NNSA
National Nuclear Security Administration

Stewardship Science Today

Office of Research, Development, Test, and Evaluation (RDT&E)

VOLUME 2 | NUMBER 1 | MARCH 2020

Stewardship Science Today (SST) highlights the stewardship science and academic programs supported by the Department of Energy/National Nuclear Security Administration (DOE/NNSA). SST is published quarterly by the NNSA Office of Research, Development, Test, and Evaluation. Questions and comments regarding this publication should be directed to Terri Stone via email at terri.stone@nnsa.doe.gov.

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CALENDAR (Subject to Change)

6/15-18/2020
SSGF/LRGF Annual Meeting, Las Vegas, Nevada
https://www.krellinst.org/ssgf/conf

6/21-25/2020
ISC High Performance 2020—The Event for High Performance Computing, Networking, Storage, Data Analytics, and AI/Machine Leaning, Frankfurt, Germany, https://www.isc-hpc.com/ (May cancel with full refund until 5/11)

6/22-7/3/2020 — Cancelled
2020 HED Summer School: Foundations of HEDP, University of Michigan, http://clasp-research.engin.umich.edu/workshops/hedss/

7/12-16/2020
CSGF Annual Meeting, Arlington, Virginia
https://www.krellinst.org/csgf/conf

INSIDE

2 Groundbreaking Stellar Opacity Experiments Reveal Inconsistencies in X-Ray Databases
3 Evaluating Turbulence Models at High Energy Densities
5 DOE/NNSA 2020 Stewardship Science Academic Programs Symposium

*Contractor Support

Welcome to this latest issue of *Stewardship Science Today* (SST). Featured in this issue are cutting-edge results from opacity experiments on Z that have been shown to reveal inaccuracies in existing X-ray opacity databases. These exciting results are leading to further research into the X-ray opacity values for other relevant elements. Stay tuned for further results in this area. We also feature work aimed at improving turbulence models for high energy density regimes being carried out through experiments at the National Ignition Facility at Lawrence Livermore National Laboratory.

Dr. William Bookless, NNSA Principal Deputy Administrator, and Ani Aprahamian, Frank M. Freimann Professor of Physics at the University of Notre Dame, discussed the benefits of SSAP during the 2020 SSAP Symposium (see page 5 for more about the Symposium).

These are exciting times for groundbreaking research at our national laboratories and partnered academic institutions. We hope to continue to attract additional early career scientists, engineers, and technicians to join our team. Featured is an article on this year's Stewardship Science Academic Programs (SSAP) Annual Review Symposium which drew a record crowd! The student posters were so outstanding that it was difficult to select winners. Congratulations to all who participated. We look forward to interacting with you at next year's symposium scheduled for February 16-17 in Santa Fe, New Mexico, and for years to come as we watch your careers develop.

Last and most importantly, please err on the side of caution and stay healthy and safe during these uncertain times.

Mark Anderson

Dr. Mark C. Anderson
Acting Assistant Deputy Administrator for Research, Development Test, and Evaluation

High Performance Collaborative Access Team Workshop

In January, a Techniques and Capabilities for High Pressure Research workshop took place at Argonne National Laboratory's Advanced Photon Source, at the High Pressure Collaborative Access Team (HPCAT) facility. The workshop focused on providing an overview of HPCAT (an NNSA-funded facility), hands-on training, and interactions with HPCAT staff and Lawrence Livermore National Laboratory (LLNL), Los Alamos National Laboratory (LANL), and Sandia National Laboratories (SNL) scientists. The two-day workshop started with opening remarks by Tod Caldwell, NNSA Federal Program Manager, and Stephen Streiffer, Director of the Advanced Photon Source. Day One featured presentations by the Stewardship Science Academic Programs' (SSAP) individual and center Principal Investigators (PIs) and

(continued on page 5)

Groundbreaking Stellar Opacity Experiments Reveal Inconsistencies in X-Ray Databases

by Thomas W. Overton (General Atomics)

Several years ago, high energy density (HED) physics experiments at the Sandia National Laboratories' (SNL) Z Pulsed Power Facility upended traditional models of how energy circulates in the sun and other stars.[1,2] Energy from fusion in the stellar core must pass through ionized elements in a star's plasma before escaping as radiation, and a critical part of these models is the opacity of these elements to the transmission of energy. Until recently, however, opacity values at stellar temperatures and pressures could only be calculated indirectly due the difficulty of recreating those conditions on earth.

