Preparing Nuclear Astrophysics for Exascale

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Abstract—Astrophysical explosions such as supernovae are fascinating events that require sophisticated algorithms and substantial computational power to model. Castro and MAESTROeX are nuclear astrophysics codes that simulate thermonuclear fusion in the context of supernovae and X-ray bursts. Examining these nuclear burning processes using high resolution simulations is critical for understanding how these astrophysical explosions occur. In this paper we describe the changes that have been made to these codes to transform them from standard MPI + OpenMP codes targeted at petascale CPU-based systems into a form compatible with the pre-exascale systems now online and the exascale systems coming soon. We then discuss what new science is possible to run on systems such as Summit and Perlmutter that could not have been achieved on the previous generation of supercomputers.

Index Terms—astrophysics, hydrodynamics, computational fluid dynamics, gravity, nuclear reactions, adaptive mesh refinement

I. INTRODUCTION

Stellar explosions create the elements that make life possible and are indispensable tools for mapping the universe. Many of these events are caused by rapid thermonuclear fusion: on time scales much shorter than a second, light elements such as hydrogen and helium are fused into heavier elements such as magnesium and iron. The fusion process releases copious amounts of energy into a small pocket of space, and the temperature of the star is almost instantly raised to billions of degrees. This results in the surface of the star being blown out into space (novae and X-ray bursts) or the complete destruction of the star (supernovae). It is known that thermonuclear explosions happen on white dwarf stars, remnants of stars like the Sun, but in many cases it is not known what triggers these events. Due to the rarity of these events and their great distance from the Earth, observational astronomy is not enough to understand their nature and it must be paired with simulation.

Simulation codes that target these events must be able to simultaneously model the star as a whole (or at least a large part of it) and the initiation of the explosion process, which happens much faster and in a much smaller region than the time and length scales that define the star as a whole. This calls for some form of adaptivity, where the parts of the star that may explode are simulated with higher fidelity (and thus more computational power) than other regions. MAESTROeX ([11]–[3]) and Castro ([4]) are astrophysical simulation codes that simulate, respectively, the time period leading up to the explosion and the explosion itself. They are built on top of the AMReX ([5]) adaptive mesh refinement framework, and provided as part of the AMReX Astrophysics Suite ([6]) of simulation codes.

MAESTROeX and Castro have been used to study the origins of X-ray bursts [7], [8] and thermonuclear supernovae [9], [10] on previous generations of supercomputers including Jaguar and Titan at ORLCF and Edison and Cori at NERSC. MPI was used for parallelism across many nodes, optionally in conjunction with OpenMP for intra-node parallelism. These systems enabled simulations that began to explore the nature of the thermonuclear fusion, but to make the simulations feasible the simulations were performed at relatively low resolutions and over relatively short simulation time scales. Unfortunately, thermonuclear explosions are so sensitive that low resolution simulations can be qualitatively wrong, and it is clear to us that much higher resolution simulations are needed than could have been run on those systems.

Pre-exascale systems that employ accelerators such as Summit and Perlmutter promise to enable such higher resolution simulations, but a substantial code refactoring effort was needed to take advantage of these architectures. (The codes had previously been used on systems such as Blue Waters and Titan but without using their GPUs.) This paper describes the software architecture of these astrophysics codes (and their dependencies, including AMReX) before and after the transition to GPU-ready status and the process taken to get there. Then performance results (at both the single node and many node levels) are presented, and the paper closes with a discussion of the new science simulation capabilities enabled by GPU-powered supercomputers.

II. SOFTWARE ARCHITECTURE AND DEVELOPMENT

The AMReX Astrophysics Suite of codes includes the grid-based hydrodynamics codes MAESTROeX, Castro, and Nyx ([11]). All three rest on top of AMReX, which maintains their

