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During the fabrication process, LANL has historically encountered a 15% pellet failure rate, which is largely a result of pellet cracking. With each pellet failure representing a programmatic burden of approximately $400K ($1.9M for each 32-pellet MMRTG produced), a strong driving force exists to identify the cause of pellet fracture. Unfortunately, the complexity of the pellet fabrication process, combined with the costs involved, make it virtually impossible to develop and implement process improvements on the production line.

Prior to LDRD researcher Adam Parkison’s project, simulation capabilities for $^{238}$PuO$_2$ product fabrication were nonexistent. Process variables were poorly understood with only limited data sets available. Parkison’s LDRD team developed a customized computer model, termed PUMA (Plutonium Modeling and Assessment), designed to simulate the full pellet fabrication process, which should help reduce the 15% pellet failure rate and reduce the programmatic burden associated with each MMRTG.

HIGHLIGHTS

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fabrication process from ceramic powder through encapsulation. Material properties measured and incorporated into the PUMA simulation include thermal conductivity, thermal expansion, reduction and oxidation kinetics, and the presence of impurities. The PUMA simulation marked a distinct paradigm shift in how the $^{238}$PuO$_2$ program approaches understanding the pellet production process.

Example of a cracked $^{238}$PuO$_2$ pellet during production, representing a programmatic burden of approx. $400K. (Image courtesy of LANL.)

**Plutonium simulation in action**

The knowledge gained through development of the PUMA model continues to guide operations at LANL within the $^{238}$PuO$_2$ program. The PUMA simulation is capable of being adapted to support several new product lines. Furthermore, due in large part to this capability, fabrication of the Light Weight Radioisotope Heater Unit (LWRHU) is currently being considered for use in space missions after a decades-long hiatus. PUMA may also be used to predict pellet behavior as the high wattage fuel being produced at Oak Ridge National Laboratory (ORNL) is added to the $^{238}$PuO$_2$ stockpile. It is also believed that the PUMA simulation could be adapted to guide fabrication of more exotic products such as the Americium-241 dioxide ($^{241}$AmO$_2$) heat sources being developed by the European Space Agency. *(LA-UR-21-23525)*

**PUMA delivers the most accurate depiction of the pellet fabrication process to date. Using this data, the pellet failure rate during fabrication due to cracking has dropped to near-zero at LANL. (Image courtesy of LANL.)*

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**Intentional “Imperfections”: Los Alamos researchers discover new capability for advanced manufacturing**

A long-standing challenge in explosives research is the development of a material that is “just right”: something that is not too sensitive and can detonate unintentionally, but also something that is not too insensitive and never detonates. Using advanced manufacturing techniques, researchers at Los Alamos have developed a process to produce explosive materials with tailored sensitivity.

In trinitrotoluene or TNT, perhaps the most well-known example of an explosive, hot spots control the dynamic behavior of the material. These hot spots often form around defects, such as air bubbles or inclusions, during the manufacture of the explosive. The uneven flow into and around these imperfections results in points of intense heat that largely control the energy necessary to initiate detonation.

Explosives have an inherent problem - they should be perfectly safe for handling and storage but detonate reliably on demand. In this video, Los Alamos researcher Virginia Manner describes the importance of understanding detonation sensitivity.
The key insight of the Los Alamos team in tailoring the sensitivity of explosives was the application of advanced manufacturing techniques to intentionally introduce voids within a fabricated material. Advanced manufacturing techniques not only allow the material to be manipulated at the mesoscale, but also eliminate variables and unintentional inclusions. With the ability to control the placement of voids within a material, the team looks to control the release of energy through a sophisticated arrangement of hot spots. The team demonstrated that the structure introduced can be used to manipulate both the detonation direction and detonation timing in a manufactured sample.

The work of the team has broad impact in detonation physics research. Following the conclusion of their LDRD project, the team found applications within the NA-115 Advanced Manufacturing Development Program mission space.