The experiments on Z, part of the Z Astrophysical Plasma Properties (ZAPP) collaboration with other national labs and academia, were the first to directly measure iron opacity at stellar conditions. To the surprise of the physics community, these experiments produced values significantly at odds with the calculated values used in the models. That meant that either the models needed adjustment or the experiments were in error.[3] The topic has even entered the domain of popular science discussion.[4]

Some of the targets used in the ZAPP experiments were manufactured at General Atomics (GA) which has supplied HED target components to SNL, Lawrence Livermore National Laboratory (LLNL), and Los Alamos National Laboratory for several decades. During the target development process, GA physicist Haibo Huang realized that characterizing the targets for these benchmark experiments would require greater accuracy than could be achieved with existing methods and commonly used X-ray opacity reference databases. There are at least five such databases maintained by four institutes, all of them now decades old: NIST-XCOM (Hubbell), NIST-FFAST (Chantler), CXRO (Henke), SNL (Biggs), and LLNL (McMaster).

To address the need for greater accuracy in target characterization, Huang's team developed customized equipment to perform high-precision X-ray transmission measurements. Their approach combined a conventional fixed-anode X-ray source and a silicon drift energy-dispersive detector. The team then worked to consolidate the five public databases into a single software package, allowing them to fit the same set of experimental data.

X-ray-database-to-element quantification is analogous to length measurement using a yardstick. If the reference standard is inaccurate, the measurement result will be proportionally off. Because comparison of these databases is not straightforward, the inconsistencies had not been apparent before this project. Within the physics community, a common perception is that X-ray databases are mature and correct to within "a couple of percent."

In fact, through this process, Huang's team discovered that element-specific values in the X-ray opacity databases deviated from each other by 5% to 10%, and sometimes far more.

To validate the new approach, Huang and his team compared X-ray opacity measurements from the GA equipment for selected elements with recent synchrotron-based values obtained by a joint team in Europe led by the French Alternative Energies and Atomic Energy Commission (CEA) and the German Physikalisch-Technische Bundesanstalt (PTB).[5] The measured values from CEA/PTB and GA agreed to ~1%, confirming that the values in the public databases were inaccurate, and the customized equipment could significantly reduce the error bar as well as providing additional support for the opacity values from the ZAPP experiments.

GA's research partners at LLNL's National Ignition Facility (NIF) and the other national labs have suggested that the new approach could immensely simplify current procedures for calibrating X-ray filters, while providing higher accuracy and more

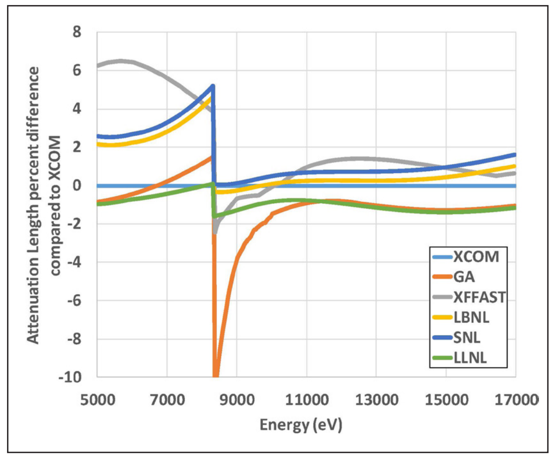

Figure 1. The direct comparison of nickel (Ni) opacity reveals significant differences among existing X-ray databases. The GA measurement observed a sharp increase in X-ray absorption above the K-edge that is not reflected in other databases but is in good agreement with recent European synchrotron data on Ni.

