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Final Report for "Verification and Validation of Radiation Hydrodynamics for Astrophysical Applications"

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Final Report for "**Verification and Validation of Radiation Hydrodynamics for Astrophysical Applications**"

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FINAL REPORT
For the period ending 09/30/2007

Prepared for:
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Final Report on

LLNL Subcontract B568673
Verification and Validation of Radiation Hydrodynamics for Astrophysical Applications

PI: Michael Zingale

LLNL Contract Technical Contact: Louis Howell

Summary

The motivation for this work is to gain experience in the methodology of verification and validation (V&V) of astrophysical radiation hydrodynamics codes. In the first period of this work, we focused on building the infrastructure to test a single astrophysical application code, Castro, developed in collaboration between Lawrence Livermore National Laboratory (LLNL) and Lawrence Berkeley Laboratory (LBL). We delivered several hydrodynamic test problems, in the form of coded initial conditions and documentation for verification, routines to perform data analysis, and a generalized regression test suite to allow for continued automated testing.

Motivation

Astrophysical simulation codes aim to model phenomena that elude direct experimentation. Our only direct information about these systems comes from what we observe, and may be transient. Simulation can help further our understanding by allowing virtual experimentation of these systems. However, to have confidence in our simulations requires us to have confidence in the tools we use. Verification and Validation is a process by which we work to build confidence that a simulation code is accurately representing reality.

V&V is a multistep process, and is never really complete. Once a single test problem is working as desired (i.e. that problem is verified), one wants to ensure that subsequent code changes do not break that test. At the same time, one must also search for new verification problems that test the code in a new way. It can be rather tedious to manually retest each of the problems, so before going too far with V&V, it is desirable to have an automated test suite. Our project aims to provide these basic tools for astrophysical radiation hydrodynamics codes.

Technical Approach

For this first period of the project, we decided to focus on the Castro code, developed in part by Louis Howell at LLNL. Castro is an adaptive mesh radiation hydrodynamics code built around the Boxlib adaptive mesh refinement (AMR) framework. Our initial goals were to create several hydrodynamic verification problems, produce the necessary analysis tools, and provided an automated regression testing framework for the code.

Based on our experience at the ASC Flash Center in Chicago, we have seen firsthand the utility of automated regression testing. To bring this testing to Castro, we decided to begin with the flashTest program developed at Chicago. This testing framework will checkout a new copy of the code (from the source control system, such as CVS) and for several user-defined tests, it will compile the code, run the test, and compare the solution against a stored benchmark.

In an ideal world, applying flashTest to our application should involve only minor changes, and the creation of a comparison tool that understands our file format. We began by adapting some convergence testing tools already in the Boxlib framework (in Parallel/util/Convergence/) to do the necessary plotfile comparisons. Most of this functionality was already there, but we added norms of the relative error (in addition to absolute error) and a more descriptive comparision summary. Our resulting changes have been committed back to the CVS repository. Adapting the flashTest routine itself to handle the Boxlib-based codes turned out to be more work than initially thought, due to differences in the build system between FLASH and Boxlib-based codes. Eventually, we decided to write our own regression test framework using ideas from flashTest. The resulting script, test.py, is available in CVS in Parallel/util/regtests/ and should work with any Boxlib-based code.

Defining a test suite is straightforward—an input file is written that describes where the source and comparison tools are, and where to store the output. Each test problem is given a section where the build location is defined (i.e. where you type make), as well as the names of the necessary input files and other job-related information. If one is starting from scratch, you will need to create the benchmark files that subsequent runs will use for comparison, this is accomplished automatically by using the '--make_benchmarks' flag to test.py. Once the list of tests is written and the benchmarks are stored, the test suite can be run as often as desired. Each time it is run, it does a 'cvs update' on the source, compiles and executes the test problems, compares to the stored benchmarks, and updates a master webpage containing the results of the test. For Castro, results from our initial runs are hosted here:

http://astro.sunysb.edu/mzingale/Castro-regtest/

The master page has a single line for each run of the entire suite. Next to the date, is the result: "ALL PASSED", "SOME FAILED", "ALL FAILED", or "BENCHMARKS UPDATED". Regardless of the result, more details can be found by clicking on the date, bringing up the summary for the test run on that day. There, each problem is listed separated, along with the status indicating whether it passed or failed. Clicking on the problem name brings up even more detail, allowing you to look at the input files, the compilation output, the execution output, and the comparison output.