1A thermonuclear supernova, often called a Type Ia supernova, is the explosion of a white dwarf star as a result of energy release associated with nuclear fusion. There is another class of supernovae caused by the collapse of massive stars. We do not examine these core-collapse supernovae in this paper.
gridding capabilities (including adaptive mesh refinement) and other key driver infrastructure such as memory management. AMReX’s core data concept for grid codes is a MultiFab, which is a (possibly disjoint) set of fluid data at a given level of mesh refinement that is distributed across multiple Fabs. (AMReX also supports simulations with particles, which is useful for electromagnetic particle-in-cell codes like WarpX ([12]) and cosmology codes like Nyx.) A Fab represents a contiguous section of space, indexed in one, two, or three dimensions, and it can have multiple fluid components such as density and temperature (that is, it is a four-dimensional array). AMReX codes mostly use an MPI + X parallelism model, where MPI is used to distribute Fabs within a MultiFab over ranks, and some intra-node parallelism model (“X”, where X is a shared memory parallel programming model like OpenMP, OpenACC, or CUDA) may be used for the Fabs within each rank. Fabs are decomposed in a tiled fashion that exposes subsets of the Fab (though the tile may span the whole array), and a typical update to the fluid state involves iterating through the full set of tiles among all Fabs owned by a rank. On the previous generation of supercomputers such as Cori, coarse-grained OpenMP was typically employed for intra-node parallelism, where each OpenMP thread worked on a tile of a Fab. See Figure 1 for an example.

The simulation codes themselves implement all physics relevant for the problem setups of interest. For example, Cas-tro includes physics capabilities for hydrodynamics, gravity, thermal diffusion, and nuclear reactions, and MAESTROeX has a similar set of capabilities. Since there is substantial overlap in the relevant physics, they both rely on a Micro-physics repository that provides modules such as the nuclear reactions. The primary difference between MAESTROeX and Castro is that the former is designed for (relatively) slowly evolving fluid flow such as convection (and can take very large timesteps), while the latter targets rapidly evolving phenomena such as detonations (and takes correspondingly smaller timesteps). For the problems of interest in this paper, both codes feature a combination of locally coupled algorithms (requiring only point-to-point communication between nearest neighbors) and globally coupled algorithms (requiring all-to-all communication).

Traditionally, codes based on AMReX and its predecessor BoxLib implemented their physics kernels in Fortran. A Fortran routine would typically include a triply-nested loop over i, j, and k (x, y, and z in space), where the bounds of the loop are determined by the spatial extent of the tile. Both C++ and Fortran driver interfaces were exposed; Castro and MAESTROeX both use the C++ interface, and the C++ driver would call the Fortran routine through the standard ISO C binding. The programming model for many AMReX codes substantially changed from this approach in preparation for the pre-exascale systems, as discussed in Section III.

Both MAESTROeX and Castro issue new releases monthly, and are co-designed with AMReX and Microphysics so that a given release version (for example, 20.04) is tagged the same way in all codes, and is compatible among all the codes. All of these software packages are freely available in a permissively-licensed open source form on GitHub. Community contributions in the form of issues and pull requests are permitted, and Section III describes a series of contributions we made to these codes to enable them to run on modern supercomputer architectures.

III. Porting to GPUs

Our early attempts at preparation of the AMReX astrophysics codes for heterogeneous architectures focused on programming models that were minimally invasive. In particular, models such as OpenACC are attractive because they allow incremental porting and allow for the maintenance of a single source (portable) code base (a property that we deemed important). However, these efforts were unsuccessful. While the codes primarily used relatively modern Fortran, some components were borrowed from older, fixed-format Fortran code. The most important example was the ordinary differential equation (ODE) integrator, VODE ([14]), which contained numerous constructs that were not compatible with OpenACC (at least as implemented in the compilers available circa 2015), such as computed go to statements. ODE integrators are the key component of nuclear reactions simulations, and so this approach was not feasible. Even in the cases where code actually compiled, we did not achieve performance better than available on CPUs. The architecture of the GPUs available at the time (e.g. the NVIDIA Kepler K20X GPU on the OLCF Titan system) was extremely unfriendly towards the significant amount of thread-local storage needed to evaluate some of the relevant physics.

The first working approach was based on CUDA Fortran. Even for CUDA Fortran, in practice only a subset of the language is supported, so a substantial refactoring of the Fortran code was done to remove all constructs that the PGI compiler effectively disallowed. We still desired portability, so the choice was made to keep the Fortran subroutines in the same format: a loop over some range of indices. But now to expose sufficient parallelism for a GPU, each thread has to be assigned a single zone rather than a tile (Figure 1). This required every part of the algorithm to be expressed in an embarrassingly parallel manner, with no explicit dependence between zones.

