Center to pursue research projects that fulfill the missions of both the Office of Science and the Laboratory, citing, as an example, plutonium measurements. Additionally, research in forensics, nuclear energy, energy security, and advanced materials would expand Lujan Center ties with both industry and the Laboratory community, he said.

The Lujan Center offers a variety of instruments that probe the structure of materials using different neutron scattering techniques and a pulsed spallation neutron source. The interactions of neutrons with matter at the Lujan Center offer unique insights that are, in many cases, complementary to the insights available from photon-based scattering capabilities at light sources elsewhere in the nation.

Bourke said he believes the Lujan Center should distinguish itself in two ways: by retaining and attracting world-class scientists and by creating "a unique set of sample environments that span a spectrum of extreme conditions." The latter could help forge the way for MaRIE (Matter-Radiation Interactions in Extremes), the Laboratory's proposed signature experimental facility for the discovery and design of advanced materials, and for which Bourke serves on its core planning team.

To attract and retain standout scientists, Bourke believes that succession planning is important to allow senior scientists more time to devote to project development and to be ambassadors for the Lujan Center and the neutron scattering community as a whole. Conversely, he believes there is a need to provide opportunities for junior staff to operate instruments. Such changes could give the Lujan Center greater visibility, he said, which is crucial both for recognition within the Office of Science and for communicating the opportunities that neutron scattering affords the larger scientific community.

Bourke has a reputation for being a good listener and a calm problem-solver, with "British-style diplomacy," according to Materials Science in Radiation and Dynamics Extremes (MST-8) Group Leader Anna Zurek, his former boss. Not one to make hasty decisions, "he definitely likes to get consensus from all parties involved," she said.

Lujan Center experience propels former students to career success

The Lujan Neutron Scattering Center provided a catapulting experience for two early-career scientists who began investigating the atomic structure of materials at the national user facility.

Former Lujan Center student Kim Tait was recently promoted to curator of mineralogy at Canada's Royal Ontario Museum and former Lujan intern Efrain Rodriguez is now an assistant professor in the University of Maryland's Department of Chemistry and Biochemistry.

More than than 300 international users visit the Lujan Center yearly, and its researchers publish more than 100 peer-reviewed scientific papers annually.

Credit Brian Boyle, Royal Ontario Museum

Tait said the type of work she did for her PhD at the Lujan Center made her stand out from the pack when it came time to find work. The native Canadian landed her dream job: serving as a curator at the largest museum for world cultures and natural history in Canada. In between writing a book on gems and minerals and organizing an exhibit on diamonds, she has continued to collaborate with Lujan Center scientists.

Lujan Center scientists Yusheng Zhao and Luc Daemen mentored Tait, who, from 2003 to 2007, studied the neutron diffraction of gas hydrates. After successfully defending her PhD at the University of Arizona, she became the associate curator of mineralogy at the Royal Ontario Museum. As curator, Tait oversees three large collections: minerals, meteorites, and gemstones.

She established an analytical facility at the museum for her research, with a powder diffractometer, a single-crystal

continued on page 4

Students . . . diffractometer and a raman spectrometer, in which she and her team of graduate students and technicians work. She is cross-appointed as an assistant professor in the Geology Department of the University of Toronto.

Rodriguez is launching a synthesis program to prepare and characterize metastable transition metal oxides for the purpose of energy storage and conversion.

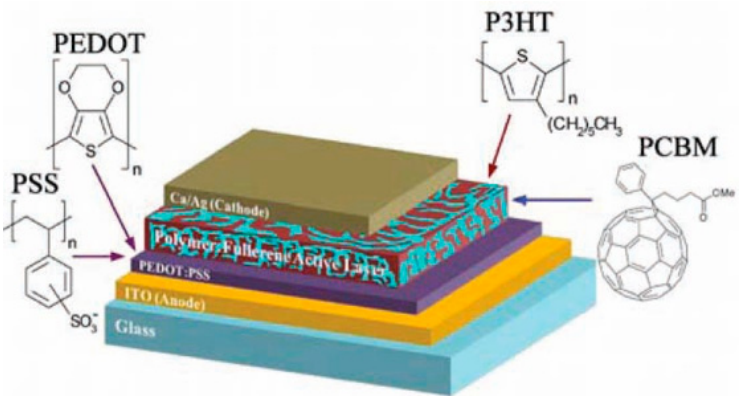
In 2003, Rodriguez, who has a bachelor's of science degree in materials science from the Massachusetts Institute of Technology, became a post-baccalaureate intern investigating the local structure of various complex oxides manganite materials using neutrons with Lujan scientists Anna Llobet and Thomas Proffen (now with Oak Ridge National Laboratory).

