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Roadmap to MaRIE

Inside

Los Alamos NATIONAL LABORATORY EST. 1943

> *"As stewards for the science we wish to conduct, we are also stewards of our workers' safety and the environment."*

Lucy Maestas

Making MaRIE's safety and environmental commitment crystal clear

Lucy Maestas has worn many important hats in her nearly 40 years at Los Alamos, but her current assignment—serving as strategic coordinator for a proposed billion-dollar-class experimental facility—tops them all.

MaRIE (Matter-Radiation Interactions in Extremes) will be used to examine materials under extreme conditions using the world's most powerful coherent, brilliant x-ray source.

"As I think about the many possibilities the MaRIE facility will provide, I feel extremely positive about being a part of the team that is bringing this facility to reality," said Maestas, who joined the MaRIE program office a year ago and set to work determining the Department of Energy technical requirements for advancing the project.

"I read as much as I could, and I asked a lot of questions!" said Maestas, who has an MBA in organizational management. She uses those skills to fulfill a broad range of functions in the MaRIE program office—from participating in outreach activities to pulling together all the necessities for successful external advisory board reviews.

In particular, Maestas spearheaded the effort to ensure that as MaRIE takes shape "its needs are not just right from a scientific aspect, but its needs must be right for workers and the environment too," she said.

"The most important contribution I've made thus far is preparing carefully wrought documents that lay the foundation for environmental, safety, and health matters," she said. This included a preliminary hazard analysis strategy and a plan to ensure MaRIE fulfills the requirements of the National Environmental Policy Act.

Lucy Maestas spreads the word about MaRIE's research possibilities at the 19th American Physical Society Shock Compression of Condensed Matter Biennial International Conference in Tampa, Florida.

To successfully craft these documents addressing MaRIE's safety and environmental commitments, Maestas gathered a team of 12 architects, engineers, environmental experts, and scientists from the Laboratory and the National Nuclear Security Administration's Los Alamos Field Office. She also ensured vital assistance was recognized with a spot award, which celebrates those who contribute significantly to the Lab's mission and values.

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Maestas cont.

Their efforts were a key element of a set of MaRIE documents Los Alamos delivered in May to the NNSA Deputy Administrator seeking approval of "Critical Decision 0," the initial step in DOE's process for advancing a project from concept to construction. The MaRIE project, she said, will continue to engage the help of such subject matter experts as it moves forward. "As stewards for the science we wish to conduct, we are also stewards of our workers' safety and the environment," she said.

In addition to building a bedrock of MaRIE champions at the Lab, Maestas travels to conferences to help recruit the next generation of Laboratory staff, describing the career opportunities available at Los Alamos. "We view MaRIE as a future facility that will require a talented workforce, which will consist of a mix of accomplished scientists and qualified engineers, technologists, and operational and support staff. We try to pique the interest of postdocs and graduate students who are developing skills in materials and laser science to help realize MaRIE the facility and take MaRIE science into the future," she said. "I describe MaRIE's capabilities of looking at materials at the mesoscale level, increasing scientists' ability to view materials changes due to age or environment. This research is vital as Los Alamos certifies the safety, security, and effectiveness of our nuclear weapons stockpile."

Science and technology on the roadmap to MaRIE

Vertical Shock Tube experiments drive understanding of unsteady turbulence

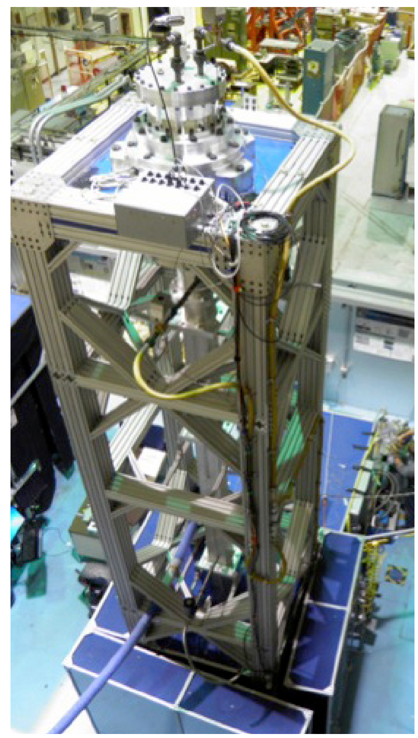
The Vertical Shock Tube (VST) experiments in Physics Division's Neutron Science and Technology (P-23) are providing new information about how "atypical" turbulence develops. A team of researchers, including principal investigator Kathy Prestridge, R&D scientist Ricardo Mejia-Alvarez, postdoctoral researcher Brandon Wilson, and research technologist Adam Martinez, are using the VST to determine the effects shock waves, initial condition perturbations, and strong density gradients have on turbulent mixing.

