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Modeling the Interaction of Laser-Produced Proton Beams with Matter

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Abstract

A major goal of this project is to significantly increase our understanding of isochoric heating of matter using laser produced proton beams, and the associated high energy density (HED) and warm dense matter (WDM) regimes generated. This will benefit research fields such as planetary science, fusion energy, plasma physics, and material science. For example, it will enhance our understanding of WDM properties of iron and silica under conditions encountered in planetary interiors and diagnostic components in fusion devices exposed to high fluxes of energetic plasma ions. The project is motivated by recent experiments that irradiated Si targets with proton beams generated by the 20 TW-laser at the SLAC MEC end-station. The HED/WDM states are probed using the 50 fs hard X-rays available in the 3rd harmonic of the LCLS. As part of this project, results from the phase contrast X-ray imaging, which shows the generation of compression waves that produces rear surface spallation, are compared with results from the 3D multi-physics multi-material code, PISALE, that combines Arbitrary Lagrangian-Eulerian (ALE) hydrodynamics with Adaptive Mesh Refinement (AMR). This comparison required modifications to several physics models in the PISALE (Pacific Island Structured-AMR with ALE) code. An important aspect of this project is the continued training of graduate students in HED physics and in conducting complex multiphysics simulations.

1 Introduction

Increasing our understanding of isochoric heating of matter and the associated high energy density (HED) and warm dense matter (WDM) generated regimes using laser-produced proton beams will benefit research in many fields, such as planetary science, fusion energy, plasma physics, and material science. The project is motivated by recent SLAC experiments that irradiated Si targets, at near constant density to eV temperatures, with proton beams generated by the 20 TW-laser at the MEC end-station. This short-lived high-temperature, high-density state is probed using the 50 fs hard X-rays available in the 3rd harmonic of the LCLS. The results of the phase-contrast X-ray imaging indicate ion energy deposition at the Bragg peak located inside the 20 μm thick Si target, and the subsequent evolution reveals the generation of compression waves that produce rear surface spallation.

In this project, we further developed and used the University of Hawaii PISALE (Pacific Island Structured-AMR with ALE) code to model these SLAC experiments. The 3D multi-physics multi-material code, PISALE, combines Arbitrary Lagrangian-Eulerian (ALE) hydrodynamics with

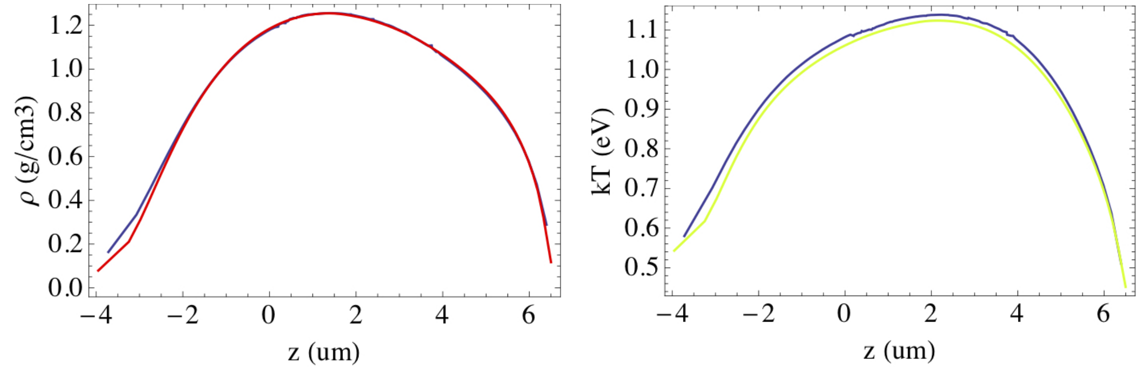

Figure 1: Comparison of PISALE and Hydra results at the end of 1 ns beam of 2.8 MeV Li ions heating an Al plate. Left image show the calculated density using PISALE (blue) and Hydra (red). Right image shows calculated temperature using PISALE (blue) and Hydra (lime).