During his Lujan Center research, Rodriguez decided to attend graduate school at the University of California, Santa Barbara, where he synthesized inorganic materials, including various technetium oxides. During his studies of this radioactive and rare element, he spent two years as a graduate research assistant at the Lujan Center with Llobet and Al Sattelberger (now a guest scientist with Materials Chemistry, MPA-MC).

After completing his PhD in 2009, Rodriguez received a National Research Council postdoctoral fellowship at the National Institute of Standards and Technology (NIST) Center for Neutron Research in Maryland, where he prepared and characterized iron-based superconductors.

Lujan Center neutron scattering capabilities contribute to understanding modern plastic solar cells

Plastic solar cells are being developed as a low-cost alternative to inorganic, mostly silicon-based, photovoltaics. They use conductive organic polymers and small organic molecules for light absorption and charge transport. The study of organic photovoltaic (OPV) materials and devices is a rapidly growing scientific field that is gaining increasing technological relevance. Recent power conversion efficiency records of above 8% have been reported. This demonstrates that OPV technology is increasingly capable of competing with other thin-film PV devices. However, many questions about basic physics of light conversion by OPV still persist. Polymer-based solar cells consist of several polymer, copolymer, and mixed polymer/fullerene layers with thicknesses less than 100 nm, as shown in the figure. Since the layers are so thin, the properties of the interfaces dominate their electrical functions. For this reason, understanding of the interface morphologies of the polymers used in these devices is required. In the series of recent papers[1-3] a multi-national and multi-laboratory group of investigators led by Prof. Adam Moulé from the University of California, Davis demonstrated how neutron reflectometry can be successfully utilized to address the structural properties of various interfaces present in the OPV devices to improve their efficiency. Due to the excellent scattering contrasts between OPV components, low absorption (which allows studying buried interfaces) and non-destructive nature of neutrons, reflectometry is a very well suited tool to address the structural properties of such polymer-based layers.



Schematic of a typical polymer solar cell with (from top to bottom) a Ca/Ag cathode, a polymer:fullerene active layer consisting of a mixture of P3HT (electron donor) and PCBM (electron acceptor), a PEDOT:PSS hole-transporting layer, and an ITO anode on a glass substrate.

Los Alamos participants include Jaroslaw Majewski and co-author on the papers postdoctoral researcher Peng Wang (both of the Lujan Neutron Scattering Center, LANSCE-LC). This work benefited from the use of the SPEAR neutron time-of-flight spectrometer at Lujan Neutron Scattering Center at LANSCE funded by the DOE Office of Basic Energy Sciences and Los Alamos National Laboratory under DOE Contract DE-AC52-06NA25396.

LANL technical contact: Jaroslaw (Jarek) Majewski

1. "The Consequences of Interface Mixing on Organic Photovoltaic Device Characteristics," D.M. Huang, S.A. Mauger, S. Friedrich, S.J. George, D. Dumitriu-LaGrange, S. Yoon, A.J. Moulé, *Adv. Funct. Mater.* **21**, 1657–1665 (2011).
2. "Investigating the Morphology of Polymer/Fullerene Layers Coated Using Orthogonal Solvents," C.W. Rochester, S.A. Mauger, A.J. Moule, *J. Phys. Chem. C*, **116**, (13) 7287-7292 (2012).
3. "Self assembly of selective interfaces in organic photovoltaics", S.A. Mauger, L. Chang, S. Friedrich, C.W. Rochester, D.M. Huang, P. Wang, A.J. Moulé, under review in *Advanced Materials* (2012).

Effect of interface-induced exchange fields on cuprate-manganite spin switches

Researchers from Argonne National Laboratory, Spain, and Los Alamos used the Asterix polarized neutron reflectometer (PNR) at the Lujan Center to elucidate the mechanism of inverse spin switching in ferromagnetic/superconducting heterostructures.

In a conventional spin-valve system the orientation of two transition element ferromagnetic films sandwiching a conducting layer directly determines whether spin scattering of one or both electron spin states takes place (Figure 1). The resistivity of the spin-valve, i.e., whether the resistivity is high or low, is the means to translate data stored in nanometer-sized magnetic domains into electrical signals like 1s and 0s that computers use.

However, the situation is very different when the ferromagnetic films are complex oxides and the conductor is a high temperature cuprate superconductor. In fact, nearly the opposite behavior (hence the name inverse spin switch) is observed. Many theories have sought to explain the inverse switch phenomena in terms of the orientation of ferromagnetic layers. The research team found compelling evidence that the orientation of the ferromagnetic layers does not directly affect the resistivity of the superconductor. In fact, the conventional explanation based on scattering of electron spins is not germane. Rather, the ferromagnetic layers induce a magnetic field in the superconductor via exchange (Figure 2a). When the exchange field opposes the applied field, the superconductivity of the YBCO layer is maximized (Figure 2b). When the exchange field augments the applied field, superconductivity is suppressed. This work highlights the importance of induced magnetization in complex oxides, and the possibility of detecting minute magnetic fields using a potentially more sensitive technology. *Physical Review Letters* published the work.