Prestridge's team is making the highest-resolution density and velocity field measurements of shock-driven mixing in the world at the VST, which is designed to study shock-driven mixing of two fluids that are struck by a shock wave. The researchers make simultaneous velocity and density field diagnostics to measure turbulence quantities in these unsteady flows using coherent optical lasers. Insight into the physics of turbulent mixing helps us understand nuclear weapons performance, improves our numerical modeling of variable-density turbulence, and provides insight into inertial confinement fusion mixing and the development of supernovae.

By studying the effects of different initial perturbations on an air-sulphur hexafluoride (SF_6) interface that is hit by a shock wave, the team can determine how quickly the flow will mix and become turbulent.

With new experiments at a shock Mach number of 1.3 (i.e., the shock is traveling at 1.3 times the speed of sound), the team has found that initial conditions with different modes produce different mixing characteristics as the flow evolves. They use coherent lasers to probe the turbulence and measure the density and velocity of the fluids. Figure 1 shows instantaneous mixing fields for three different initial condition experiments, demonstrating that the more length scales in the initial perturbations, the more complex the mixing interface after shock.

An aerial view of the Vertical Shock Tube, located in P-23's turbulence laboratory.



An important result from these initial experiments is that the mixing region is not uniform for any of the initial condition types, and many mixing quantities vary throughout the mixing region. This result is illustrated in Figure 2, where normalized values of the density and density-specific volume covariance are shown throughout the mixing regions. The dashed line at the center of the graph is the center of mass of the mixing region and the light dotted lines are the edges of the mixing regions. The mixing is non-uniform and asymmetric. This makes modeling this mixing of two gases much more complex than single-gas turbulence.

The work is an example of science on the road to MaRIE, the Laboratory's proposed experimental facility for Matter-Radiation Interactions in Extremes. Using MaRIE's multi-probe diagnostic hall, simultaneous measurements of density and velocity can be made at the micron frontier in extreme shock loading conditions including in more opaque or dense fluids, helping scientists understand compressibility and other effects in turbulent mixing.

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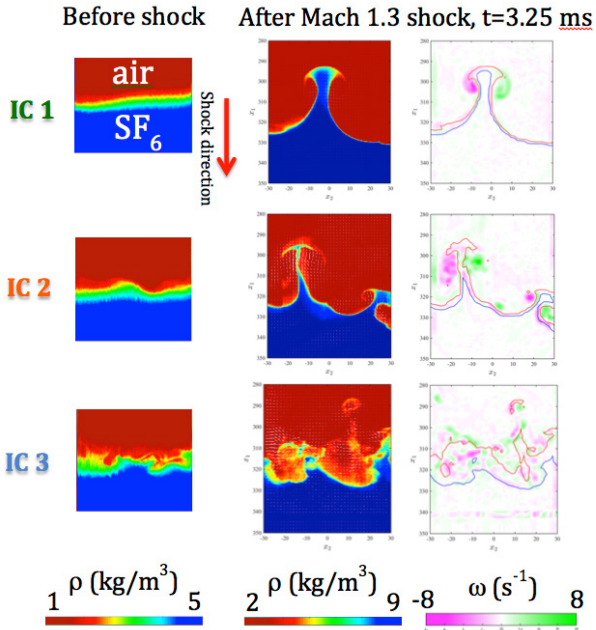


Figure 1. Three different initial condition experiments at Mach 1.3. First column shows density fields for the three initial condition types, increasing in interface complexity in each row. Second column shows the density field of the shocked interface 3.25 ms after the shock crosses the initial condition. Third column shows the vorticity field, or amount of local rotational motion, with the edges of the mixing layer marked with red and blue lines along the 25% and 75% density contours.

Vertical Shock Tube cont.

Prestridge presented the recent experimental results at the American Physical Society's 19th Biennial Conference on Shock Compression of Condensed Matter in Tampa, Florida in June.

New to the Extreme Fluids team is postdoctoral research associate Alex Craig (P-23), who recently earned his PhD in aerospace engineering from Texas A&M University. Having recently completed his postdoctoral appointment, former Extreme Fluids team member Brandon Wilson has joined Advanced Engineering Analysis (W-13) as an R&D engineer.

This work, which supports the Laboratory's Nuclear and Particle Futures pillar, is funded via NNSA Science Campaigns (John Scott, Los Alamos program manager).