Principle investigator Alexander Mueller describes: “This work ideally will make high explosive (HE) materials safer and make their energy delivery more precise. Due to a precise application of HE power, this work will have implications in what technologies these material can be applied to; worker safety in industry and military that handle and use these materials; and, hopefully, when developed to a high level, a reduction of unintended casualties from conventional weapons. It will also allow for weapon designers to explore new concepts, due to both the new effects that can now be used to manipulate the dynamic behavior of the HE and the agility gained by reducing the design-manufacture-test cycle through the use of these techniques.” *(LA-UR-21-23577)*

**LDRD Quarterly Highlights**

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**LDRD researchers earn DOE Early Career awards**

Five recent Early Career awardees are from LANL, LLNL, and SNL. Notably, four of those winners have LDRD experience. This high association with LDRD experience is not surprising. Early involvement in LDRD projects has been found to have significant impact on career advancement, as LDRD projects allow principal investigators to gain technical skills and experience in project management and mentorship.

DOE’s Early Career program supports exceptional scientists working in the agency’s priority research areas. The LDRD researchers were selected for their work related to Advanced Scientific Computing Research, Basic Energy Sciences, Fusion Energy Sciences, and Nuclear Physics. Miles Beaux from Los Alamos has established plutonium capabilities for scanning probe microscopy that do not exist anywhere else. Matt Durham, also from Los Alamos, is a key player in the Office of Science’s Nuclear Physics Heavy Ion program due to his work with the Pioneering High Energy Nuclear Interaction Experiment (PHENIX). Dr. Andrea Schmidt from Livermore is driving innovative work in magnetically driven Z-pinch plasmas. Lastly, Dr. Drew Kouri from Sandia is leading efforts focused on fusion of simulation and experimental data.

The DOE’s official announcement and full list of awardees is at the [Early Career Research Program](#) webpage.
Livermore researchers analyze near-surface nuclear detonations to better predict potential damage

An LDRD-funded research team at Lawrence Livermore National Laboratory (LLNL) is taking a closer look at the effects of nuclear weapon blasts close to Earth’s surface. Previous efforts to correlate data from events with low heights of burst revealed a need to improve the theoretical treatment of strong blast waves rebounding from hard surfaces.

Investigators compared theory with numerical simulations of different nuclear yields, heights of burst, and ambient air densities. They focused on nuclear blasts in non-ideal environments, such as blasts over mountainous terrain, or in the presence of rain or snow. These types of environments change the blast wave in operationally significant ways.

Results of their high-fidelity blast simulations indicate that the shock wave produced by a nuclear detonation continues to follow a fundamental scaling law when reflected from a surface. These findings enable investigators to more accurately predict the damage a detonation will produce in a variety of situations, including urban environments.

“Having the capability to accurately predict the damage of a high-yield device in a wide array of cases is of paramount interest to our national security,” said LLNL scientist Greg Spriggs. “This information enables us to pre-compute potential damage and guide emergency response personnel in the event that the United States is attacked or in case of a catastrophic accident.”

This latest research spawned from decades of data collected during LLNL’s work scanning and analyzing films of old atmospheric tests. “The more we know about the effects of nuclear detonations in different environments, the better prepared we will be to respond,” Spriggs said.

More information about research related to near-surface nuclear detonations can be found on LLNL’s website. (LLNL-WEB-458451)

Livermore research team doubles creation of antimatter using high-intensity lasers

Scientists at LLNL achieved a nearly 100 percent increase in the amount of antimatter (also known as positrons) created in laboratory experiments. Using targets with specially designed microstructures on the laser interface, investigators shot a high-intensity laser at the targets to generate the antimatter beams. Previous research using a tiny gold sample created about 100 billion particles of antimatter. The new experimental setup doubled that quantity.
In this illustration depicting the team’s research approach, laser light enters the microstructure in front of the gold target, driving high-energy gamma photons (orange) and particles, including the electron-positron antimatter pairs (blue and green). The experimental data shows that the micro-structure doubled the energy conversion from lasers to antimatter (relative to a target with no structure). (Image courtesy of LLNL.)

“These experimental results are important for the Livermore positron project and its goal to make enough electron-positron antimatter to study the physics of gamma-ray bursts,” said Hui Chen, a plasma physicist who leads the LDRD-funded project. “In addition, we found that the experiments also created a high-energy, mega-electron-volt (MeV) x-ray backlighter that can penetrate very dense objects, which is important for many aspects of high-energy-density science research.”

