Lawrence Livermore National Laboratories Perspective on Code Development and High Performance Computing Resources in Support of the National HED/ICF Effort

C. J. Clouse, M. J. Edwards, M. G. McCoy, M. M. Marinak, C. P. Verdon

Disclaimer

This document was prepared as an account of work sponsored by an agency of the United States government. Neither the United States government nor Lawrence Livermore National Security, LLC, nor any of their employees makes any warranty, expressed or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States government or Lawrence Livermore National Security, LLC. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States government or Lawrence Livermore National Security, LLC, and shall not be used for advertising or product endorsement purposes.

Lawrence Livermore National Laboratories Perspective on Code Development and High Performance Computing Resources in Support of the National HED/ICF Effort

C. J. Clouse, M. J. Edwards, M. G. McCoy, M. M. Marinak, C. P. Verdon

July 2015

Introduction

Through its Advanced Scientific Computing (ASC) and Inertial Confinement Fusion (ICF) code development efforts, Lawrence Livermore National Laboratory (LLNL) provides a world leading numerical simulation capability for the National HED/ICF program in support of the Stockpile Stewardship Program (SSP). In addition the ASC effort provides high performance computing platform capabilities upon which these codes are run. LLNL remains committed to, and will work with, the national HED/ICF program community to help insure numerical simulation needs are met and to make those capabilities available, consistent with programmatic priorities and available resources.

The HED/ICF mission is supported by a suite of codes. The development of these codes has, and currently is supported through, both the ICF funding and ASC funding. HYDRA is currently the mainline computational tool for the ignition effort within ICF and is supported predominately through the ICF program. Generally, new capabilities that are of principal importance to the ignition mission are developed in HYDRA first and then added to ASC supported tools like LASNEX and ARES. Capabilities that are more generally applicable to other WCI missions are developed in ASC simulation tools and then are evaluated for applicability to ICF. Occasionally, because it is only 2D and lacks the considerable complexities associated with the requirement to run massively parallel, development of new ICF capabilities in LASNEX may precede and help inform developments in HYDRA .

Longer term, as next generation platforms are sited in 2018, LLNL's weapons program will assure that HYDRA, key existing ASC codes, and a new code under development specifically targeted to these platforms, will be available for use so that the ICF ignition effort can continue to compute at the leading edge.

Overarching Vision for Code development in Support of HED/ICF

LLNL's long term vision for numerical simulation capabilities in support of HED/ICF is to have more than one numerical design code at LLNL with all the essential algorithms and capabilities needed for simulation of HED/ICF experiments. The current reality is that program drivers and resources limit the pace at which we can attain that vision. Therefore, we have taken an approach that leverages the different capabilities within the existing design codes to help identify and inform the importance of different numerical models and/or algorithm implementations. This, coupled with experimental results, is being used to help inform what enhancements are required within our numerical simulation codes

and their priority for development and implementation. In addition to these considerations it is also our goal, at least for the foreseeable future, to allow for some differences between the codes (particularly where little validation data exists) as a way to assess the impact of those differences on design options.

Near Term ICF Plans

Increased emphasis on high resolution simulations
The push toward higher resolution simulations as well as better accountability of initial conditions, such as capsule mounting perturbations and capsule defects, is helping to narrow the gap between simulation predictions and experimental results. Currently, these simulations are being run with HYDRA at unprecedented problem sizes. ARES, with its ALE-AMR capabilities, will also be used to run at high resolution with cost savings in memory and run time. In addition, the high order Eulerian hydro scheme found in the Miranda code is being implemented into ARES as an alternate hydro option. Miranda has already been used to study hydrodynamic instability growth in ICF implosions at high resolution, but has been limited in its usefulness due to a lack of other relevant physics. Integration in ARES will provide the additional physics needed and provide for the evaluation of an alternate hydro scheme as a long term component of the ICF code suite.

Improved characterization of drive conditions
To account for LPI and cross beam energy transfer, reduced models grounded in first principles are being developed to more accurately characterize the drive conditions. A better characterization of asymmetries in drive conditions is another major factor in helping to explain simulation to experiment discrepancies.

Inclusion of Magnetic Field Effects
While all the ICF simulation tools, ARES, HYDRA and LASNEX, are able to include magnetic field effects on bulk fluid properties in implosion simulations, magnetic field effects on thermal and charged particle transport are currently limited to 2D LASNEX simulations and need to be accounted for in 3D simulations. Development priorities supporting magnetically driven experiments at Z have been formulated in consultation with managers in the simulation program at Sandia National Laboratory. A complete treatment of 3D magnetic fields and their effects on thermal and charged particle transport is under development. The latter effect will be included in the Monte Carlo charged particle transport package, developed under ASC that HYDRA and ARES share.