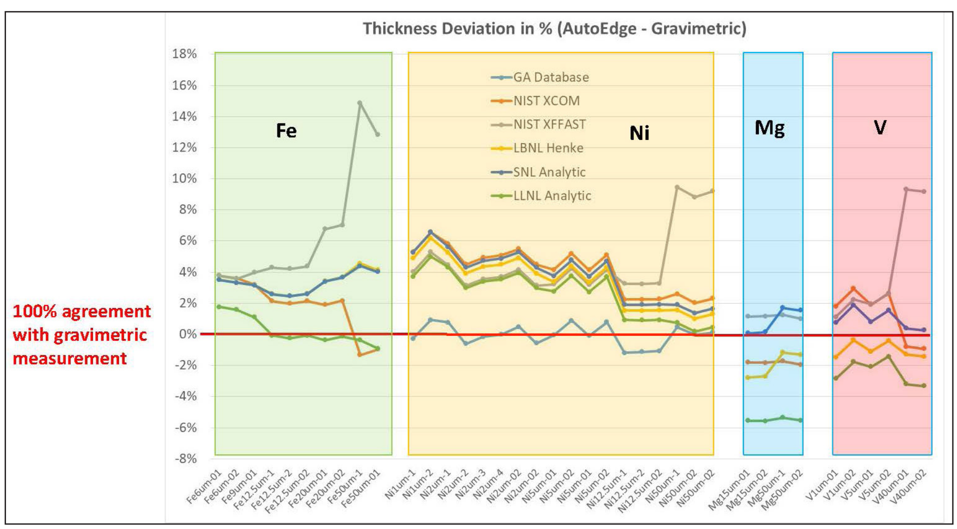

Figure 2. Inaccuracies in existing X-ray databases leads to significant error in measurement (not limited to Ni, as shown for Fe, Mg, V), whereas GA's refined X-ray database controls such error to 1% for Ni. Research on other elements is in progress.

systematic data. Since Brookhaven National Laboratory's National Synchrotron Light Source went offline in 2014, there has been no designated beamline in the United States for X-ray filter calibration, leaving a void in the U.S. national programs.

Meanwhile, the stellar opacity experiments at SNL are being replicated on NIF in a multi-laboratory collaboration. If the results can be repeated, the research has significant importance for both fundamental science and national security.

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This work is supported in part by the Department of Energy/National Nuclear Security Administration under Award Number DE-NA 89233119CNA000063. ◆

Evaluating Turbulence Models at High Energy Densities

by Kumar Raman, Jason Bender, Channing Huntington, Steve MacLaren, Sabrina Nagel, and Shon Prisbrey (Lawrence Livermore National Laboratory)

The RESHOCK campaign at Lawrence Livermore National Laboratory is investigating the evolution of turbulent, unstable plasma interfaces that arise in many high energy density (HED) applications including ICF implosions.[1] New National Ignition Facility (NIF) experiments, along with related studies of turbulent shear flows[2,3] provide data and model validation for plasma interfaces in the HED regime. A common approach to modeling such interfaces involves the use of Reynolds-Averaged-Navier-Stokes (RANS) models with parameters partly constrained by theory and experiments, but which need to be tuned for each application. The tuning process is not unique, and the ability of one set of tuned model parameters to predict similar systems with different shock strengths or material densities has not been well tested.

Our experiments measure the mixing-layer width of an unstable interface and are specifically designed to challenge RANS-type mix models where turbulence is assumed to be fully developed. RANS models, to be applicable, require that the mixed state exhibits a broad spectrum of length scales without memory of the detailed initial condition.[4] We utilize precise control of the initial interface conditions along with a repeatable drive history and then compare the measured mix-width growth to RANS model predictions over the time interval when we believe we have a fully-developed, turbulent flow.