However, some parts of the software had previously been written in a way to maximize expected performance on vector CPU architectures. A classic example is the core stencil operation in the hydrodynamics routine, where a slope at a given index is calculated by looking at several zones to the left and right. The CPU code first calculated the slopes for all zones in the x dimension (say), stored them in a local array, and then read from that array in a second loop that used two values from the slope array to reconstruct a polynomial approximation of the fluid state. Converting this to a fully thread parallel format required redundantly calculating two slopes for each zone, which implied more total floating point operations when summed across all threads, but exposed massive parallelism. (The original approach can be
recovered on NVIDIA GPUs through the use of on-chip shared memory and synchronization points, which we have not yet explored.) Fortunately, the refactoring effort ultimately led to a performance improvement on CPUs as well, due largely to decreasing the memory footprint of the code (the code was memory bandwidth bound on CPUs as well).

This approach was quite promising and early testing on GPU-enabled systems demonstrated a nice speedup for pure hydrodynamics tests on the NVIDIA V100 GPU, compared to server-class CPU nodes. However, a challenge remained: as mentioned previously, the driver framework is in C++, so the way that GPU offloading was achieved was to write CUDA C++ kernels that called the Fortran routines as device functions evaluated on a per-zone basis. These Fortran routines themselves often called other Fortran device functions, sometimes in different Fortran modules. This meant that there was limited capability of the compiler to optimize the kernels through inlining and other approaches. Another significant drawback was that for every array passed from C++ to Fortran, the bounds of the array had to be copied (since in the Fortran routines the arrays were indexed starting from offsets corresponding to the index within the grid). For the functions with many Fabs passed to them, simply maintaining the array bounds in per-thread stack memory resulted in overflowing the 255 available registers on Volta, resulting in register spilling and very low occupancy. It was not clear how this could be circumvented without a major refactor.

At the same time, many codes running on US Department of Energy systems were evaluating and porting their codes to run on top of the C++ performance portability frameworks Kokkos ([15]) and RAJA ([16]). These frameworks expose abstraction layers where the work done (the body of a loop) is separated from the implementation of the loop evaluation on a target architecture. The loop body is captured as a lambda function. AMReX implemented a similar approach, tailored to the context of its application base. A generalized “parallel for” construct does the work of generating a CUDA kernel and mapping individual indices to threads; the application code needs only to define the work done at a given index \((i, j, k)\).

The parallel for construct works correctly for standard CPU builds, and the abstraction layer permits AMReX to easily test new programming model backends without requiring every application developer using the library to learn all of the details of the new programming models.

This approach ended up being quite similar to the ones provided by the previously mentioned performance portability frameworks. The reason why AMReX provides this as a distinct implementation, rather than requiring codes to use something like Kokkos, is that many AMReX-based codes, including the ones discussed here, do not use AMReX merely as a library, but rather as the overall framework for the code, where AMReX defines much of the base infrastructure and provides a substantial amount of tooling. As a result, AMReX has traditionally tended to develop software targeted at the most common use cases of its users. For example, the vast majority of parallel loops in Castro and MAESTROeX are tightly nested three-dimensional loops over a contiguous region of logical index space constituting a box (see Fig. 1). The AMReX parallel for construct accepts as arguments this C++ \texttt{Box} object, as well as the lambda defining the work, making it extremely convenient for application codes to offload loops in a way that is readable in the context of AMReX-based software. This flexibility permits experimentation with the backend layer without changing user code. We have tested Kokkos during this effort and found that it could achieve performance comparable to the AMReX implementation of many of our loops (though it typically required some parameter tuning relative to the base choice of CUDA threadblock size in Kokkos).

Given the confluence of these and other factors, we began to contribute a major refactoring effort of most of the physics code in Castro and MAESTROeX from Fortran to C++. In almost all cases, kernels sped up by one or two orders of magnitude, resulting in a very large total performance improvement. Our C++ results have been promising enough that all future code development we contribute to the AMReX Astrophysics Suite is likely to take place in C++. (These results should not be taken to imply that Fortran is a poor
choice for accelerated systems, as we had good success with Fortran. It was the haphazard combination of C++ and Fortran that was suboptimal for us.)