When enough energy is squeezed into a very small space, such as during high-energy particle collisions, particle-antiparticle pairs are produced spontaneously. When energy transforms into mass, both matter and antimatter are created in equal amounts. In these experiments, intense laser-plasma interactions produce very high-energy electrons, whose energy, when interacting with the gold target, can generate electron-positron pairs.

Investigators used previous results and new simulations to design microstructures, which could either enhance or diminish this interaction, leading to enhanced or suppressed positron generation. The agreement between the simulations and the experiment provided researchers with the confidence that they were capturing the most important physical mechanisms.

The ability to create numerous positrons in a laboratory opens the door to new avenues of anti-matter research, including an understanding of the physics underlying various astrophysical phenomena such as black holes and gamma-ray bursts, as well as a pathway toward creating a dense electron-positron plasma in the laboratory. The research also brings scientists one step closer to being able to use laser-generated positron sources for the variety of national security applications.

More information regarding the team’s research regarding antimatter creation can be found on LLNL’s website. (LLNL-WEB-458451)

Livermore scientists explore direct drug delivery with carbon nanotube porins

Modern medicine relies on an extensive arsenal of drugs to combat deadly diseases, but getting those drugs into disease-ridden cells has remained a major challenge for modern pharmacology and medicine. To tackle this difficulty, an LDRD-funded research team at LLNL, in collaboration with investigators from the University of California, Merced, and the Max Planck Institute of Biophysics, are studying the use of carbon nanotubes to enable direct drug delivery from liposomes through the plasma membrane and into the cell interior by facilitating fusion of the carrier membrane with the cell.

Drugs are often poorly soluble, strongly toxic to other tissues, or face rapid degradation in the organism’s chemical environments. They can accumulate in non-target tissues, bind to other cellular components, or may not internalize efficiently into the target cells.
Liposomal delivery systems aim to mitigate these problems by encapsulating drugs in external carriers that circulate through the bloodstream. However, these systems involve a trade-off between enhancing liposomal stability on the way to the target and easing payload release into the cytosol of the target cell.

Most current liposomal delivery strategies rely on the endosomal pathway for cell entry, which is inherently inefficient and often results in degradation of the drug. Commonly used cationic lipids, which enhance liposomal fusion with the target membrane and enhance endosomal escape, proved to be toxic.

“We thought that carbon nanotube porins—short pieces of carbon nanotubes inserted into lipid membranes—could mimic viral fusion peptide functionality and help to fuse the liposomal carriers to the membranes of cancer cells,” said chemist Alex Noy, who leads Livermore’s research team.

In a series of experiments, the team demonstrated that a nanomaterial platform containing small-diameter carbon nanotube porins can function as a potent promoter of membrane fusion. Moreover, when Noy and his team loaded their liposomes with a potent chemotherapeutic agent, these carriers delivered the drug to cancer cells, killing a majority of the cells.

“Our results open an avenue for simple and efficient drug delivery carriers compatible with a wide range of therapeutics,” said Nga Ho, an LLNL postdoctoral researcher who participated in the study. Potential applications include highly efficient delivery of DNA and RNA vaccines across the plasma membrane.

More information regarding using carbon nanotube porins for drug delivery can be found on LLNL’s website. (LLNL-WEB-458451)

Livermore physicists leverage quantum sensors to search for sterile neutrinos

Sterile neutrinos are theoretically predicted new particles that offer an intriguing possibility in the quest for understanding the dark matter in our universe. Unlike the known “active” neutrinos in the Standard Model of particle physics, sterile neutrinos do not interact with normal matter as they move through space, making them very difficult to detect.

An interdisciplinary research team led by LLNL investigators, in collaboration with experts from the Colorado School of Mines, demonstrated the power of using nuclear decay in high-rate quantum sensors in the search for sterile neutrinos. The findings are the first measurements of their kind, and are expected to jump-start an extended project to look for one of the most promising candidates for dark matter.
During this LDRD-funded research, the team conducted experiments where they implanted radioactive beryllium-7 atoms into superconducting sensors developed at LLNL. When the beryllium-7 decays by electron capture into lithium-7 and a neutrino, the neutrino escapes from the sensor, but the recoil energy of the lithium-7 provides a measure of the neutrino mass. If a heavy sterile neutrino with mass $m_c^2$ were to be generated in a fraction of the decays, the lithium-7 recoil energy would be reduced and produce a measurable signal, even though the elusive neutrino itself is not directly detected.