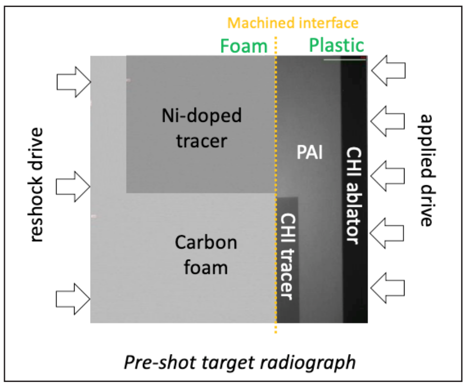

Figure 1: Pre-shot radiograph with the different materials and regions labeled. The direction of the applied drive and reshock drive are also labeled.

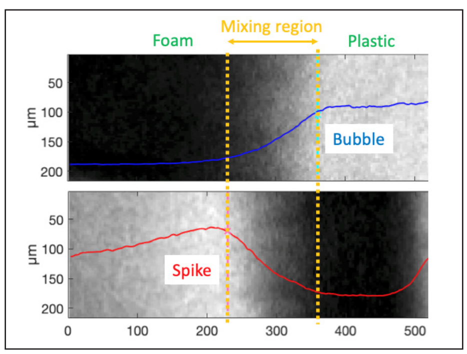

Figure 2. Experimental radiograph. The dashed lines mark bubble and spike front positions determined by where the contrast starts to transition from light to dark. The distance between the dashed lines is the width of the mixing region.

The RESHOCK platform uses an experimental geometry (see Figure 1) that allows us to control the relative timing and magnitude of the opposing shocks that propagate through the unstable interface. Conditions at the unstable interface are controlled by: (1) the initial densities on both sides of the interface, (2) the geometry of the ripple pattern, consisting of wavelengths uniformly distributed between 10 and 20 microns and a 1 micron average amplitude, designed to grow quickly while dominating other target non-uniformities, and (3) precise, repeatable drive conditions. The time interval between the arrival of the initial and second shocks at the interface is set by the time needed for the mixing layer to grow a few times larger than the initial wavelength, meeting a nominal criterion for a turbulent transition.[5,6] The arrival of the second shock then aggressively drives the flow into what we believe is a fully-developed turbulent flow.[7] We measure the growth of the turbulent mixing zone after the reshock via radiography (see Figure 2) until boundary effects start to dominate. We use dopants in parts of the plastic and foam to produce an inverse radiograph which allows us to extract an accurate mix-width. Figure 3a shows the mix-width time history from a series of radiographs compared with a RANS model. Here the model is calibrated to the nominal (blue) data and then used to predict the impact of a stronger reshock (red).

RANS models typically have many internal parameters—some of which can interact with each other and influence the predicted mix width. To help determine the uniqueness of a given set of parameters, we run a large suite of simulations in which relevant RANS parameters are systematically varied and then compare with the experimental results to determine

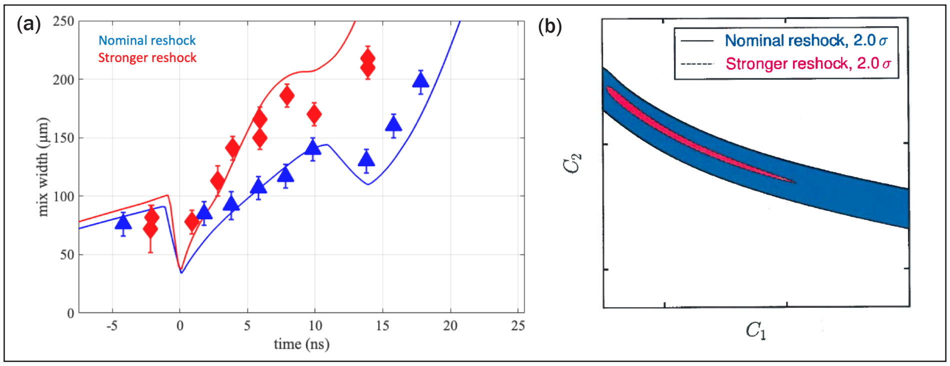

Figure 3. (a) Comparison where we (non-uniquely) calibrate the model to nominal data then predict the effect of a stronger reshock. Origin of time axis is the time the interface is reshocked. (b) Results from a large suite of simulations where the two parameters (C_1, C_2) were systematically varied. The resultant simulated mix-width was then compared to the measured values to produce a regions within the two parameter space that provide a 2σ match to the data. The axes schematically represent the range of a priori acceptable values for the parameters C_1 and C_2, but only a portion of the parameter space matches the data.