Tests can fail when the code changes, either due to bug fixes (in which case, you'll want to update the benchmarks) or new bugs introduced. The comparison output shows the magnitude of the change. Different optimization or minor reorganization of code will show relative errors near machine precision, as might be expected. Whenever unexpected changes are discovered, the user can look at the result of the cvs update (also posted on the test result pages) to see which files changed since the last test, and then use this information to zero in on the offending changes.

The development of the test suite is ongoing, and already collaborators at LBL are using it for Castro development and we are using it at Stony Brook for another Boxlib-based code. We expect it to work for any lab code built around these frameworks, and would be happy to assist anyone in getting it up and running.

With the testing framework developed, we turned to investigating pure hydrodynamics problems. Several standard 1-d shock tube problems were run, as well as the Sedov blast wave test (a point explosion problem). The results are shown here:

http://astro.sunysb.edu/mzingale/Castro/

Analytic results were produced using an exact Riemann solver. We see good agreement between the analytic results (solid lines) and the Castro results (points). When we found discrepancies, we pointed these out to the developers, and were able to work together to improve the results.

To analyze these results, we needed simple tools to extract one-dimensional slices out of plotfiles or produce angle-averaged profiles of the data. As these tools did not exist, we created them for the benefit of all in the project, and committed them to the CVS repository in fParallel/data_processing/. fextract reads in a plotfile and produces a 1-d slice of the data along any coordinate axis. fsedov reads in a Sedov test plotfile and produces average state quantites as a function of radius. Both of these tools are well commented and should be directly applicable to more advanced test problems we plan to run in the future.

Research or Other Technical Results

The main results of this project were the creation of the tools and testing infrastructure to perform verification tests on Boxlib-based codes. We set up several standard hydrodynamics verification problems, and documented them in the form of Readme files placed in the source code directories, together with instructions on how to perform the comparisons with the analytic solutions.

Looking forward to the next contract year, we will continue this model, this time moving on to radiation verification problems in the same framework. Our goal is to provide a well-documented test suite that can be applied to any astrophysical radiation hydrodynamics code.

Papers and Book Chapters Supported in Part by the Subcontract

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References

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Final Report for "**Verification and Validation of Radiation Hydrodynamics for Astrophysical Applications**"

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Final Report on

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Verification and Validation of Radiation Hydrodynamics for Astrophysical Applications

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LLNL Contract Technical Contact: Louis Howell

Summary

The motivation for this work is to gain experience in the methodology of verification and validation (V&V) of astrophysical radiation hydrodynamics codes. In the first period of this work, we focused on building the infrastructure to test a single astrophysical application code, Castro, developed in collaboration between Lawrence Livermore National Laboratory (LLNL) and Lawrence Berkeley Laboratory (LBL). In this contract period, we focused on radiation transport problems with Castro. We used the understanding of the radiation transport algorithm as implemented in Castro to make suggestions for improvements to the code so that it can be used for general astrophysical radiation transport problems.

Motivation

Castro is meant to be a general community radiation hydrodynamics code for astrophysical problems. When we started this contract period, a single group radiation hydrodynamics solver was implemented, so this became the main focus of this contract period. We proposed to do some straightforward single group problems that are typically used to test other astrophysical codes. In particular, we proposed to implement a Gaussian diffusion test, radiation flux-divergence test, and the light front test. A multigroup radiation solver was also developed for Castro, requiring different test problems. Overall, our goal for this contract period was to learn about the radiation solvers in Castro, implement some basic radiation test problems, and begin to understand what changes are necessary to perform astrophysical problems.

Technical Approach

As in the previous contract period, we performed our work using the Castro code. The hydrodynamics portion of Castro is developed at Lawrence Berkeley National Laboratory and the radiation components are developed at LLNL.