“This research lays the groundwork for even more powerful searches for these new particles using large arrays of sensors with new superconducting materials,” said physicist Stephan Friedrich, who leads LLNL’s research team.

More information regarding LLNL’s search for sterile neutrinos can be found on LLNL’s website. (LLNL-WEB-458451)

Medical diagnostic capability developed through Sandia LDRD investments enables rapid response to the coronavirus pandemic

The coronavirus pandemic highlighted the criticality of having portable, automated, highly accurate technology that can rapidly detect threats in environmental and clinical settings. Fortunately, Sandia has a long history of developing novel detection systems. SpinDX, a Sandia LDRD-enabled technology was utilized in 2020 for rapid detection of viral antigens and SARS-CoV-2 antibodies during the coronavirus pandemic. As a result, SpinDX was able to offer healthcare professionals a powerful way to diagnose SARS-CoV-2 at all stages of the disease.

Sandia chemist Chung-Yan Koh, left, and former Sandia bioengineer Chris Phaneuf demo the SpinDx diagnostic device. (Photo by Jules Bernstein.)
LDRD investments in “lab-on-chip” technology have allowed researchers to create portable diagnostic devices enabling the rapid detection of chemical and biological agents. Beginning in the mid-1990s, the development of a handheld chemical analysis system called µChemLab helped spur the growth of Sandia’s now enduring capability in biological science and technology. Additional investments from LDRD, government, and technology partnerships over the next two decades led to improvements in detection capabilities for national security and medical applications.

SpinDX came out of a need to rapidly identify trace levels of biotoxins to combat terrorism. After initial LDRD investments in 2009, SpinDX continued to receive funding from multiple sponsors, including the U.S. Armed Forces Radiobiology Research Institute, National Institutes of Health, and National Institutes of Allergy and Infectious Diseases, to address critical issues in biodefense and healthcare. Numerous companies have licensed SpinDX as a platform for point-of-care diagnostics testing, water pathogen testing, and other applications.

Investments in SpinDX continue to pay dividends through seven patents and eight commercial licenses, the development of new partnerships, and the expansion of novel applications beyond what was first envisioned beginning with the original LDRD in 2010. Sandstone Diagnostics licensed SpinDx from Sandia in 2012 and have continued to refine and develop the technology. In 2019, they started promoting their Torq™ system. Torq consists of a compact, battery-powered centrifuge and specially designed discs that spin and separate blood samples immediately following collection. Torq combined with other companies’ medical tests, allows lab-quality sample collection and preparation almost anywhere for rapid response COVID-19 testing. (SAND2021-3609 R/SAND2021-5909 M)

NNSA, Army, Air Force and Navy programs integrate Sandia’s multi-mission radio frequency architecture

Major NNSA, Army, Air Force, and Navy programs are now utilizing advanced real-time multi-mission sensors that can send/receive/process arbitrary signals with large instantaneous bandwidth using multiple channels. These radar capabilities, which enable smarter sense, analyze, and respond cycles, evolved through LDRD investments over the past four years.

In 2017, a Sandia LDRD team, led by PI Jacques Loui, sought to develop a multi-mission digital radar architecture to simplify and modularize a radar’s radio frequency frontend by replacing application-specific analog detection methodology with flexible and programmable digital signal processing. After a year of work, they successfully obtained real-time digital-detection radar impulse response from a prototype and demonstrated multi-channel synchronization.
With such positive results, the Sandia Multi-Mission Radio Frequency Architecture (MMRFA) LDRD team continued the effort into 2019 and demonstrated an ultra-wide-band multimission modular digital radar architecture that overcame limitations of single-application analog radar designs by leveraging commercial-off-the-shelf (COTS) hardware, existing/new firmware/software intellectual properties, and available radio frequency (RF) apertures. They demonstrated several Sandia firsts in real-time ultra-wideband sensing, including multi-channel clock synchronization, advanced arbitrary waveform generation, frequency domain channelization, and single-stage-heterodyne conversion using advanced COTS and custom RF modules.