model sensitivities or possible uncertainties. Figure 3b shows how two different parameters interact and map out a region of acceptable correlation with the measured mix-width growth. The figure indicates that, to some extent, we can trade these parameters against each other with regard to obtaining a best match to the data. On the other hand, the optimal parameter spaces for the two series do not perfectly coincide implying the degeneracy is not complete, i.e., that only a smaller subset of the RANS parameters that fit the nominal data would provide an acceptable fit if extrapolated to the stronger reshock data set. Comparisons of this type, done over many data sets, provide insight into the RANS parameter space, highlight potential issues with extrapolating from calibration data, and guide optimizations of the framework for current and future HED applications.

Two caveats should be noted. The first is that we can measure the mix width but are unable to directly verify that the flow is fully turbulent due to current diagnostic limitations. Technically speaking, the diagnostic limitations mean that we cannot measure flow properties at intermediate-length scales, which for a fully-developed turbulent flow would show a decoupling of the large scales driven by bulk forcing and the small scales where energy is dissipated.[9] For our experiment, some characteristic numbers are about ~100 microns for a bulk scale, nominally the width of the mixing region, and ~1 micron for the upper end of the intermediate scales, whereas dissipative scales are much smaller (see Ref. 10 for details of these estimates) which may be compared with the 25 micron spatial resolution of the imaging system. The second is that the mix width is not the optimal quantity for a modeling comparison, since many parameter sensitivities are exhibited more through the internal structure of the mixing region than its overall width.[11,12,13]

Hence, more work is needed to move beyond large-scale feature evolution to more fully validate a turbulence model for the HED regime. We look forward to when HED diagnostics advance, in spatial resolution and in other respects, to enable measurements of the turbulent flow field that are routine for conventional flows (for example, see Ref. 14). We expect such diagnostic advancements, coupled with the precise control of initial and driving conditions inherent to HED experiments, to be a powerful combination for studying turbulent mixing in the HED regime.

The ability to measure the mix width in the HED regime and then vary the initial conditions of the turbulent mixing over a large range of densities and shock pressure allows a strong test for the validity of a tuned RANS mix model. Future experiments that can minutely probe the relationship between turbulent length scales will be more constraining than the bulk measurement of the mix-width, but, as seen by the data being produced by the RESHOCK campaign, the bulk measurement of mix-width in the HED regime is already providing a test bed for common mix models in the HED regime.

Acknowledgements

The dual-shock drive platform that we use was developed by Los Alamos National Laboratory for the Shock-Shear NIF campaign.[3] We acknowledge Ted Baumann for developing the novel foams required for the analysis technique in Figure 2 and the critical role of NIF target fabrication and operations in making and fielding the targets. We thank Oleg Schilling and Ye Zhou for discussions on turbulence and modeling.

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This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. ◆

DOE/NNSA 2020 Stewardship Science Academic Programs Annual Review Symposium

The 2020 Stewardship Science Academic Programs (SSAP) Annual Review Symposium was held in Washington, DC on February 26-27, 2020. The Symposium, which hosted a record of more than 350 attendees, featured overviews of work to date from ongoing grants and cooperative agreements from the following programs: Stewardship Science Academic Alliances, High Energy Density Laboratory Plasmas, and the National Laser Users' Facility.

Highlights of the Symposium included keynote speaker Dr. William Bookless, NNSA Principal Deputy Administrator, along with presentations on recent accomplishments from grantees, presentations from the NNSA national laboratories, and poster session and reception. The posters on display were truly excellent. It was difficult to select the following Outstanding Poster Award winners.