Technical Contact: Kathy Prestridge

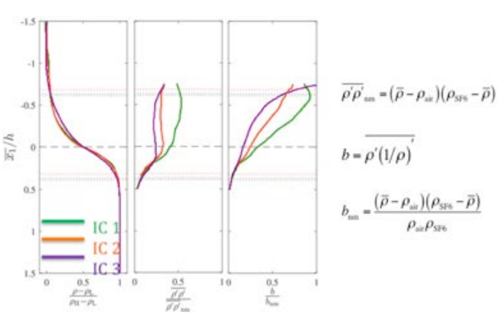
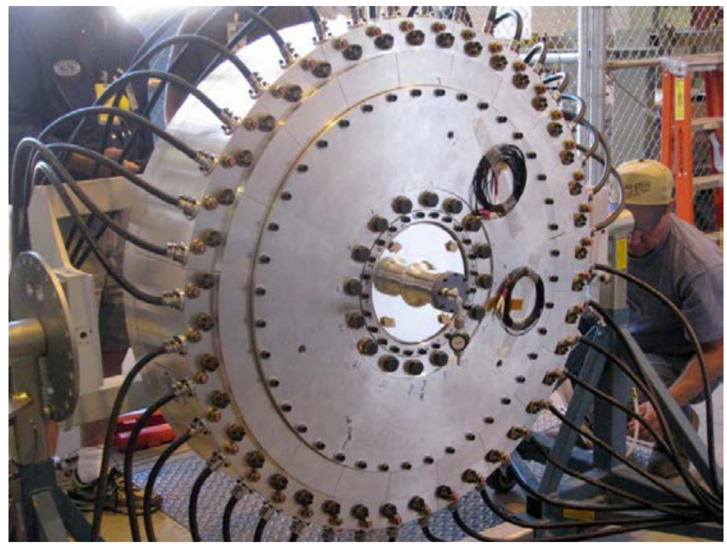


Figure 2. Average profiles of scalar quantities through the mixing regions of the three different experiments pictured in Figure 1.

PHELIX at pRad enhances movie-making of materials in extreme environments

A new pulsed power driver for the Proton Radiography Facility (pRad) at the Los Alamos Neutron Science Center is producing images of higher spatial resolution than previously attainable, serving as a valuable tool for scientific experiments key to understanding and maintaining the U.S. nuclear stockpile.

PHELIX (for Precision High Energy Density Liner Implosion eXperiment), combined with pRad technology, produces more than five times the axial imaging data at higher spatial resolution in one experiment than was available with Atlas, a previous Los Alamos pulse power facility for liner-on-target experiments.



The PHELIX transformer with the liner load cassette at the center. The photograph was taken during initial testing prior to installation into the boxcar. The black coaxial cables connect the transformer to the capacitor banks (not shown).

Recently this capability was featured in an invited talk by David Oro at the Shock Compression in Condensed Matter conference in Tampa, Florida. Damaged surface hydro (DSH) experiments performed with PHELIX explore shocked-ejected particle transport into gas in converging geometries. For these experiments a cylindrical liner-on-target configuration is employed. To control the initial conditions, micron-sized tungsten (W) particles are used in place of shock-formed ejecta. The inner surface of the cylindrical target is coated with a 100-μm thick layer of W powder. The liner impacts the target generating a shock that launches the W particles off the target surface. The time history of the trajectory of the converging shocked-ejected particulate is captured in 21 proton radiographs recorded during the experiment.

Three experiments of this type have been executed, one into vacuum, one into argon at 8.3 bars, and one into xenon

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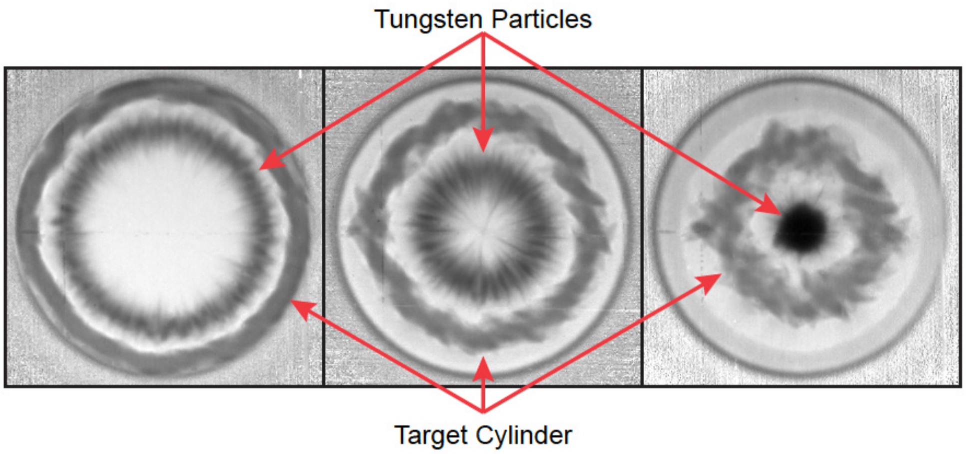

Three of the 21 proton-radiographs taken down the liner load central axis during the experiment. From left to right, the images were taken at approximately 30 μs, 34 μs, and 39 μs after the start of current flow. In the first image we see the cloud of tungsten particles and target cylinder enter the field of view. In the second image, the fastest traveling particles have reached the center. In the third image, most of the tungsten particles have accumulated at the center.

