Modeling Warm Dense Matter Experiments using the 3D ALE-AMR Code and the Move Toward Exascale Computing

Alice Koniges[1,a], Wangyi Liu[1], John Barnard[2], Alex Friedman[2], Grant Logan[1], David Eder[2], Aaron Fisher[2], Nathan Masters[2], and Andrea Bertozzi[3]

[1] Lawrence Berkeley National Laboratory
[2] Lawrence Livermore National Laboratory
[3] University of California, Los Angeles

Abstract. The Neutralized Drift Compression Experiment II (NDCX II) is an induction accelerator planned for initial commissioning in 2012. The final design calls for a 3 MeV, Li+ ion beam, delivered in a bunch with characteristic pulse duration of 1 ns, and transverse dimension of order 1 mm. The NDCX II will be used in studies of material in the warm dense matter (WDM) regime, and ion beam/hydrodynamic coupling experiments relevant to heavy ion based inertial fusion energy. We discuss recent efforts to adapt the 3D ALE-AMR code to model WDM experiments on NDCX II. The code, which combines Arbitrary Lagrangian Eulerian (ALE) hydrodynamics with Adaptive Mesh Refinement (AMR), has physics models that include ion deposition, radiation hydrodynamics, thermal diffusion, anisotropic material strength with material time history, and advanced models for fragmentation. Experiments at NDCX-II will explore the process of bubble and droplet formation (two-phase expansion) of superheated metal solids using ion beams. Experiments at higher temperatures will explore equation of state and heavy ion fusion beam-to-target energy coupling efficiency. Ion beams allow precise control of local beam energy deposition providing uniform volumetric heating on a timescale shorter than that of hydrodynamic expansion. The ALE-AMR code does not have any export control restrictions and is currently running at the National Energy Research Scientific Computing Center (NERSC) at LBNL and has been shown to scale well to thousands of CPUs. New surface tension models that are being implemented and applied to WDM experiments. Some of the approaches use a diffuse interface surface tension model that is based on the advective Cahn-Hilliard equations, which allows for droplet breakup in divergent velocity fields without the need for imposed perturbations. Other methods require seeding or other methods for droplet breakup. We also briefly discuss the effects of the move to exascale computing and related computational changes on general modeling codes in fusion energy.

1 Introduction

Warm Dense Matter (WDM) is an emerging and challenging field that is at the crossroads of strongly and weakly coupled plasmas, degeneracy and non-degeneracy, and solid, liquid and vapor states. The basic physical properties, e.g., opacities, conductivities, dielectric functions, heat capacities, and phase transitions, are not well understood for WDM conditions. The response of material to dynamic loading, e.g., droplet and bubble formation, is of fundamental interest and depends critically on the controlling physical parameters. The experimental challenge is to create sufficiently warm (0.5 -5 eV), nearly uniform matter at near solid densities. Our approach is to use a heating source that penetrates a sample,