The High-Performance Digital Radar (HPDR) significantly advanced the state-of-the-art for Sandia radar system architectures by replacing static analog waveform generation and detection with agile digital waveform synthesis and signal processing. The project culminated with a successful flight test that demonstrated integration of the HPDR with an operational radar and creation of high-resolution synthetic aperture radar imagery.

In 2020, the MMRFA team demonstrated the first ever instance of real-time, parallel and fast Fourier transform-matched filtering of large instantaneous bandwidth signals. Pulse compression, important for imaging applications, requires real-time digital matched filtering when using agile waveforms. To overcome motion compensation challenges, the team implemented real-time pulse extension with efficient interpolative post processing that improved bandwidth utilization without performance (resolution and throughput) degradation. They also configured and tested simultaneous dual-channel receive operation that improved range performance while doubling data throughput. This set an important precedent that facilitates the configuration and setup for simultaneous multi-channel digital signal processing of agile waveforms in the future. *(SAND2021-3609 R)*

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A high-resolution Digital Synthetic Aperture Radar image from the successful initial flight test in 2019. Teams from Sandia and the U.S. Air Force, under the guidance of NNSA, performed a critical B61-12 flight test. (Image courtesy of SNL.)

**Sandia’s CTH software code used to design and improve high-velocity and high-temperature national security applications**

CTH is one of the most highly used computational structural mechanics codes on Department of Defense high-performance computing platforms, and the number one code at Sandia in terms of computing hours. This software, which solves multi-dimensional problems characterized by large deformations and strong shocks within various material configurations, is currently being used to in the design and improvement of high-velocity and high-temperature national security applications that ultimately help protect the country.
Sandia’s CTH journey started more than 30 years ago with its predecessor codes, CHARTD and CSQ, which were developed in the 1970s for one-dimensional problems and expanded to simulate problems in two- and three-dimensions in the 1980s. CTH software was then created to expand Sandia’s production shock physics code suite to 3D. The code, written in FORTRAN 90 and C, was modified to run on massively parallel computers in 1992-1993 and enhanced with parallel adaptive mesh refinement.

In the last 20 years, many Sandia LDRD projects have contributed to the development and application of CTH, which can successfully analyze a variety of materials for high-speed impact, penetration, perforation, and explosive detonation. Applications are numerous and include astrophysics, safety assessments, accident investigations, blast design, threat assessments, fracking predictions, and medical research. CTH was used to mimic the entry process of the Chelyabinsk asteroid in Russia, simulate the penetration (a first-of-its-kind simulation), breakup and fireball of Comet Shoemaker-Levy 9 hitting Jupiter, and aid in the accident investigations of the Space Shuttle Columbia disaster and the USS Iowa naval training accident. (SAND2021-3609 R)

Leveraging R&D: The Long-Term Impact of the SDRD Program

The long-term value of the Site Directed Research and Development (SDRD) program is demonstrated by projects whose benefits to the NNSA’s mission and then to program emerge over many years. An SDRD project’s lifespan may be only one to three years long, but research that is subsequently adopted by programs and funded by programmatic dollars can mature and provide the basis for long-lasting technologies. Following the evolution of our SDRD projects over five or more years demonstrates how our initial R&D investments yield a high return of programmatic capability.

The two SDRD projects we highlight below have reshaped the programs they impacted.

Multiplexed Photonic Doppler Velocimetry

The SDRD program began investigating multiplexed photonic Doppler velocimetry (MPDV) concepts in FY 2010. When this investigation began, its scope was limited, focusing simply on finding “a better way to do optical velocimetry.” That initial effort quickly expanded, however, and soon an accelerated effort to develop MPDV into a key enabling technology for future stockpile stewardship experiments began.
A team of NNSS scientists, in collaboration with researchers from Lawrence Livermore National Laboratory (LLNL) and Los Alamos National Laboratory (LANL), set out to address the challenge of developing a better, faster, and more economical way to gather a large amount of detailed data on the reliability of the U.S. nuclear weapons stockpile without nuclear explosion testing.