PHELIX cont.

at 8.3 bars. The image quantity and quality from pRad provides a level of detail both in time and space not before available for these types of experiments. While these experiments employ pRad's X3 magnifier, PHELIX can also be operated with the X7 magnifier trading off field-of-view for higher resolution.

The study of the details of hydrodynamically evolving features under extreme conditions is important for validating hydrodynamic algorithms in weapons computer codes. PHELIX gives researchers another tool to achieve these conditions in a controlled fashion that is compatible with advanced diagnostics such as pRad.

And unlike Atlas or Pegasus, both of which required large rooms and fixed positioning, PHELIX is small, the size of a travel trailer, and can be placed in the pRad beamline for experiments and removed to make way for others.

The work is an example of science on the roadmap to MaRIE, the Laboratory's proposed Matter-Radiation Interactions in Extremes facility that will provide the capability to image over microseconds timescales thick samples of materials undergoing a dynamic event.

PHELIX, which logged its first shot at pRad in 2013, is an air-insulated capacitor bank providing greater than 400 kJ of stored energy, generating peak currents above 5 MA to implode centimeter-size liners in 10-40 μs, attaining speeds of 1-4 km/s.

To achieve the desired peak current with a compact pulse-power system, PHELIX employs a two-stage Marx generator, the output of which is connected through coaxial cables to a unique multi-turn-primary, single-turn-secondary, current step-up toroidal transformer. Current from the secondary flows along annular transmission plates to a central "cassette" containing the liner load. PHELIX experiments are self-confined. By adjusting the charge voltage for each shot, researchers can tune the magneto-hydrodynamic push on the liner to match experimental needs.

Funded by Science Campaign 1: Primary Assessment Technologies (LANL Program Manager Stephen Sterbenz), the creation of PHELIX was a collaboration of Physics, Computational Physics, Accelerator Operations and Technology, Materials Science and Technology divisions, and National Security Technologies LLC. The pRad capability is primarily supported by the NNSA Science Campaigns. PHELIX supports the Lab's National Security mission and Materials for the Future science pillar.

Technical contact: David Oro

Ultrafast laser driven shocks allow observation of initial chemistry behind the shock front in nitromethane

Predictions for the timescale of shock-induced chemistry in detonating nitromethane range from 10 ns for empirical reactive burn models[1] to tens of picoseconds for quantum molecular dynamics models.[2] Until recently, there were no experimental means to directly probe this discrepancy of 3 orders of magnitude variation in kinetic predictions. Recent ultrafast shock chemistry experiments performed at Los Alamos have demonstrated that substantial chemical reactions occur in tens of picoseconds near detonation conditions in nitromethane.[3]

Nitromethane is one of the simplest and most thoroughly studied explosives, yet very little is known about the shock induced chemistry that drives detonation. Fast shock induced chemistry is an essential characteristic of detonation, yet this chemistry remains a mystery for all explosives in use today. Researchers at Los Alamos have been developing tabletop ultrafast laser driven shock capabilities (see photo next page) for more than 15 years to enable observation of the chemical events that support detonation.

These capabilities, which were highlighted in an invited talk by Shawn McGrane at the recent Shock Compression in Condensed Matter conference in Tampa, Florida, have been employed to measure the properties within the first

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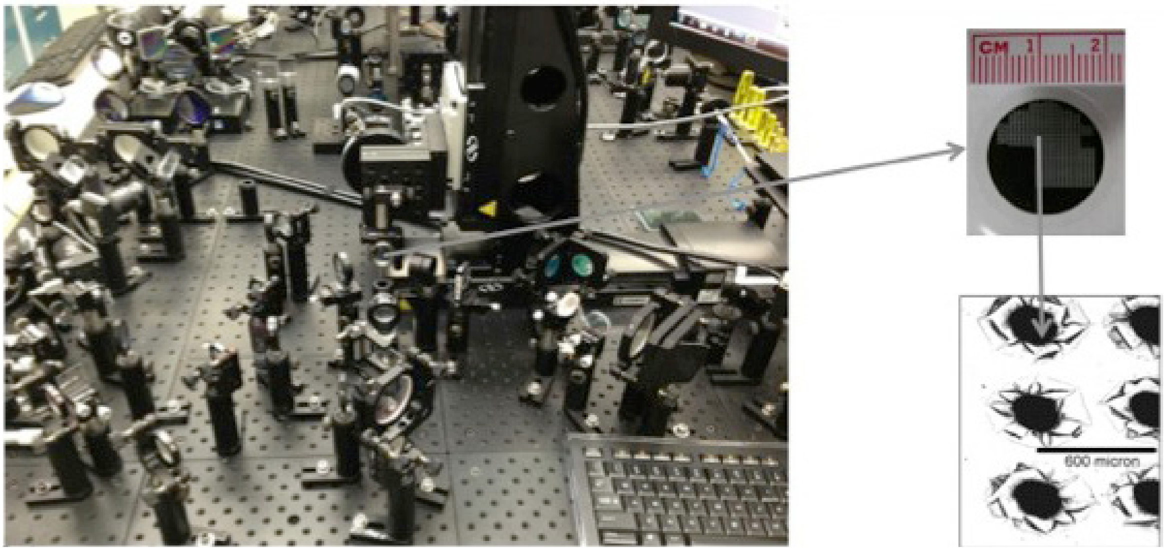


A tabletop laser system drives hundreds of microscale shock experiments a day with picosecond synchronization to numerous optical diagnostics.