[a] e-mail: aekoniges@lbl.gov

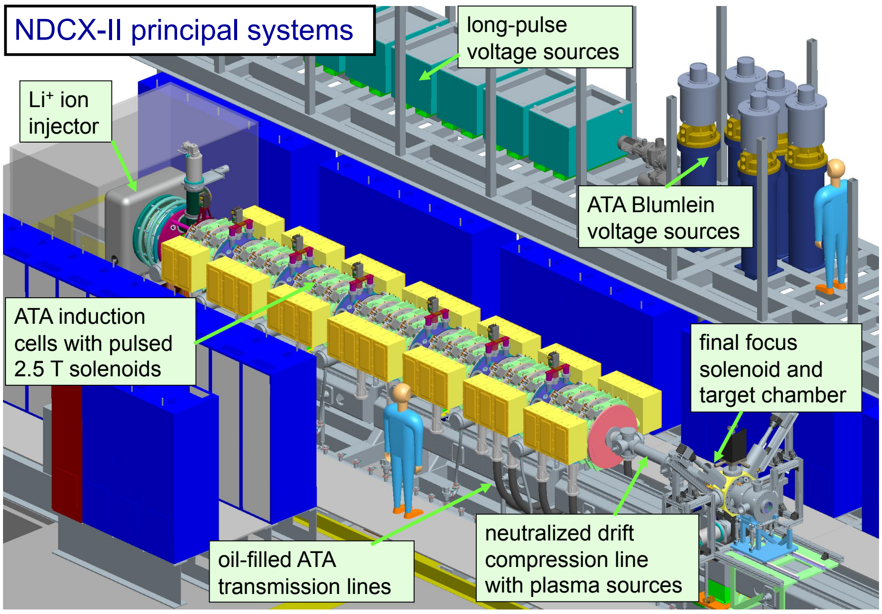

Fig. 1. The NDCX-II machine at LBNL.

e.g., high-energy ions, with a pulse short enough to achieve heating prior to significant hydrodynamic motion. Accurate modeling of experiments is critical to obtain a true understanding of WDM properties and related phenomena. We are developing a 3D open-source, multi-physics, multi-material code ALE-AMR, for modeling the WDM regime. Recently changes in computer architecture are forcing radical changes in computational modeling for the drive to exascale computing. In this paper, we also discuss the effects of these computational changes on large scale energy modeling codes such as ALE-AMR.

2 The NDCX-II Facility

A key feature for NDCX-II is time-of-flight longitudinal "drift compression" of a section of the beam to achieve a high intensity pulse; this is a process analogous to chirped-pulse compression of a short-pulse laser beam. A head-to-tail velocity gradient is imparted to the ion beam by a set of induction cells (accelerating elements), and the pulse then compresses as it drifts down a beam line, in a neutralizing plasma environment which provides space-charge compensation. NDCX-II will accelerate a beam containing 20-50 nC of Li+ ions to 1.2-3 MeV and compress it into an sub-ns pulse at the target with an 1-mm radius spot size. (Initial operation will have longer pulses and larger focal spots as discussed below.) The machine is an induction linac with custom voltage waveforms to control the longitudinal space charge forces and compress the pulse. Overall longitudinal compression factors of 500X are required to achieve a 1-ns pulse, but most of that compression occurs in the accelerator [1]. To be cost effective, NDCX-II reuses and modifies induction cores and cells and some of the pulsed power hardware from LLNL's decommissioned Advanced Test (electron) Accelerator (ATA). Up to 46 cells could be used on NDCX-II but the initial configuration will consist of 27 cells that reach an ion energy of 1.2 MeV. Figure 1 shows the layout of the NDCX-II facility. Extensive particle-in-cell computer simulation studies have enabled an attractive physics design that meets the stringent cost goal [1]. The blumleins (blue cylinders in the figure) can energize the ferrite cores in the induction cells with voltage pulses up to 250 kV for 70 ns. In order to minimize the accelerator length and to optimize the usage

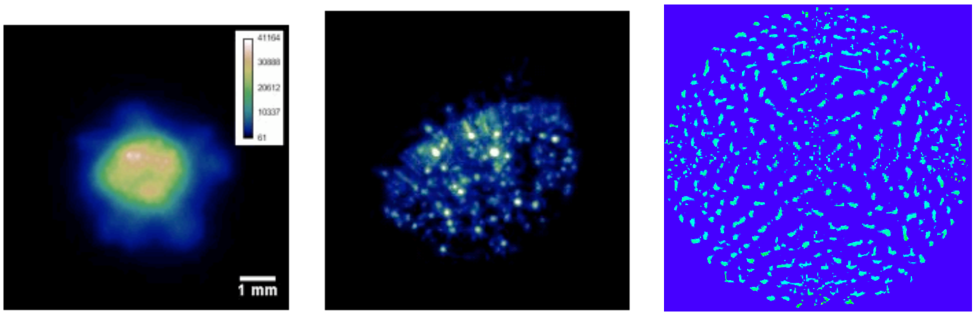

Fig. 2. (left) Gated camera image (gate width = 6 μs) of a carbon target heated by a NDCX-I beam. (center) Shower of hot platinum debris fragments/droplets 500 μs after the beam pulse. (right) Preliminary ALE-AMR simulation for a surface tension model in 2D with symmetry.

of pulsed power, an initial stage of non-neutral beam compression, at the first few induction cells after the injector, will shorten the pulse length from 500 ns to less than 70 ns. Long-pulse voltage generators are used at the front end while blumleins power the rest of the acceleration. The shorter pulse (sub-ns) and longer ion range as compared to NDCX-I will allow more nearly isochoric heating of the target.