Adaptive Mesh Refinement (AMR). The PISALE code has physics models that include laser/ion deposition, radiation hydrodynamics, thermal diffusion, anisotropic material strength with material time history, advanced models for fragmentation, and surface tension models. The PISALE code calls a Scalable Structured-AMR Application Infrastructure (SAMRAI) library. The PISALE code has an ion beam deposition package that has been used to model Li ions. The results of using the ion package were validated by a comparison with the results of the LLNL Hydra code for Li ions heating an Al plate, as shown in Fig.~(1). Modeling new experimental configurations generally requires modifications to the code in addition to determining new parameters for the various models that are used in the simulations. One advantage of PISALE over some codes used to model DOE funded experiments such as those at SLAC, is that graduate students and postdocs can modify the source for a particular experiment. For example, graduate students worked on the PISALE surface tension and other packages to model SLAC experiments where an x-ray free electron laser (XFEL) beam heated water and hydrogen droplets. We obtained excellent agreement of the calculated initial dynamics of water droplets compared to experimental optical images. This work, funded by DOE grant SC-0021374, also studied target fratricide, where a following droplet is significantly perturbed by the explosion of the heated droplet. The effect was observed for water droplets, but is difficult to study experimentally for hydrogen because of the 10x smaller droplets. The PISALE simulations showed that target fratricide is also important for hydrogen droplets.

In the next section, we discuss some recent improvements to the PISALE code and computational resources associated with this project. We follow with sections that provide a summary of the SLAC experiments and associated PISALE simulations. We then discuss training, professional development, and dissemination of results. We provide a summary at the end.

2 Recent Improvements to PISALE and Computational Resources

The PISALE codebase contains a Partial Differential Equation (PDE) solver framework, and the solution of these PDEs on modern High Performance Computing (HPC) platforms has enabled PISALE to make contributions to many diverse applications. The first version of the code was used to solve pure gas dynamics problems such as Sedov blast wave simulations. The addition of elastic/plastic flow terms and anisotropic material failure models with material history, combined with multi-material capability and laser/ion beam models, greatly expanded the range of applications that can be modeled. PISALE has a range of different strength and failure models that can be used for impact and other applications. Thermal conduction and radiation transport are coupled to the basic conservation law equations and solved by implementing the diffusion approximation, which uses a nodal radiation energy and a zone-averaged nodal temperature.

As part of this project, we evaluated and extended the ion beam package in PISALE. Previous work using the package was restricted to a monoenergetic beam of Li ions. We have determined the appropriate stopping formula for the full range of measured proton energies interacting with a Si sample. We have modified the ion beam package in PISALE to have multiple ion beams with different ion properties, including ion energy, spot size, and fluences as a function of time. The PISALE exploits complex numerical techniques for fully anisotropic stress tensors, interface reconstruction for multiple materials, and a flexible strength/failure infrastructure for analytic or tabulated material models and equations of state. We have determined the appropriate equation of state and material strength/failure model for the Si material used in the SLAC experiments. In the PISALE code, a void material with an associated volume fraction is introduced when a material failure occurs. This can result in spall planes that will be compared to measured spall generation, which is imaged using the 50 fs XFEL beam.

The primary computational system at NERSC during the initial portion of this project was Cori, which is a Cray XC40 with a peak performance of about 30 petaflops. During this project, we ported PISALE to the new Perlmutter system at NERSC. We worked on making PISALE run effectively on Cori (and Perlmutter), including determining the specific modules needed to port and create the code. In addition to the AMR library, SAMRAI, used by PISALE, the code has a number of dependencies, such as Boost, HYPRE, HDF, etc. that must be updated and complied concurrently to be included in the full PISALE build. (Generally, dependent libraries need to be compiled with the same compiler versions for maximum portability.)

We applied for and received sufficient resources on the Cori and Perlmutter systems at NERSC to complete all the required simulations for this project. We validated the many changes we made to the PISALE coding to make it compatible with the version of the C++ standard that is used by the latest compliers on the NERSC systems. We continuously update the repository for the code using Git for version control. We run a suite of test problems to validate any changes made to the PISALE code's HED branch. We are continuing to make major changes to the data structures and other aspects of the PISALE code to make it compatible with recent versions of SAMRAI. The version of SAMRAI we are using provides higher performance and better parallel scalability. We are still working on compatibility with a version of SAMRAI that uses RAJA to obtain better portability, including running on systems using GPUs. Perlmutter, based on the HPE Cray Shasta platform, is a heterogeneous system comprised of 3,072 CPU-only and 1,792 GPU-accelerated nodes, with a performance of 3-4 times that of Cori. We currently use the CPU-only nodes and will be able to exploit the full capability of the system when we run on GPU-accelerated nodes as well.