Los Alamos researchers include M.R. Fitzsimmons, M. Zhernenkov. Collaborators are Y. Liu, L.Y. Zhu, A. Hoffmann, and S.G.E. te Velthuis (ANL), C. Visani, N.M. Nemes, J. Tornos, M. Garcia-Hernandez, C. Leon and J. Santamaria from Spain. Reference: "Effect of Interface-Induced Exchange Fields on Cuprate-Manganite Spin Switches," *Physical Review Letters* 108, 207205 (2012).

The DOE Office of Basic Energy Sciences supported the ANL and LANL portions of the research. The Lujan Center is a national user facility supported by DOE Basic Energy Sciences. The work supports the Lab's Energy Security mission area and the Materials for the Future and Science of Signatures science pillars.

Technical contact: M.R. Fitzsimmons

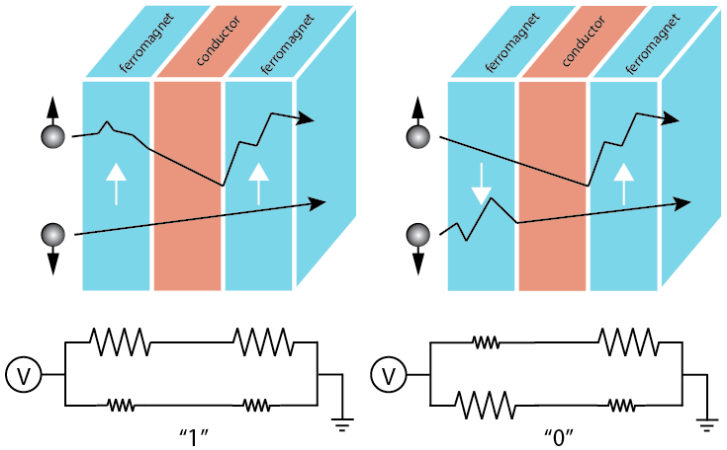


Figure 1 (top): Trajectories of electron spins, up and down, as they traverse the ferromagnet/conductor trilayer. Kinks in the trajectories indicate scattering of the electron and increased resistivity. (bottom) Electrical circuit representing electron scattering as resistance. The low resistance circuit is depicted as a "1".

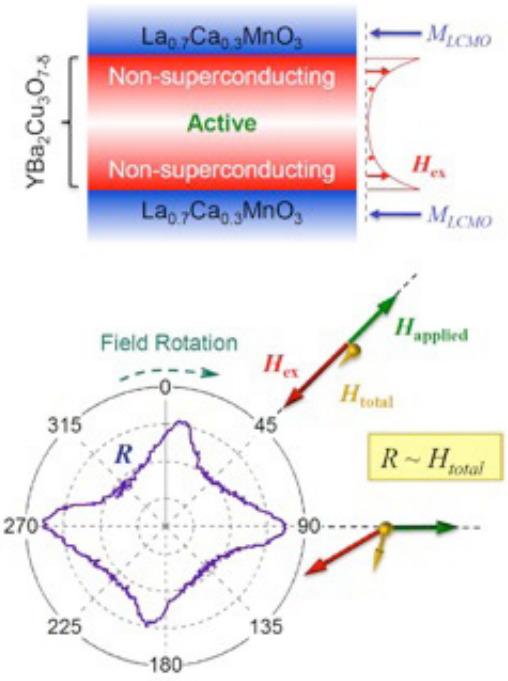


Figure 2 (upper): Schematic picture of the exchange field induced in YBCO by proximity to LSMO. The exchange field decays with distance from the interface. The superposition of the exchange field from each side of YBCO can either cancel or augment the applied field thus affecting the strengthening or suppressing the superconducting properties of the YBCO, respectively. (lower) Dependence of the resistance R upon the orientation of the applied field. When the exchange field Hex negates the applied field, superconductivity is strengthened.

HeadsUP!

WSST Fest a success

Laboratory workers had the opportunity to learn about employee-driven safety programs and successes at the recently held WSST Fest. The event included information booths by organizational Worker Safety and Security Teams, a safety showcase with safety products and services from Laboratory suppliers, and health screening sessions for employees. To see a slideshow of the event, please see int.lanl.gov/news/newsbulletin/QuickTimes/wsst-fest-2012.mov.

New home for Employee Assistance Program

The Employee Assistance Program has moved to the Occupational Medicine building at TA-3 from the Los Alamos Neutron Science Center.