Support for Direct Drive
Priorities relating to direct drive and magnetic drive have been formulated in consultation with managers in the simulation program at Rochester LLE. While support for spherical direct drive simulations is in HYDRA, developments in support of modeling NIF polar direct drive targets are central to this effort and will be pursued.

Improved Plasma Physics Models
The Boost Sciences for Stockpile Certification (BSSC) effort, which is partially funded by ASC, has been investigating basic plasma physics properties, such as charged particle transport properties in a DT gas

with ICF ablator impurities, using first principles MD and plasma kinetics codes. ASC has recently hired a new plasma physicist from PPL that will provide improved models, shared between ARES and HYDRA, that are informed by this work. In addition, HYDRA is collaborating with researchers at Imperial College and the University of York in the UK to obtain a more accurate assessment of non-local transport in hohlraum plasma profiles making use of a kinetic code.

Preparations for Sierra

Both ARES and HYDRA are heavily involved in the Sierra Center of Excellence (CoE), in which members of those code teams work with experts from IBM and NVIDIA to learn how to optimize their codes for the next generation (2018) ASC Sierra architecture. The CoE is an ASC funded effort intended to move the community on to heterogeneous architectures that include GPU accelerators. GPU programming expertise has been brought in to help. The shared ASC Monte Carlo transport capability used by ARES and HYDRA is involved in both the Sierra COE and a similar Trinity COE effort at LANL and has already demonstrated excellent progress.

Longer Term Plans

Accelerator enabled improvements to physics

Accuracy of the NLTE physics is limited to the number of atomic excitation levels that can be included in the simulation. Deficiencies in the current number of levels routinely used in simulations have already been observed, but increasing the number of levels raises the cost exponentially. Much of this computation could be well optimized for a GPU, potentially making higher fidelity simulations relatively cheap. GPU optimization of the NLTE kernels will be investigated.

In addition, LPI interactions are currently simulated off line with PF3D and will be included in the short term through sub-grid models. Advanced architectures could potentially provide the capability to run interactive LPI models in which the hydro and LPI conditions are updated iteratively, assuring self-consistency.

Next-Gen ICF modeling

Advanced hydro options will be investigated with a variety of ASC codes. These studies will provide insight into potential options for future ICF applications. These models are generally higher order algorithms with high ratios of floating point operations to memory fetches, making them ideal for efficient operations on anticipated advanced architectures. They have also shown greater robustness to mesh imprinting that can destroy spherical symmetry in an implosion. It is expected that any new hydro scheme would then leverage off the infrastructure being developed for Next-Gen ASC applications, including the use of a common Toolkit of computer science infrastructure components, use of a standardized Datastore for storing all mesh information and standardized interfaces to the Datastore, allowing for a modularly developed suite of physics capabilities.

In the Next-Gen framework, the Toolkit and Datastore are intended to replace the roughly 40% of source code typically devoted to such infrastructure needs in our large multi-physics applications. It is expected that HYDRA will be retrofitted to make as much use of the Toolkit and Datastore as possible to

help minimize the long term maintenance cost of HYDRA and more easily leverage new modular physics capabilities written to the Datastore interface.

Collaborations

HYDRA is expected to expand its role of a simulation tool available to external collaborators in which they are able to provide new capabilities. To enable this, we would provide, on a case-by-case basis, the necessary environment and information for collaboration and would provide direct assistance with the integration of the package into the code, if needed. Since tight quality control must be maintained, collaborations may be limited to "trusted" partners, but the executable can be made available to a wider audience. The executable will be made available on the LLNL CZ machines (unclassified collaboration zone, accessible by sensitive country foreign nationals) for availability to collaborators and also might well be made available to collaborators at other sites under defined security controls. The ARES executable and source code will be made available to "trusted" collaborators eligible for RZ (unclassified restricted zone not available to SFNs) account access.

In addition, the ASC program maintains very substantial resources in the CZ and more limited resources in the RZ. LLNL's ASC Program will establish banks and a process to make available computer time to community members working on DOE funded ICF projects. Depending on the demand, there may have to be some proposal process. This is in addition to the resources already provided to the LLNL ICF effort, which consumes about 22% of the ASC computer banks at LLNL. In addition, while the HYDRA team has been working to gather simulation needs from the external community and to try to respond to those needs, the process has been informal. A more formal process of tracking requests for simulation improvements, tracking requests for computer time and coordinating collaborative development activities will be established.