3 SLAC Experiments: Laser-Produced Proton Beams

Laser-produced high-energy (MeV) proton beams can be used for isochoric heating of solid targets. In the SLAC experiments associated with this project, the 20 TW-laser at the MEC end-station interacts with a polypropylene target producing high energy electrons that pull out protons. The protons are accelerated from the rear surface of the target in a well-defined, highly directional beam, normal to the target surface, and deposit their energy within the secondary sample (the target to be isochorically heated) at the end of their range of travel. In contrast to our work on XFEL beam heating of water and hydrogen droplets, the XFEL beam is used to investigate the dynamics of this beam/matter interaction. The combination of the high intensity short pulse laser

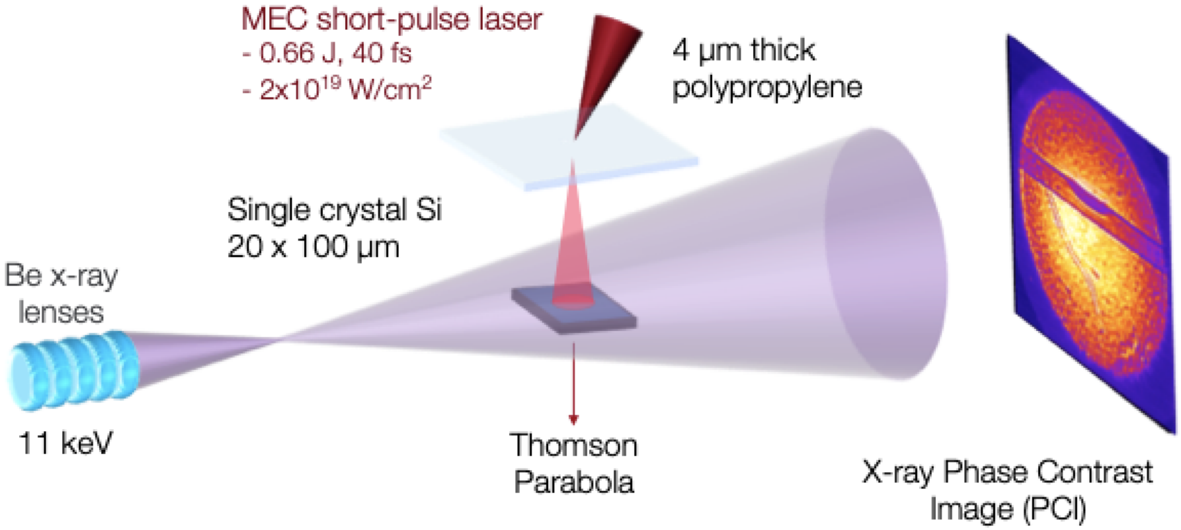

Figure 2: Experimental configuration using proton beams generated by the 20 TW-laser at the SLAC MEC end-station to heat a Si target. This short-lived warm dense matter state sample is imaged using the 50 fs, 11 keV X-ray LCLS beam.