From a memory management perspective, our design goal from the beginning was to implement all relevant physics on the accelerators, so that data motion back and forth to the CPU would occur negligibly often. (This is not possible when the GPU memory is oversubscribed; the code should almost always be run in a way where this does not happen to obtain optimal performance.) Consequently, we chose CUDA Unified Memory due to its ease of use. This strategy was successful and in the present MAESTROeX and Castro codes data motion between the CPU and GPU only occurs in a few places (checkpointing the simulation state to disk, and MPI transfers, depending on whether CUDA-aware MPI is used). The only serious difficulty was that the codes frequently allocate temporary memory in the simulation timestep loop for scratch calculations. These frequent allocations are tolerable on CPUs but disastrous in CUDA, where memory allocation is orders of magnitude slower. Fortunately, AMReX had previously implemented a simple caching (pool) allocator, where in the asymptotic limit memory allocations and frees do not actually allocate or free memory on the GPU; rather, they obtain or release handles to previously allocated data. Similar approaches are frequently in use elsewhere in the GPU community, for example in the Umpire library ([17]). (Major deep learning frameworks such as TensorFlow and PyTorch also implement caching allocators for the same reason.) We contributed a change to AMReX to make the caching allocator the default for the CUDA-enabled build and that resolved the performance obstacle.

Looking forward, we believe we are well situated to take advantage of new computational architectures as they come online. We have a single source code that can run on both traditional CPU node architectures and modern heterogeneous architectures (and in fact our GPU porting work ended up resulting in a net increase in performance on CPUs). The AMReX abstraction layer for parallel loops allows offload to multiple backends that support lambda functions, so at present we can simply run them serially for CPUs (utilizing OpenMP for coarse-grained parallelism) and in parallel on GPUs. As of the time of writing, AMReX has already begun developing backends for HIP and DPC++, targeting OLCF Frontier and ALCF Aurora, respectively, and many of the core constructs already work on those architectures and have been tested on the currently available versions of AMD and Intel hardware. Of course, there will still be some technical differences to sort out in how each vendor’s implementation of lambda capture interfaces with some of our code constructs. We anticipate that our overall performance limiters on non-NVIDIA GPU architectures will be similar to those on NVIDIA GPUs, namely size and bandwidth of the register file and caches, and to a lesser extent DRAM bandwidth and size.

On the memory front, it is unclear whether those platforms will have an analogue of CUDA’s Unified Memory, or if so what its performance characteristics would be, but we do not anticipate this being a serious problem. The AMReX memory allocator wrapper can easily switch between different underlying memory allocation APIs provided by the platform. Because our codes are now in the state where the data is already on the GPU for the duration of the simulation, it will not be difficult to switch to a memory allocation API that provides device-only data, as we do not ever dereference our simulation data on the CPU. (When we write a checkpoint file, it involves making a copy to CPU memory, not migrating the data to the CPU.) We can already prototype this in CUDA, and so we will be able to do much of the preparation work for these architectures ahead of time.

IV. PERFORMANCE MEASUREMENTS

In a hydrodynamics code, performance is typically measured in terms of throughput: how many zones are updated per microsecond, which has the property that it is O(1) for a modern high-end CPU server node running a standard pure hydrodynamics test case such as the one presented in Section IV-A. This metric, or the related zones/second metric, has been reported for a few other astrophysical fluid dynamics codes. Cholla ([18]) reported 7 zones/$\mu$s/sec for a hydrodynamics algorithm quite similar to the one used in Castro on the NVIDIA Kepler K20X GPUs on Titan. GAMER ([19]) and K-Athena ([20]), which evolve magnetic fields in addition to standard hydrodynamics, report peak throughputs of 55 zones/$\mu$s/sec on NVIDIA P100 and 100 zones/$\mu$s/sec on NVIDIA V100, respectively. Under optimal conditions Castro achieves around 25 zones/$\mu$s/sec on NVIDIA V100 (this number should not be directly compared against the numbers from other codes, which have different algorithms). In this section we describe two test cases that demonstrate our performance with an eye toward scaling behavior. Simulations were run on the OLCF Summit system (IBM AC922 server nodes with 2 IBM Power9 CPUs and 6 NVIDIA V100 GPUs each).