At Stony Brook, the bulk of the work was performed by Eric Myra, the research scientist supported on this project. Overall, Eric was supported half-time for about 5 months. Although Eric has considerable experience in the field of radiation transport, he had no exposure to the Castro code, therefore time was needed to get up to speed on this code. We worked closely with Louis Howell and Mike Singer at LLNL to understand the details of the radiation transport algorithm implemented. This process was greatly helped by a brief trip to Livermore over the summer. Unfortunately, Eric has left stony brook for another academic position, and therefore will not be available for working on this project in the next contract period.

We implemented each of our test problems in the CVS repository for the Castro code. For each problem, we also provided simple documentation explaining the problem and expected results, and, where applicable, a sample solution.

Research or Other Technical Results

The main results of this project were setting up test problems in the Castro framework and providing documentation for those problems in the form of text files committed to the project CVS repository.

Overall, the following test problems were implemented and documented:

- The gray lightfront problem in 1-, 2-, and 3-d Cartesian was added, and verified to agree with the analytic solution.
- The gray lightfront problem in 1-d spherical was implemented and verified.
- The 1-d and 2-d Gaussian diffusion test was implemented and verified. 3-d can easily be added following the 2-d implementation.
- The 2-d flux divergence test was added and compared to the analytic solution. 1-d and 3-d were not implemented, but can be added in a straightforward manner.

The work on these problems was done in close collaboration with Louis Howell and Mike Singer. This collaboration allowed the code to evolve to our needs and we identified features needed for various test problems.

The above list are single group problems and matches the list outlined in the original contract. We also began exploring multigroup problems. A multigroup lightfront problem was added, and appears to give a valid solution, however, we are still working on understanding the full behavior of the multigroup radiation solver. Finally, work began on implementing the radiating sphere problem, however, we have not yet successfully gotten this to run.

In addition to implementing test problems, we also made some improvements to the code infrastructure:

- A new comparison routine (fParallel/data_processing/fcompare.f90) was implemented that can compare two plotfiles in 1-, 2-, or 3-d. (The previous routine did not work with 1-d plotfiles).
- refinement on radiation was added.

We also continued to monitor the code's behavior on basic hydrodynamics problems implemented last contract period.

Over the course of this work, a number of places where code improvements are needed were identified. These changes would be necessary in order to perform astrophysical radiation hydrodynamics calculations with Castro. We list the major improvements needed here:

- The opacities need to be abstracted out of the radiation solvers and put into a separate routine (ideally in the fParallel/extern/directory). This would allow for the user to easily implement different opacities. The opacity routine should take as input (as a minimum) density, temperature, and composition. With these quantities, any opacity module would be able to perform an EOS call to get other thermodynamic quantities (such as chemical potentials). Probably a single interface to return both absorption and scattering opacities would work to begin.
- The general stellar equation of state in the Castro framework (Frank Timmes' helmholtz free energy-based EOS) already includes the radiation pressure. Doing radiation hydrodynamics calculations with Castro would double count the radiation contribution.
- A user-modifiable, problem-specific framework for specifying the radiation group boundaries is required.

Some results of the radiation tests appear at: http://astro.sunysb.edu/mzingale/Castro/

Papers and Book Chapters Supported in Part by the Subcontract

Some of the results of our radiation verification appeared in a poster by Mike Singer (LLNL) for the 2008 Granlibakken conference on radiation transport.

References

N/A

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Summary

The motivation for this work is to gain experience in the methodology of verification and validation (V&V) of astrophysical radiation hydrodynamics codes. In the first period of this work, we focused on building the infrastructure to test a single astrophysical application code, Castro, developed in collaboration between Lawrence Livermore National Laboratory (LLNL) and Lawrence Berkeley Laboratory (LBL). In the second and third periods, we began exploring and testing the radiation capabilities of Castro. Specifically, in the ~5 month period of this contract, we worked on 2 separate projects with Castro: extending the verification efforts to multigroup photon radiation problems and starting the exploration of radiating shocks.