3 Modeling Work

Simulations of NDCX-II targets require a large number of models/packages to capture the essential physics. The ALE-AMR code has ion, x-ray and laser deposition, radiation hydrodynamics, thermal diffusion, anisotropic material strength with material time history, and advanced models for fragmentation including void insertion [2]. We are recently adding surface tension models to the code and benchmarking the ion beam package with analytical stopping distance results and other ion beam implementations in hydro codes. A study of including surface tension models into the code using the advective Cahn-Hilliard equations has been described[3]. When solid material fails in the code, a small volume of void is inserted in the zone. If the zone is stretched due to tensile forces or a divergent velocity field, the majority of the volume increase in the zone is due to void growth. The interface reconstruction scheme allows for void regions in neighboring zones to merge and can produce fragments of material surrounded by void. It is possible that a similar model can be used for the breakup of droplets in simulations with surface tension. Figure 2 shows a typical NDCX-I (the predecessor to NDCX-2) gated image and the shower of hot platinum debris produced as a result of the beam pulse (middle). A very first ALE-AMR simulation of the droplet breakup is given in the far right image. Although the simulation uses symmetry for simplicity at this point, and we have simplified the beam heating process with an initially-heated droplet, the ALE-AMR image of the droplet breakup shows a nice visual similarity to the experimental results.

4 High Performance Computing

From the perspective of memory volume or arithmetic throughput, the needs of computational scientists are, for all practical purposes, unbounded. As computing power grows, resolution increases, time scales are extended, and the number of phenomena that can be studied together, in context, increases. Application codes have moved from one, to two, to three-dimensional geometries, often on unstructured and dynamically changing grids. In the next generation of application codes there will be a continued drive towards higher fidelity through full multiphysics simulations of real-world phenomena. For WDM, this is particularly important as we strive to model the physics capturing different regimes of material state (solid fragments, molten droplets, vapor and radiating plasma) all on an irregular moving adaptive mesh.

One driving force that is causing applications to undergo a revolutionary change is the underlying change in architecture due to new multicore and heterogenous computing nodes that are currently being designed primarily to increase performance without severe increases in energy consumption. Concurrency will increase exponentially, and neither memory bandwidth nor volume will keep up with the growth in arithmetic performance. Locality must be exploited in a way that allows the memory hierarchy to be used with good power and time efficiency. Soft error rates will increase, and it will no longer be enough to simply drop an occasional checkpoint to achieve resilience. Some of our work on the ALR-AMR is to both exploit these changes to allow for more complicated physics models, while at the same time making sure our simulations run effectively at scale on new architectures such as the NERSC Hopper Cray XE6.

5 Summary

Success at NDCX-II requires an integrated experimental/computational effort. The 3D multi-physics multi-material code, ALE-AMR, is unique in its ability to model hot radiating plasmas and cold fragmenting solids. It is an open science code without export control restrictions that can model NDCX-II. NDCX-II experiments will explore WDM issues such as equation of state effects and heavy ion fusion beam-to-target energy coupling efficiency. Modeling results can be used to plan experiments, critique shots, and compare with experiment data using synthetic diagnostics. We are exploring the addition of surface tension models to the physics of ALE-AMR. Using this new code we hope to explore the process of bubble and droplet formation (two-phase expansion) of superheated metal solids using ion beams. The code has been shown to scale to thousands of CPUs at NERSC, allowing the complex 3D modeling that makes this effort possible. Next generation computing implies an architectural revolution, that with the additional of advanced programming techniques, can further the development of such integrated experimental and computational programs.

6 Acknowledgements

This research used resources of the National Energy Research Scientific Computing Center, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. Work by LBNL was supported by the Director, Office of Science of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. Work by LLNL was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Security, LLC, Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.
This work is dedicated to the memory of Frank Bieniosek (1953 - 2011) who contributed the NDCX-I experimental data images.

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