A. Blast Wave

The Sedov-Taylor blast wave ([21]) is a standard performance benchmark in computational fluid dynamics, often implemented in hydrodynamics benchmark codes such as LULESH ([22]) and Laghos ([23]). A source of energy is deposited in a very small space at the center of the computational domain; a blast wave then forms which evolves self-similarly in space and time. In a multiphysics code such as Castro, the Sedov problem exercises the coupling between the hydrodynamics and equation of state physics modules. The communication pattern for this problem is local (the hydrodynamics algorithm in Castro only requires communication between neighboring regions of the domain.) However, the amount of work per zone is relatively small (compared to the science problems of interest for Castro) and this problem quickly exposes weak scaling limits as the number of nodes increases.

Figure 2 demonstrates the weak scaling of Castro’s implementation of the Sedov-Taylor problem on Summit. Three
scaling scenarios are presented. Weak scaling is typically defined as keeping work per processor fixed while increasing the number of processors, and for this canonical weak scaling case we distributed a grid of 256$^3$ zones across the 6 GPUs on the node. This test was performed on 1, 8, 64, and 512 nodes, and the results are depicted by the solid curve in the figure, with crosses at each data point. The loss in efficiency primarily being due to MPI communication (corresponding to a weak scaling efficiency of about 63%, the characteristic of the architecture than about how closely we achieved optimality in our implementation of the physics algorithms, as for small problem sizes we would mostly be measuring the bandwidth of CPU-GPU transfers during an oversubscription scenario. In practice, there is a relatively narrow range of grid sizes that make sense to run on GPUs.

Considering these three effects, determining optimal GPU performance and load balancing is a problem that is best solved empirically by varying the size of the computational domain and the size of the boxes within it. AMReX provides runtime parameters to control both the number of zones in the domain, and the maximum and minimum (per-dimension) widths of a box. The domain decomposition algorithm in AMReX tends to prefer larger boxes, so for a given domain size, increasing the maximum box width effectively decreases the number of boxes. We ran the Sedov test at power-of-two node counts up to 512 nodes, and in each case we ran several simulations, keeping the minimum box width at 32, but varying the maximum box widths between 32, 48, 64, 96, and 128. We ran these at two different domain sizes (the smaller domain being a factor of 0.75 smaller per dimension than the larger one, e.g. $192^3$ and $256^3$ for the single-node case). The dashed curves in Figure 2 represent the best (circles) and worst
(squares) throughput over all of these combinations at each node count (normalized to the value of the canonical weak scaling throughput on one node). The “best case” demonstrates what is possible to achieve with careful tuning by the user, while the “worst case” demonstrates what happens if the user is careless and neglects to consider these properties.

Our conclusion is that very high performance can be achieved on pre-exascale systems compared to previous architectures, but careful tuning of runtime parameters is necessary for the user to achieve optimal performance, much more so than was required for users of these codes on previous architectures. This is in line with the scaling results of other grid codes (see [19] for an example of an order of magnitude performance variation between small and large grids). Unfortunately, this sometimes encourages the user to select spatial resolutions that are optimal for the system architecture rather than optimal for the science problem, but that seems to be the price we must pay for accelerated computing on today’s architectures.

B. Reacting Bubble

MAESTROeX’s hydrodynamics algorithm is different from Castro’s: the updates require a global communication step (in particular, a linear solve implemented using the multigrid method). This exposes a fair amount of work but also significantly more MPI communication in relative terms. However, the core nuclear astrophysics problems of interest for MAESTROeX involve thermonuclear fusion. The numerical solution of the equations representing the nuclear fusion process is purely zone-local work, and takes the form of a coupled set of ODEs. The size of this ODE system depends on the number of atomic isotopes represented: a greater number of isotopes generally yields higher fidelity but at greater computational expense.

Thermonuclear fusion is a highly energetic process. For many nuclear fusion processes, the energy release is a very strong function of the temperature $T$ of the surroundings. For example, the energy generation rate of the process that fuses three helium nuclei into a carbon nucleus may have a temperature dependence as sensitive as

$$f(T) = T^{40}.$$ 

Other fusion processes are comparatively less sensitive to the temperature, some dramatically so. As a result there is a wide range of evolutionary timescales involved, some as short as picoseconds and some much longer. The resulting coupled ODE system generally needs to use an implicit time integration method (otherwise the whole system would be forced to march along at the smallest timescale, which would be inefficient). Implicit methods typically require a linear system solve. If there are $N$ types of atomic nuclei represented, the size of the matrix representing the linear algebraic system is approximately $N^2$, so the computational expense grows quickly with the number of atomic isotopes simulated.