The EAP is a counseling and referral service that assists employees in addressing behavioral health issues. Its phone number remains 667-7339. EAP's free, confidential counseling services are available to all badge holders and their family members. Questions? Contact James Barber or Lisa Celosse at 667-7339.

Reminder: Rains are here, but continue practicing fire safety

Increased humidity and rain has lessened fire danger on LANL property and in the nearby forests. But LANL emergency operations managers remind employees to continue practicing fire safety.

Employees should:

- Smoke only in designated smoking areas and discard cigarette butts in proper receptacles.
- Don't park cars along shoulders in forest roads; engines running can emit sparks that start a fire.
- Report, and if possible, remove downed branches, heavy growth of shrubs that can ignite and quickly explode into a large fire.
- Practice defensible space at work and at home.

Employees are reminded to call 9-1-1 if they spot a fire on or off Lab property, and to call Emergency Operations at 7-6211 if they spot a potential hazard, such as a power line that may be in danger from a tree or a downed power line. Employees also should call Emergency Operations if they encounter wildlife.

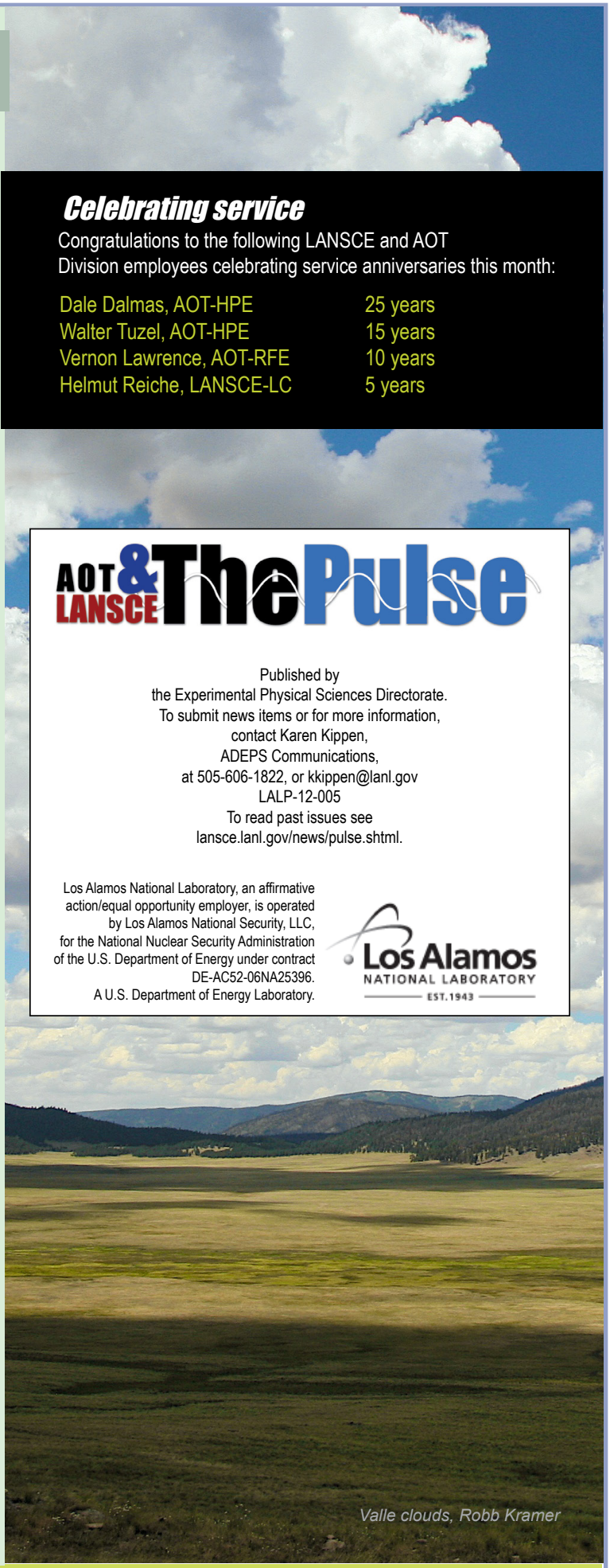
Celebrating service

Congratulations to the following LANSCE and AOT Division employees celebrating service anniversaries this month:

Dale Dalmas, AOT-HPE	25 years
Walter Tuzel, AOT-HPE	15 years
Vernon Lawrence, AOT-RFE	10 years
Helmut Reiche, LANSCE-LC	5 years

AOT & LANSCE The Pulse

Published by
the Experimental Physical Sciences Directorate.
To submit news items or for more information,
contact Karen Kippen,
ADEPS Communications,
at 505-606-1822, or kkippen@lanl.gov
LALP-12-005
To read past issues see
lansce.lanl.gov/news/pulse.shtml.



Valle clouds, Robb Kramer