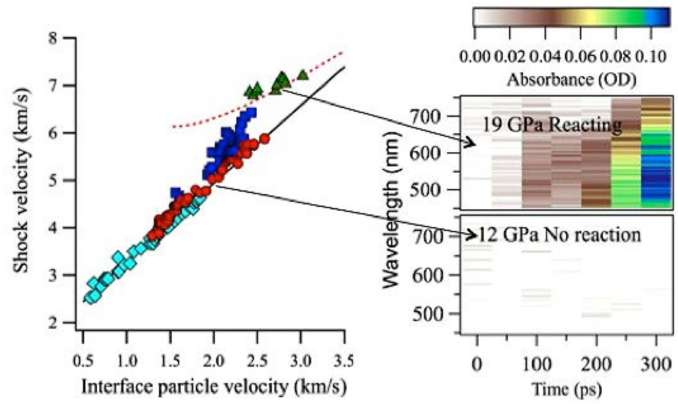
Ultrafast cont.

300 ps behind the shock front in nitromethane. Interferometric and transient absorption results are summarized in the figure. The observed reactions at 19 GPa are significantly faster than predicted by reactive burn models of nitromethane[1] that have been parameterized to fit a broad range of data on detonation wave profiles and shock to detonation transitions. However, the measured interferometry data agree with the properties of the predicted products (the red dashed curve). In contrast, the observed reaction rates are similar to those predicted by quantum molecular dynamics[2], but the chemical species appear to be different, since the optical properties observed disagree with predictions.[4]

As the experimental measurement specificity improves, details of the theory and simulations will be tested even more stringently. The current optical measurements of shocked chemistry at picosecond timescales are setting the stage for time resolved x-ray chemical measurements that could be performed at a facility like MaRIE (Matter-Radiation Interactions in Extremes). Eventually, iteration between improvements in theory and experiment will converge upon a complete story of the essential chemistry of detonating nitromethane, and other explosive materials.

This work supports the Laboratory's Stockpile Stewardship mission and Materials for the Future science pillar by furthering understanding of shock induced chemistry with the long-term goal of achieving predictive reactive burn modeling of high explosives. The team includes Kathryn Brown, Cynthia Bolme, McGrane, and David Moore (Shock and Detonation Physics, M-9). This work is funded by Campaign 2: HE Science (Project Leads Margo Greenfield and Dan Hooks) and has previously been supported by Los Alamos's Laboratory Directed Research and Development program (Program Manager Bill Priedhorsky).

Technical contact: Shawn McGrane



Shocked nitromethane exhibits chemical reactions as seen through deviations from the black solid line on the Hugoniot plot (left) and through the transient absorption of the products (right). On the left plot, diamonds are plate impact data[5] recorded on nanosecond to microsecond timescales; the red circles, blue squares, and green triangles are ultrafast laser shock driven data measured in <300 ps. The red circles are not reacting in the first 300 ps, the blue squares are beginning to react over 300 ps, and the green triangles are reacted within tens of picoseconds. The black curve is an unreactive reference Hugoniot[6], and the red dashed line is the predicted product curve[1].

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Livescu named ASME Fellow

State-of-the-art simulations exemplify science on the roadmap to MaRIE

Daniel Livescu (Computational Physics and Methods, CCS-2) has been named an American Society of Mechanical Engineers (ASME) Fellow. An authority in the field of fluid mechanics who has made significant contributions to the Los Alamos National Laboratory/Department of Energy stewardship mission as a principal investigator for the NNSA Defense Science Programs, Livescu received the award in the ASME research and development category. Fellows in this category have made noteworthy invention, discovery, or advancement in the state of the art as evidenced by publication of widely accepted materials, by receipt of major patents, or by having products or processes in the marketplace.

Livescu received a doctorate in mechanical and aerospace engineering from the University of Buffalo and joined the Laboratory in 2001. His research focuses on direct-numerical simulation of turbulence and large-scale flow computations. Livescu has led numerous open science proposals, including on Lawrence Livermore National Laboratory's Dawn and Sequoia supercomputers and Los Alamos's Roadrunner. The Roadrunner proposal resulted in the first successful implementation of a large fluid dynamics code on the computer cell architecture. He has performed the largest simulations to date of turbulent flows, approaching or exceeding the parameters achieved in typical experiments. The simulations have revealed new or unexpected physics and helped to develop the Laboratory's turbulence models.