In addition to the compute demands the memory demands are also non-trivial. Modern GPUs such as V100 have a very small amount of thread-local memory (255 single-precision data registers). With $N \sim 10$ isotopes the Jacobian of the system alone is enough to fill up these registers, and other physics involved guarantees that we will encounter register spilling. We are exploring methods to address this, including using sparse linear algebra (many nuclei do not fuse with other nuclei and the reaction rate is zero, so we do not have to explicitly represent it). But as it stands now, even though this is a compute intensive process it is not perfectly efficient on GPUs.

A useful test case demonstrating both the hydrodynamics solve and the nuclear reactions solve is a reacting bubble problem [25]. A hot bubble is placed in a plane parallel atmosphere. The conditions of the atmosphere are similar to those found in the center of the white dwarf stars we are interested in, prior to their potential explosion as supernovae. This temperature perturbation is large enough to begin localized thermonuclear fusion of carbon in the bubble, causing it to become buoyant and rise up through the atmosphere. Despite being a much simpler problem than would be modeled in a typical science run (we only model $N = 2$ reacting nuclei), it nevertheless includes all of the relevant physical processes. The scaling of this problem is shown in Figure 3. The problem was run on one node and then increased by factors of 2, 3, 4, and 5 per dimension (run on 8, 27, 64, and 125 nodes, respectively).

The performance characteristics of this problem are quite different from the one studied in Section IV-A. At single node scale the throughput is approximately 11 zones/$\mu$sec (for reference, this is about a factor of 20 higher than the single-node CPU throughput). The wall time is dominated by the nuclear burning and the parallel communication needed for the multigrid solve in the hydrodynamical system, which are approximately equally balanced. However, at high node counts the parallel communication dominates – at the highest node

![Weak scaling of MAESTROeX reacting bubble](image-url)
count studied, about 6x more time is spent in the multigrid solve than in the nuclear reactions solve, and the multigrid solve is extremely communication bound. The globally coupled nature of the system means that it is harder to scale this problem to the full size of a system like Summit – but it is also an opportunity, because it means that if we solve the problem more accurately with a more complete set of atomic nuclei, it will be easier to scale.

While scaling tests are useful, what we really care about is what new science we can investigate. Systems such as Summit can process a given problem much faster than we would have solved the same problem on a previous supercomputer, which enables broader parameter studies. But in particular the increased power of these systems enables wonderful new science capabilities. Let’s now turn to an example of a problem that is well matched to a modern accelerated architecture.

V. SCIENCE RESULTS

A promising candidate for thermonuclear supernovae is the merging of two white dwarf stars in a binary star system. The merger might occur gradually as the stars spiral into each other due to the emission of gravitational waves, as predicted by general relativity ([26], [27]). Or it might occur due to the head-on collision of two white dwarfs, triggered by oscillations in the binary orbit caused by a nearby companion ([28], [29]). In this section we examine this collision hypothesis. The collision problem is quite computationally tractable: it is easy to determine exactly how much simulation time will pass before the stars collide, given an initial setup. When the stars collide, the kinetic energy of their motion will rapidly be converted into heat, quickly increasing the temperature and initiating nuclear reactions. As discussed in Section IV-B, these thermonuclear reactions release copious amounts of energy, heating the nearby material and therefore increasing its reaction rate in a positive feedback loop. This will almost certainly lead to a thermonuclear detonation, possibly destroying one or both stars. The question is only where and when the detonation happens, which determines whether this process is a possible cause of supernovae or some other astrophysical event. (By comparison, in the gradual inspiral case, it is not definitively known if a detonation will occur at any point in the process, so the amount of time needed to simulate the system is not well bounded.)

On a system such as Titan at OLCF or Edison at NERSC, we typically would have simulated this process in three dimensions on a uniform grid up to $512^3$ in size. We ran such a case on Summit to demonstrate this (the upper panel of Figure 4). The two white dwarf stars (which are of equal size) are initially situated at a distance equal to twice their diameters, moving toward each other at significant speed. The stars collide with each other about seven seconds later (in simulation time) and cause rapid thermonuclear fusion. We terminate the run when the temperature reaches four billion Kelvin, as this is the point at which a detonation and subsequent explosion is imminent. The simplest science question to answer here is: how much time passes before the detonation begins? The longer the stars are colliding before the explosion occurs, the more time there is to fuse elements at the contact point between the stars into heavier elements such as nickel, the signature of a supernova. If the detonation occurs promptly when the stars make initial contact, only lighter elements such as magnesium and silicon will be created, and this event will likely not explain supernovae (but might still be visible as some other astronomical event).