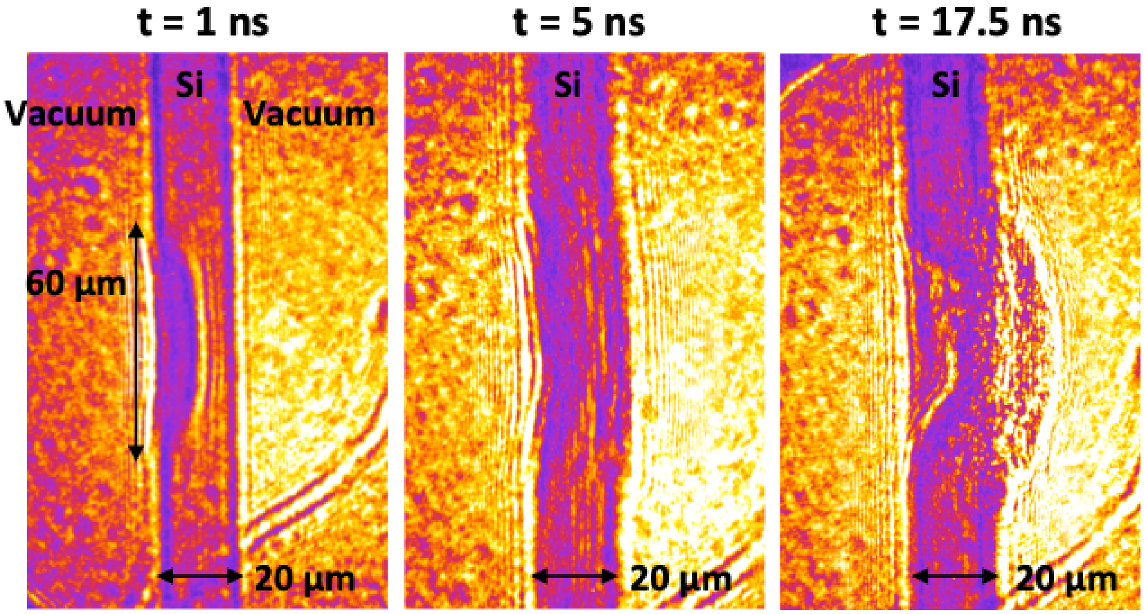

Figure 3: Measured response in Si target from proton beam arriving from the left.

system at MEC, able to create MeV proton beams to isochorically heat matter, with the LCLS, allows unprecedented access to the creation and interrogation of this exotic state of matter.

We show the experimental configuration in Figure 2. The 20 TW MEC short pulse laser is focused on 4 μm thick polypropylene foil, producing an energetic proton beam heats isochorically a 20 μm thick single crystal Si sample located 300-500 μm from the proton source. The measured proton spectrum is shown in Figure 4. The heated target is spatially and temporally diagnosed using the MEC X-ray imager (MXI) diagnostic operated in PCI mode, where phase changes are freely propagating over long distances to detect and quantify density gradients. The 11 keV X-ray collimated LCLS beam is focused to a micron-size spot before the Si sample using a Be compound refractive lens (CRL) stack to image the interaction onto a phosphor screen (YAG). The fluorescence is then re-imaged by a high-resolution optical system coupled to a sCMOS camera with an effective pixel size of 150 nm.

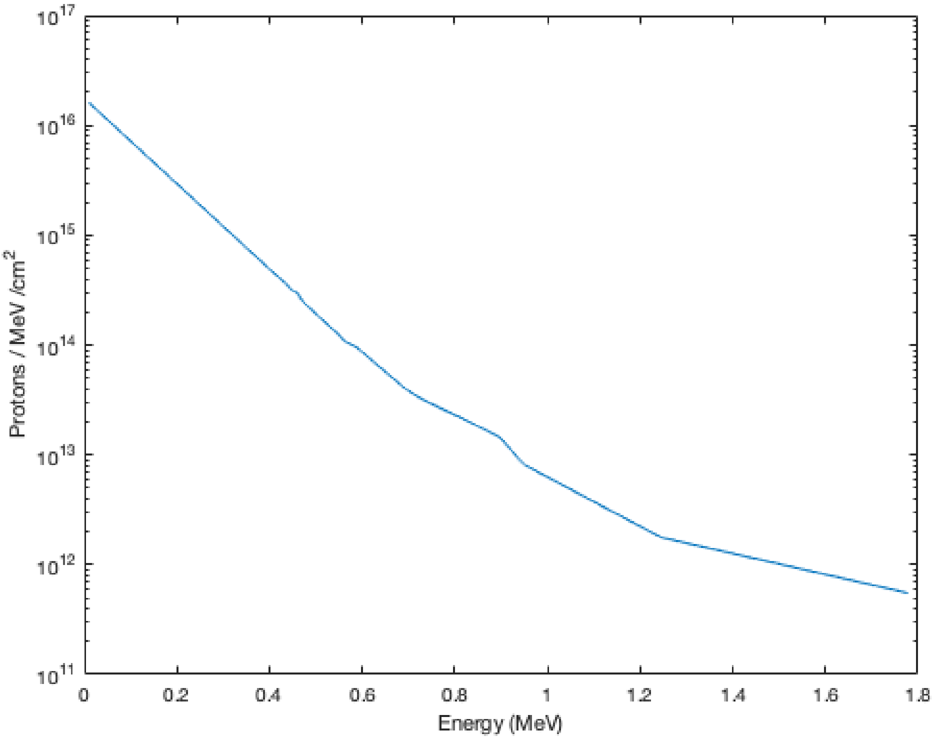

Figure 4: Measured proton spectrum generated by the 20 TW-laser striking polypropylene target.

Typical experimental results obtained during the LCLS experiment are shown in Figure 3. The MeV proton beam arrives at the target from the left. These measurements visualize the density evolution as a function of time indicating the deposition of MeV protons at 1 ns, compression wave generation at 5 ns, and material failure and spallation at 17.5 ns delays. Although X-ray diffraction diagnostics were implemented during the experiment, bremsstrahlung x-ray background generated by the short-pulse interaction significantly impacted the quality of the data.