By the time FY 2011 ended, the MPDV development team had built a demonstration system and completed proof-of-concept experiments. In 2012, the Gen-1 MPDV system was completed and fielded on the Gemini experimental series at the U1a Complex at NNSS. The 128-channel Gen-1 MPDV system allowed researchers to collect more high-fidelity data from a single integrated experiment than all of the previous comparable experiments combined, and the resulting data from these experiments have changed the way the nuclear weapons community views large-scale experiments within the science-based stockpile stewardship strategy. The achievements attained by the MPDV development team led to several awards, including an R&D 100 award in 2012.

The technology grew and capability expanded rapidly due to significant programmatic efforts that followed. The Gen-2 MPDV system was developed in 2013 and was fielded at the Dual-Axis Radiographic Hydrodynamic Test (DARHT) facility at LANL as well as at Site 300 at LLNL. Efforts to improve the design and performance of MPDV systems and components continued, and in August 2014, the MPDV diagnostic was used on the Leda experiment at U1a. The Leda experiment was completed with 100 percent data return and paved the way for the follow-on experiment series, Lyra.

The Gen-3 MPDV system was fielded for the first time on Orpheus, the first experiment in the Lyra series executed in September 2015 at U1a; the resulting data showed a large increase in signal-to-noise ratio over the Gen-1 system fielded on the Gemini series. The system was also fielded on the remaining experiments in the Lyra series, Eurydice and Vega, which took place at U1a in March and December 2017, respectively. These experiments demonstrated the MPDV’s capability to gather shock physics data in unprecedented detail.

The innovation and development of MPDV has provided experimenters with a powerful diagnostic tool that is capable of collecting data crucial to furthering our understanding of weapons physics and advancing the science-based Stockpile Stewardship Program. The MPDV has brought about a paradigm shift in shock physics diagnostics, and the MPDV technology will continue to play an important role in upcoming and future stockpile science experiments.

**Broadband Laser Ranging**

Broadband laser ranging (BLR), another key optical diagnostic for current and future stockpile stewardship experiments, also has its roots in the SDRD program. BLR measures the precise position of a rapidly moving surface, and it is complementary to PDV because PDV data do not always yield complete information about the material position. Independent position measurements made with BLR complement velocity data from PDV. BLR is also compatible with PDV in that BLR and PDV can be fielded together and share the same probes pointed at the same target.
The work began as a one-year feasibility study in spring 2014 when scientists at NNSS Special Technologies Laboratory began investigating a BLR technique for use in an optical distance measurement system for dynamic experiments. By summer 2014, they had finished building a prototype BLR system and began fielding it on small-scale experiments. The study yielded encouraging results. As a result, in 2015, a BLR R&D team consisting of researchers from NNSS, LLNL, LANL, and Sandia was formed and began designing and building a BLR system suitable for larger-scale experiments.

In December 2015, a 2-channel BLR diagnostic system built jointly by NNSS and LLNL scientists was successfully fielded on a hydrodynamic test at LLNL Site 300. In 2016, a LANL-built BLR system and an NNSS-built BLR system were fielded on the Silverleaf experiments, a series of four experiments conducted at LANL in preparation for the Nightshade experimental series of the Red Sage campaign at U1a. The Silverleaf experiments provided experimenters with an opportunity to learn how to field a BLR system.

In March 2017, an 8-point BLR system was fielded alongside MPDV for the first time on the Eurydice experiment of the Lyra series at U1a. The system was also fielded on the final experiment of the Lyra series, Vega, in December 2017. The results from these experiments have demonstrated that BLR is the next level of diagnostics, enabling researchers to obtain orders of magnitude more distance measurements than was possible with traditional electrical pins.

In 2020, a 16-point BLR system was fielded on the Red Sage campaign experimental series at U1a and on the 3687 experiment at the DARHT facility. More recently a 48-point BLR system was installed at Site 300 at LLNL. We anticipate that BLR systems will continue to grow and expand, playing an increasingly important role as one of the main diagnostic tools for stockpile science research. (DOE/NV/03624--1037)