This problem fits comfortably within 16 nodes and, at that scale, completes in under 15 minutes. This is a significant speedup: a typical run on Edison might have used a couple hundred nodes and run on the timescale of many hours. This problem is reasonably balanced in performance terms: the early part of the evolution is just the free fall of two objects toward each other through their mutual gravitational pull. This involves the hydrodynamics module (whose performance was noted in Section IV-A) and the gravity module (which involves a global linear solve similar to, though a little easier than, the one described in Section IV-B). The throughput for this part of the evolution is excellent. When the stars make contact and nuclear fusion begins, the simulation of the nuclear reactions quickly becomes the bottleneck, becoming about 5 times more expensive than the gravity solve, and the throughput drops substantially. However, the throughput is still quite good relative to previous systems (nuclear reactions are expensive to simulate on CPUs too), and the thermonuclear ignition point is soon reached. The fact that we can simulate this whole process in less than ten node hours means that we could easily now run a parameter sweep over the initial conditions (which would ultimately be necessary, given the wide range of possible binary systems in nature) and learn about whether this class of systems might explain at least some supernovae.

There is, however, a serious flaw with this type of simulation. Given the size of the domain, the spatial width of a grid zone is 50 kilometers (compare to the radius of the stars, nearly 10,000 kilometers, which is the same order of magnitude as the radius of the Earth – these stars are quite dense). The length scale over which a thermonuclear detonation begins to propagate in this stellar material is not especially well known but is very likely smaller than 10 kilometers ([30], [31]) and possibly much smaller, so our simulations are unresolved. Worse still, [32] and [33] observe that the thermonuclear fusion process is numerically very unstable at this resolution. As we discussed, this type of stellar material is susceptible to thermal feedback loops that rapidly ignite it. (Unlike air on Earth, this type of matter does not expand much when heated due to quantum mechanical effects, so the heat from nuclear reactions easily gets trapped and causes even more energy release.) Unfortunately, grid zones themselves can artificially act as their own cauldrons for this feedback process. This occurs if the timescale for heat to be transferred to neighboring zones is much longer than the timescale for heat to be generated in that zone. We inspected the ratio of these timescales for simulations at this resolution and found that the energy generation timescale was often an
Fig. 4. Collision of two white dwarfs at the point of thermonuclear ignition (simulation time is noted in the upper left corner). Contours of the density of the stellar material are shown on a logarithmic scale (scale shown at right). At this time, the contact point between the stars is actually denser than the center of either of the stars and has a temperature measured in the billions of degrees. The stars are approaching each other from the left and right, respectively, and much of the material in the contact point between them has pancaked outward (up and down, from the perspective of the page) since it has nowhere else to go. (Upper) Low-resolution simulation typical of the state of the art result possible in 2015, which is not numerically converged. A red dot marks the location in space of the thermonuclear ignition, which is at 4 billion Kelvin. (Lower) Similar to the upper figure, but we have resolved the contact point by an additional factor of 16 in space. Thermonuclear ignition has occurred at an earlier time (though that is partially explained by better resolution of the contact point), and the central contact region has still not become very dense. This event would not explain thermonuclear supernovae. However, it is also still not fully resolved, so astrophysical conclusions should not be drawn from it.
order of magnitude smaller than the heat transfer timescale, meaning that we could not distinguish between a physically correct thermonuclear detonation and a spurious one caused by numerical instabilities.

As a result, on previous systems we experimented with performing this simulation in two dimensions (using an axisymmetric cylindrical coordinate system that restricted us to problems symmetric about the axis joining the two stars). This freed up computational power from the third dimension to be used for adaptive mesh refinement in the contact region between the stars. In two dimensions, we were finally able to get to the sub-kilometer resolutions necessary to contemplate fully resolving this process. However, this was only possible for very specific configurations that are physically unrealistic (we cannot expect the stars to exactly line up when they collide, and it is difficult to simulate processes such as rotation of the stars about their own axes in an axisymmetric coordinate system).