Technical Approach

We implemented the radiating sphere test problem, first described by Graziani (2008). We followed the implementation described in Swesty and Myra (2009). The appeal of this problem is that it exhibits a non-trivial multigroup diffusion, and has an analytic solution. This problem provided a useful testbed for debugging the multigroup photon solver. Castro gets very good agreement with the analytic solution. We also implemented both a gray and multigroup radiation source test problem which tests the radiation energy source term to the gas energy equation. We see excellent agreement to the gray radiation analytic solution. We also implemented a multigroup version of this problem. Although no analytic solution exists in the multigroup case (to our knowledge), the late-time values for the energy should be the same as the gray radiation case. Castro's multigroup solution agrees well with the asymptotic value, with the understanding that small numbers of groups underestimate the initial energy of the blackbody (just discretization error).

Doug Swesty is new to the project this year, and brings with him many years of experience in radiation hydrodynamics. To begin getting acquainted with Castro, Doug reviewed the code and literature describing the algorithm and wrote up a detailed document describing how Castro's radiation solver compares to those in use in astrophysics. Castro does not include dynamic diffusion, a term in the radiation energy equation that couples the radiation field to the fluid velocity. To understand how the absence of this term affects the radiation hydrodynamics solutions, we ran some simple radiating shock tube problems with Castro and compared against Doug's V2D code (Swesty and Myra 2009). These tests showed that the agreement between the codes improves when the problem is optically thin. The document describing these comparisons was committed to the Castro CVS repository in `CASTRO/Parallel/Castro/Exec/RadShock/doc/`.

Our long-term goal for Castro is to study instabilities in radiating shocks. To begin, we decided to try to reproduce some published radiating shock solutions, as originally posed by Ensman (1994). This problem involves the generation of a radiative shock by means of a piston. In the Newtonian case this can effective be modeled on a fixed Eulerian grid by a Galilean boost into a frame co-moving with the piston. This results in initial conditions that have the entire mass of fluid initially moving to the left with uniform velocity at t=0. The problem produces a strong shock that moves rightward. The material behind the shock cools radiatively producing a postshock profile in temperature that reflects this radiative cooling. We have been attempting to model this shock using Castro with limited success. Our results do not match those of Ensmann, nor do they match the results of Hayes et al. (2006) who used this problem as a verification problem for the ZEUS-MP code. Puzzlingly, the results of Ensman and Hayes et al. do not agree either. The Hayes et al. results show a postshock temperature profile that is concave-upward while the Ensman results show a postshock profile that is convex-downward.

Before we can have confidence in Castro's ability to model multi-d radiating shocks, we need to understand the differences we see between Castro and published solutions. Our efforts to compare Castro are complicated by missing terms (dynamic diffusion) in the coupling of the radiation and hydrodynamics. We have attempted to make a comparison through a two-step process. First we have attempted to compare reproduce the results of Ensman using V2D code of Swesty & Myra. This code has the ability to turn the dynamic diffusion terms on and off. Our objective was to carry out the Ensman problem for both cases. Once we had established the importance of dynamic diffusion, by comparing simulations with and without dynamic diffusion, for this particular problem, we intend to compare Castro's results for this problem to both V2D and ZEUS-MP (we have obtained the ZEUS-MP code and have used it to obtain numerical results for this problem). However, the V2D results do not match those of ZEUS-MP and, in fact, qualitatively resemble the results of Ensman code VISPHOT. This is puzzling and we continue to try and track down the origin of the differences between V2D and ZEUS-MP. Without making this comparison we have no way of understanding whether Castro is giving the correct answer or not.

At present, Swesty is still testing V2D in comparison to ZEUS-MP in the hopes of determining which solution is correct. Once a resolution is found, we work on understanding the range of validity of Castro on the radiating shock problem. We expect this work to continue into the next year, outside of this contract.

A separate project during this contract period was to add documentation describing all of the test problems produced so far into the new Castro User's Guide. At this point, all of the hydrodynamics tests have been documented, and the radiation tests are starting to be documented there. This is ongoing. Finally, the PI is working with the Castro developers on a code paper, expected to be submitted to the Astrophysical Journal.

Papers and Book Chapters Supported in Part by the Subcontract

Abstract for the 215th American Astronomical Society Meeting, *CASTRO: A New AMR Radiation-Hydrodynamics Code for Compressible Astrophysics*, Ann Almgren, J. Bell, M. Day, L. Howell, C. Joggerst, E. Myra, J. Nordhaus, M. Singer, M. Zingale

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