David Bernstein, The University of Iowa, *Transverse and Stopping Forces in Strongly-Magnetized Plasma from Molecular Dynamics Simulations*

Benjamin Brugman, Michigan State University, *Strength, Deformation, and Equation of State of Tungsten Carbide to 66 GPa*

Paul Fanto, Yale University, *State Densities of Nuclei in Static-Path Plus Random-Phase Approximation*

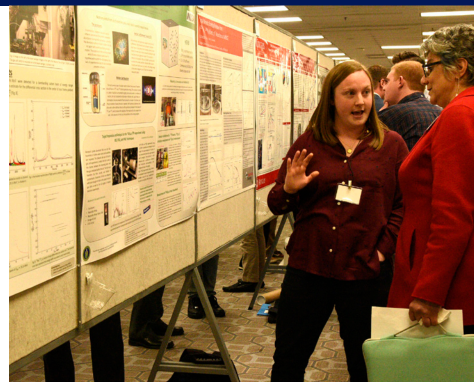
Daniel Felton, University of Notre Dame, *Radiation Induced Assembly of Uranium Peroxide Nanoclusters*

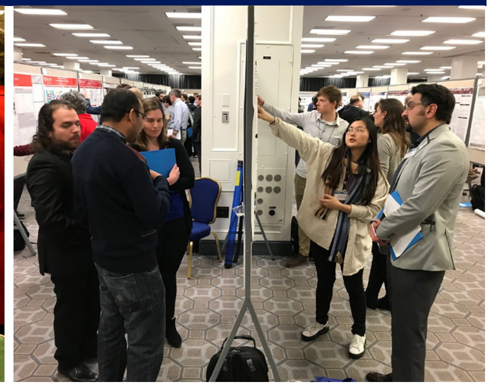
Maren Hatch, University of New Mexico, *Development of Novel Dual View, Four Frame Imaging System and Other Diagnostics to Study Electrothermal Instabilities on Mykonos*

Rebecca Toomey, Rutgers University, *A Measurement of* $^{18}O(\alpha,n)^{21}Ne$ *for Nuclear Physics and Nonproliferation*

Ashley Williams, University of South Florida, *Probing Metastability of Carbon at High Pressures by Predictive First-Principles Simulations*

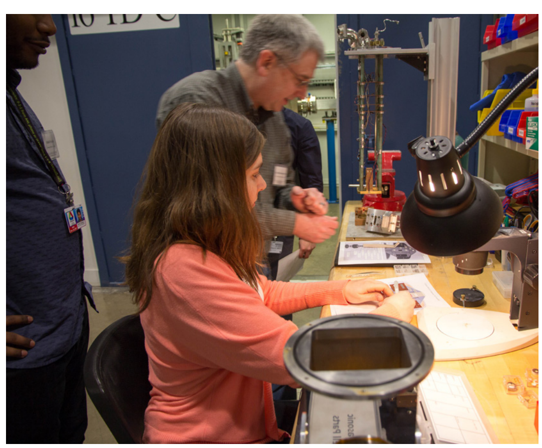
Shu Zhang, University of California, San Diego, *Pump-Depletion Dynamics and Saturation of Stimulated Brillouin Scattering in Shock Ignition Relevant Experiments* ◆





2020 SSAP Symposium Poster Session. *This year, 118 graduate student posters were featured. There were 82 non-graduate students, including Principal investigators, advisors, and NNSA and national laboratory personnel, who served as judges. Both numbers are new records! Top and right: Students answer questions about their cutting-edge research. The eight talented graduate students who received an Outstanding Poster Award at this year's symposium are pictured below. From left to right: Ann J. Satsangi, SSAA Program Director, Zhang, Williams, Toomey, Hatch, Felton, Fanto, Brugman, Bernstein, and Michael Kreisler, Science Advisor to NNSA.*

HPCAT Workshop *(continued from cover)*



HPCAT's director and staff. Day Two provided hands-on demonstrations and training to use the facilities. The workshop brought together a diverse community, which included NNSA/SSAP PIs, scientific staff from three national labs (LLNL/LANL/SNL), various early career university faculty, and HPCAT staff. In all, it was a successful workshop with over 50 participants, including students and postdocs. ◆