His work is an example of science on the roadmap to MaRIE, the Laboratory's proposed experimental facility for materials science at the mesoscale. MaRIE experiments will provide unprecedented spatial and temporal resolution data and enable validation of the turbulence calculations performed by Livescu. MaRIE experiments will leverage the increased computational capacity enabled by exascale computing, resulting in high fidelity simulations of flow environments.

Livescu has mentored 11 postdoctoral researchers and 10 doctoral students (as thesis co-advisor). Many of them now hold faculty positions at prestigious universities or are Laboratory staff members.

ASME promotes the art, science, and practice of multidisciplinary engineering and allied sciences around the globe and includes more than 140,000 members in 151 countries.

Preparing for exascale simulations of materials in extreme environments

On July 29, 2015, President Obama issued an Executive Order creating the National Strategic Computing Initiative, to address the myriad challenges required to deploy and effectively utilize an exascale-class supercomputer (i.e., one capable of performing 10^{18} operations per second) in the 2023 timeframe. Since physical (power dissipation) requirements limit clock rates to at most a few gigahertz, this will necessitate the coordination of on the order of a billion concurrent operations, requiring sophisticated system and application software, and underlying mathematical algorithms, that may differ radically from traditional approaches. Even at the smaller workstation or cluster level of computation, the massive concurrency and heterogeneity within each processor will impact computational scientists.

The multi-institutional, multidisciplinary Exascale Co-design Center for Materials in Extreme Environments (ExMatEx), has initiated an early and deep collaboration between domain (computational materials) scientists, applied mathematicians, computer scientists, and hardware architects, in order to establish the relationships between algorithms, software stacks, and architectures needed to enable exascale-ready materials science application codes within the next decade.

ExMatEx, which was launched in 2011, has two ultimate goals: (1) identifying the requirements for the exascale ecosystem that are necessary to perform computational materials science and engineering simulations (both single- and multi-scale), and (2) demonstrating and delivering a prototype scale-bridging materials science application based upon adaptive physics refinement. Such simulations provide higher physical fidelity while simultaneously providing the massive concurrency and asynchrony that are required to efficiently utilize the emerging hierarchical, heterogeneous platforms such as Trinity (Los Alamos National Laboratory), Sierra (Lawrence Livermore National Laboratory, LLNL), and the subsequent generation of exascale supercomputers.

Scientific users are key stakeholders in the co-design process and have been engaged from the start. In June, this reached a peak with ExMatEx Center Director Tim Germann giving the opening plenary lecture "Exascale computing and what it means for shock physics" at the 19th Biennial Conference of the APS Topical Group on Shock Compression of Condensed Matter, and Deputy Director Jim Belak giving a plenary lecture "Preparing for the future of computing: Bridging scales within the Exascale Materials Co-design Center" at the 3rd World Congress on Integrated Computational Materials Engineering.

Over the next year, ExMatEx will demonstrate its scale-bridging challenge problem at scale on Trinity, to simulta-