4 PISALE Simulation Results

To model these new SLAC experiments, we use experimental data for the proton spectrum, shown in Figure 4, as input to PISALE. All the protons leave the polypropylene foil with a duration of less than 100 ps. However, the arrival time at the Si sample is a function of their energy, with their highest energy ones arriving first. We divide the protons into different energy groups with

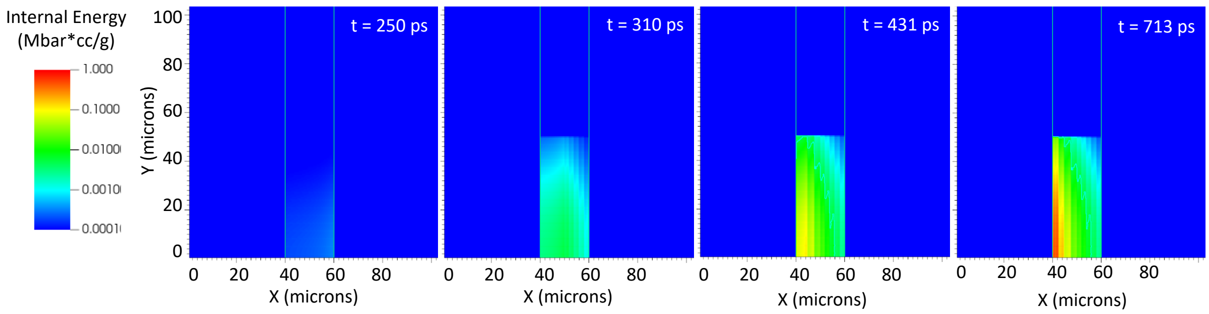

Figure 5: Calculated internal energy per unit mass of 20 μm thick Si target heated by proton beam arriving from the left at four times.

corresponding different arrival times. Given the distance between the polypropylene foil and the Si sample, all of the proton energy deposition is complete in about 1 ns. In addition to arriving at different times, the ions with different energies deposit their energy at different locations in the Si sample. We explored using different number of energy groups, and the results shown in this report are for 17 energy groups going from 0.05 to 1.8 MeV with almost 60% of the energy in the proton beam being in the 0.2 to 0.6 MeV energy range. Less than 10% of the proton beam energy is below 0.2 MeV.

In Figure 5 we show results from the PISALE simulation for the internal energy per unit mass inside the 20 μm thick Si target heated by the 50 μm radius proton beam coming from the left. The first image is at 250 ps when only protons with energy greater than 1.3 MeV have started to arrive at the target. One can see a small amount of heating in the center of the beam. Note the log scale. The next image is at 310 ps, with heating seen in the entire beam with the deposition relatively uniform through the thickness of the Si target. This is expected for these high-energy protons. At 431 ps, some of the lower-energy protons with shorter stopping distances start to arrive, and we see a higher internal energy on the front side of Si target. In the far right image, we show results at 713 ps when protons in the lowest-energy group have started to arrive, and most higher-energy protons have deposited their energy or have passed through the Si target.

The calculated response of the Si target to heating by the proton beam is shown in Figure 5, where we show the density with a linear scale at four times. In the far left image at 1.4 ns, we see the shock moving to the right with a narrow density enhancement location about 3 μm into the Si target in the center of the beam path. In the next image at 2 ns, the density enhancement has broadened and is about 7 μm into the Si target. This corresponds to a velocity of 6.7 μm/ns. This is consistent with the observed velocity obtained from images at 1 and 5 ns in Figure 3. The start of rear surface motion in the simulation is seen in the 6 ns image in Figure 5. Rear-surface spall is seen in the image on the far right at 9 ns with some melting of the Si target. The PISALE simulations are in agreement with experimental data, including shock speed and rear-surface spall.

The project has expanded the capability of the PISALE code to model complex ion beams with varying energies, arrival times, and other beam properties. This is beneficial for ongoing modeling efforts in modeling laser-produced ion for the formation of color centers relevant to photon qubits funded by DOE grant DE-SC0024403.

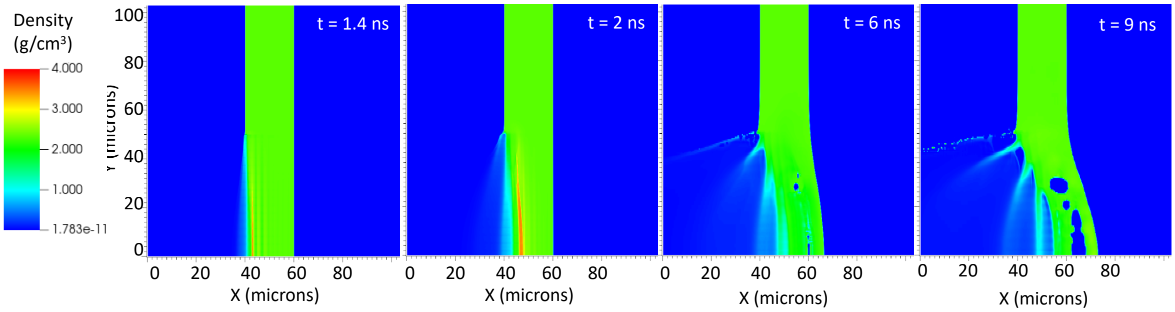

Figure 6: Calculated response of 20 μm thick Si target following heating by proton beam at four times.Measured response in Si target from MeV proton beam arriving from the left.

5 Training, Professional Development, and Dissemination of Results

The project provided many opportunities for training and professional development. Working with our collaborator, Prof. Siegfried Glenzer from Stanford University and SLAC, we continued training a Stanford graduate student, Claudia Parisuaña, in HPC simulations, HED/WDM physics, and using visualizations to compare calculated and measured quantities. This student also did excellent work simulating droplet dynamics following heating by an XFEL beam. We also continued to train an applied math graduate student, Jack McKee, at the University of Hawaii (UH) on how to build and run the PISALE code, as well as relevant HED/WDM physics. This student was a major contributor to extending the capability of the ion beam package in PISALE and in running the majority of the simulations shown in the previous section. The two senior UH personnel of this project, Koniges and Eder, participated in additional NERSC training with a focus on being able to use the GPUs on the new Perlmutter system. Additionally, Koniges and Eder both contributed to the training of the entire scientific community through their SC22 and SC23 tutorials, "OpenMP Common Core: a "Hands-On" Exploration." The PI of the project continued to expand her professional development by educating herself in software management techniques. She was requested to present PISALE capabilities and University of Hawaii ideas to members of the DOE Exascale Computing team. She was also appointed to the prestigious Advanced Scientific Computing Advisory Committee (ASCAC). We continued to make extensive use of Zoom and Slack in addition to more traditional means for PISALE code development and collaboration.

The results of this project have been broadly disseminated to communities of interest. The PISALE website (https://pisale.bitbucket.io/) provides background on the code, a list of associated papers, a short description of funded grants, including this project, photos of team members, and a gallery of visualizations. This site has been widely disseminated to students and researchers of interest. At the 64th Annual Meeting of the APS Division of Plasma Physics, October 17–21, 2022, Spokane, WA, the PI gave a poster, "Modeling Plasma Physics Phenomena with a Complex Multiphysics Code." Claudia Parisuana gave an update on her PISALE work in a poster at the 65th Annual Meeting of the APS Division of Plasma Physics, October 30–November 3, 2023, Denver, CO. Prior to this meeting, the PI and senior personnel Eder attended the "SimNet Meet 'n Greet" event and gave a poster "PISALE: A Research Friendly Tool for Modeling HED LaserNetUS experiments on HPC Platforms." A Best Paper Award was received for, "A Survey of Recent Applications of the PISALE Code and PDE Framework," by A. Koniges, et al., associated with the ADVCOMP

2023 conference.

6 Summary

We extended the capability of the PISALE code to model an additional class of experiments using laser-produced ions to heat a range of materials. We focused on recent SLAC experiments using protons to heat Si samples. We have determined the appropriate stopping formula for the full range of measured proton energies interacting with a silicon sample. We have modified the ion beam package in PISALE to have multiple ion beams with different ion properties, including ion energy, spot size, and fluences as a function of time. Using strength and failure models for Si, we compared observed and calculated spallation associated with proton heating. This work is relevant to diagnostic components in fusion devices exposed to high fluxes of energetic plasma ions. The PISALE code was shown to perform well on both the Cori and Perlmutter HPC systems at the DOE's NERSC facility. We also made significant improvements to the build systems to improve portability and made major changes to the PISALE code to allow it to use more recent versions of the SAMRAI library with the goal of using GPUs in the future.