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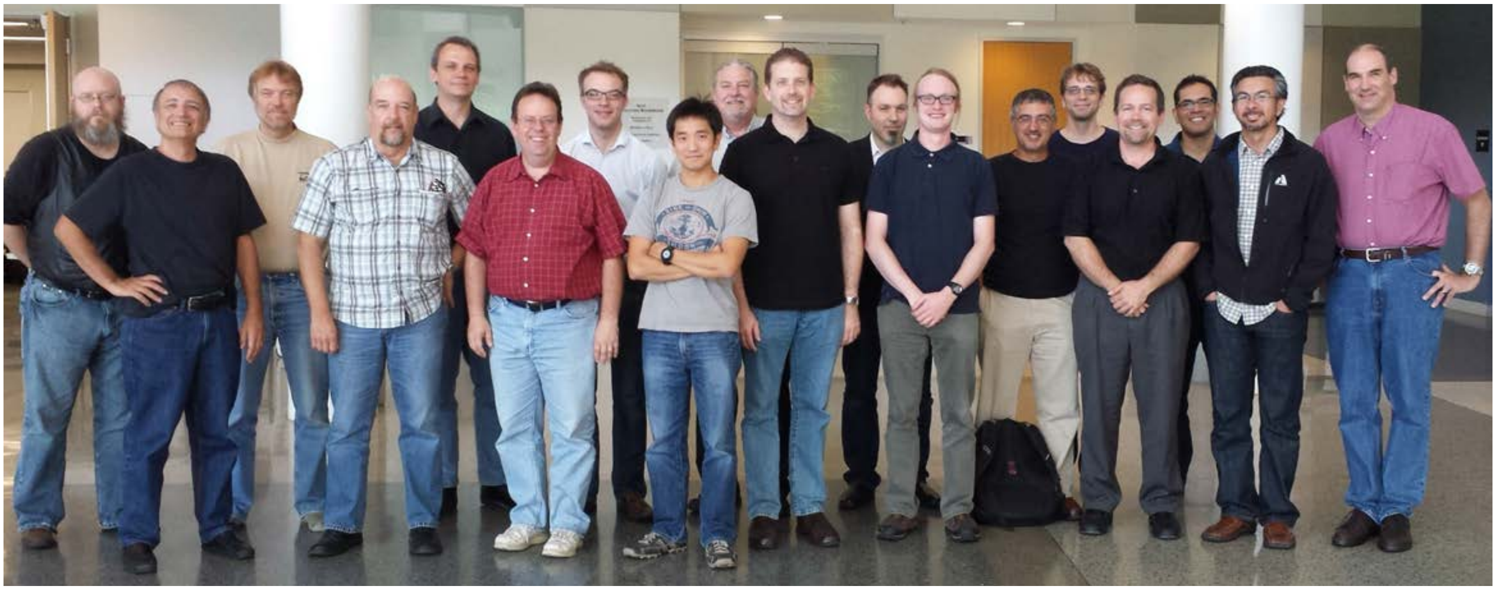
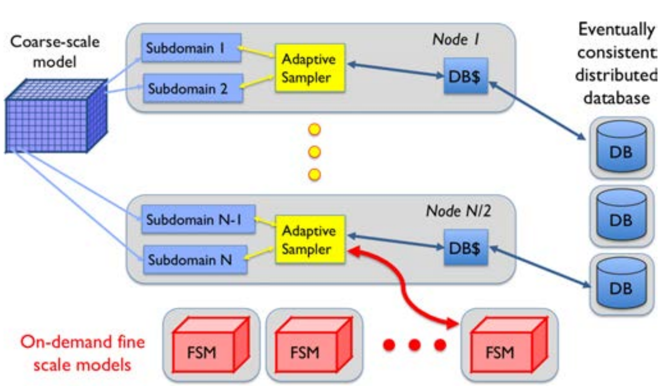


ExMatEx team members attending the September 2014 All-Hands meeting on the Georgia Tech campus. External stakeholders and collaborators, including processor and supercomputer vendors, computer science, and materials science and engineering research groups, also participate in these regular meetings.

Exascale cont.

neously test its adaptive sampling algorithm, task-based execution model, and underlying software stack, including the database and runtime system. This model of a tantalum Taylor anvil impact test will use adaptive sampling to construct a fine-scale response surface with (poly-) crystal plasticity models of increasing fidelity (and computational expense), from a simple Taylor model to VPSC (a homogenized approach) to VPFFT (a full-field, spatially resolved model). This Trinity scale-bridging demonstration, and in particular Trinity-specific optimizations such as using "burst buffer" flash memory nodes for the database query and interpolation, and Knights Landing many-integrated-core (MIC) nodes to accelerate the fine-scale computations, is supported by Los Alamos's Laboratory Directed Research and Development program.

ExMatEx is supported by the U.S. Department of Energy, Office of Science, Office of Advanced Scientific Computing Research, and supports the Information Science and Technology and Materials for the Future Science Pillars. Center Director Tim Germann (Physics and Chemistry of Materials, T-1) and Deputy Director Jim Belak (LLNL) lead ExMatEx, which also includes participants from Sandia National Laboratories, Oak Ridge National Laboratory, Stanford University, California Institute of Technology, Purdue University, and Georgia Tech.



Target multiscale applications are composed of various pieces, or components, that must interact with each other in a dynamic and adaptive fashion as the code runs.

Technical contact: Tim Germann

To learn more about MaRIE, please see marie.lanl.gov or contact Cris Barnes, capture manager, at cbarnes@lanl.gov.

Roadmap to MaRIE, featuring science and technology highlights related to Los Alamos National Laboratory's proposed experimental facility, is published by the Experimental Physical Sciences Directorate. For information about the publication, please contact adeps-comm@lanl.gov.

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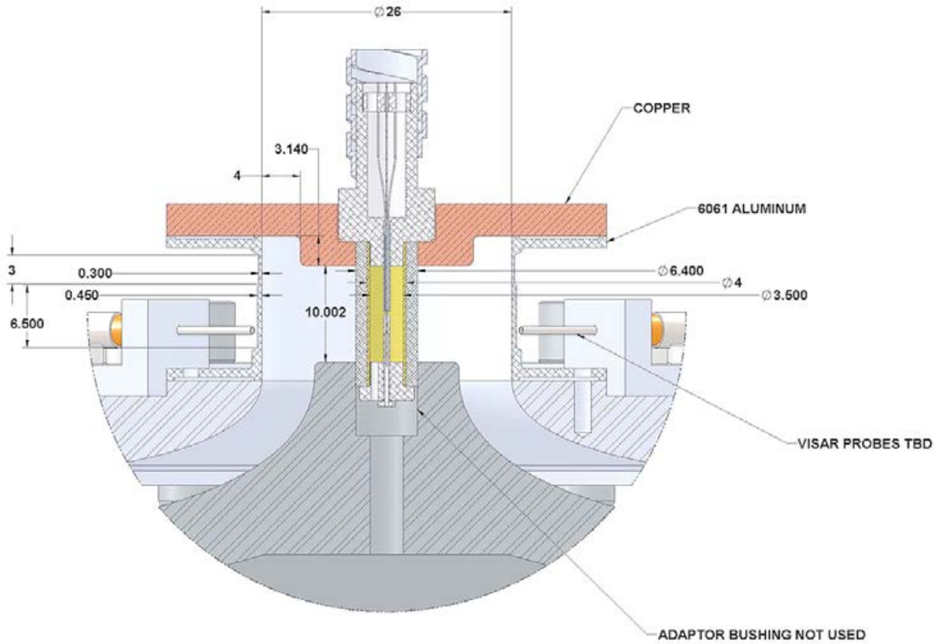
NNSA National Nuclear Security Administration

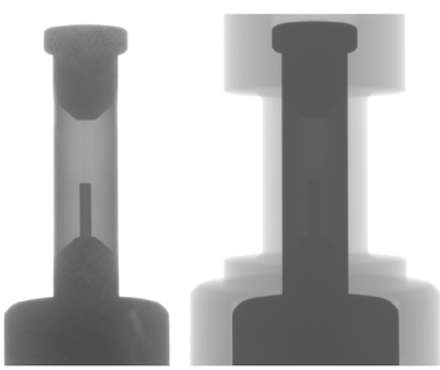
Z Machine cylindrical compression experiments on depleted uranium

Researchers executed the first containment experiment (Shot #2824) using depleted uranium in a thin walled cylindrical geometry at Sandia National Laboratories' Z machine. The team developed a new experimental geometry to acquire quasi-isentropic (nearly constant entropy) compression data at significantly higher peak pressures than previously achievable.

Los Alamos National Laboratory, General Atomics, and Sandia National Laboratories (SNL) collaboratively designed and fabricated the depleted uranium target (see figure). The extreme length-to-diameter aspect ratio required the depleted uranium blanks to be formed by electric discharge machining at Los Alamos. General Atomics precision machined the depleted uranium blanks to final specification and fabricated the target. Key to the success of these experiments was fine-grained uranium, which mattered due to the constrained geometry of these shots. The 15-mm-long cylindrical target was composed of an inner liner made of depleted uranium (inner radius 1.75 mm, 250 µm wall thickness), and an outer liner (the pusher) made of aluminum (inner radius 2.0 mm, 1200 µm wall thickness) that contained the electrical current and magnetic field throughout the implosion.



Cutaway cross-section image developed during the depleted uranium target design project phase depicts the experimental configuration of the target assembly. The platform has cylindrical symmetry. The crosshatched gold region (image center) represents the depleted uranium target. The crosshatched gray region that borders it represents the aluminum liner or "pusher." (All dimensions are in mm.)



Radiographic images of the target assembly taken at two different contrast or intensity levels. (Left): Image showing semi-transparent depleted uranium thin walled cylinder. Fiber optic probe for PDV diagnostics can be seen through target center. (Right): Image showing semi-transparent aluminum liner or "pusher" with depleted uranium thin walled cylinder appearing as fully dense solid.

The diagnostics included six internal photon Doppler velocimetry (PDV) probes to measure the response of the depleted uranium inner surface to the pressure drive, six velocity interferometer system for any reflector (VISAR) probes, and two PDV probes that measure the velocity of the external surface of the aluminum anode can. All internal PDV probes returned excellent data. The depleted uranium liner was tracked to the maximum possible velocity and was quasi-isentropically compressed to the peak pressure predicted via magnetohydrodynamics simulation. Radiologic containment during dynamic actinide (i.e., uranium, plutonium, etc.) experiments on the Z machine is dependent on a set of explosively driven ultrafast closure valves. As predicted, Shot #2824 contained the uranium in the chamber.

Los Alamos and SNL have collaborated on actinide dynamic experiments for more than 10 years. This new experimental configuration will facilitate the exploration of actinides behavior to significantly higher pressures and densities. The kind of data obtained for the validation equation of state and other physics performance properties is an example of Science on the Roadmap to MaRIE (Matter-Radiation Interactions in Extremes), the Laboratory's proposed experimental facility for control of time-dependent material performance. Similar studies could be performed at unprecedented scales using MaRIE's advanced capabilities.

The Los Alamos team includes: Franz Freibert (Nuclear Materials Science, MST-16), Nenad Velisavljevic (Shock and Detonation Physics, M-9), and David Alexander (Metallurgy, MST-6). NNSA Defense Programs funded the research through the Dynamic Materials Properties Science Campaign. The work supports the Lab's Materials for the Future science pillar.

Technical contact: Franz Freibert

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