Now, though, with the computational power unlocked by modern GPU server nodes, we can actually attack this problem in its full three dimensional glory. The lower panel of Figure 4 is similar to the upper panel, but with higher spatial resolution. The stars themselves are refined by a factor of 4 at all points in the run (a spatial resolution of 12.5 km). Additionally, when any material heats up to \(10^9\) K, we refine it by an additional factor of 4 (3.125 km). The power of adaptive mesh refinement is that the additional work added is not proportionally larger (which would be a factor of 4\(^6\)): the stars only occupy 0.5% of the volume of the simulation domain, and the high-temperature region is another factor of 100 smaller in volume. Consequently we can run this setup on only 48 nodes and still fit it fully in the memory of the 288 GPUs used. In order to maintain hydrodynamic stability, the length of a timestep is inversely proportional to the spatial resolution, so completing the simulation up to the point of ignition still took significantly more time: approximately 5000 node hours. Nevertheless, this is a new result that qualitatively would not have been possible for us on previous systems.

The key science takeaway from this simulation is that the enhanced resolution helps us answer qualitative questions about the collision process. The low resolution result ignites at a relatively early time in the collision process: the high density contact point has not had enough time to fuse its light elements into heavy elements. This may look like a “failed” supernova, if we were able to observe it. However, if the ignition had occurred a little bit later, this could have possibly explained some supernova events, and it was plausible that it would go this way with higher resolution. However, the higher resolution simulation goes the other way: the ignition occurs even earlier, and there is no way for this process to explain the supernovae we observe, if we take the simulation result at face value. With that said, we do not believe this simulation is numerically converged either, as our two-dimensional simulations suggest we need to achieve at least another order of magnitude in spatial resolution for that, and our diagnostic measurements indicate that the zonal burning timescale is still shorter than the energy transfer timescale. While we cannot yet say anything definitive from this result, we now believe we are far closer to a realistic answer, and further improvements in computational performance will help us get there.

VI. CONCLUSION AND OUTLOOK

Stars are three-dimensional objects and need to be modeled that way, with high fidelity required to accurately model thermonuclear fusion processes. Unfortunately, until now we have been able to achieve either high resolution in two dimensions, or low resolution in three dimensions, but not high resolution in 3D. Because low resolution simulations are qualitatively incorrect, we have been pursuing much of our science for the last few years in 2D, for both white dwarf mergers and X-ray bursts. We have made progress in this way but it is not a path to truly answering our science questions of interest.

There is still much work to be done. The simulation of Section V was performed by simulating only \(N = 13\) elements. This is the bare minimum to say anything qualitatively correct about the thermonuclear fusion process in these supernovae, and high-fidelity science simulations require at least an order of magnitude more isotopes to be tracked. Furthermore, we have not achieved the spatial resolution needed to overcome the numerical instabilities associated with simulating thermonuclear fusion. We are not sure if it is possible to get a full grasp on this problem on today’s systems; however, we are confident we have made great strides toward that goal.

Our future work will, for the near term, focus primarily on enhancing the performance of the solutions of coupled ODE systems for the nuclear reactions. There are several avenues opened now that we have ported the ODE integrator (and physics modules that evaluate the reaction rates) to C++ and substantially modernized it in the process. For example, we can straightforwardly replace the dense linear system with a sparse linear system. We know what the sparsity pattern is for each combination of isotopes, and that pattern does not change over time. This allows us to use an optimal sparse representation rather than a generic storage format. Although using this to decrease memory requirements is most beneficial for very large sets of isotopes, this would be helpful even for the smaller networks like the one used in this science simulation (which has about 40% of the dense matrix empty).

Along related lines, it is even possible to write the exact sequence of operations needed for the linear solve using code generation tools.

Another avenue of our pursuit relates to using the CPUs as part of the simulation rather than letting them idle. A system like Summit has > 95% of its peak theoretical computational throughput in GPUs, so one might think that attempting to use the CPUs effectively is fruitless, and this is probably true for a problem like our hydrodynamics solve. However, our ODE solves for nuclear reactions have the property that the work may be incredibly nonuniform among zones. In the extreme case where one zone in a box is igniting while all of the others are quiescent, the computational cost may vary by multiple orders of magnitude across zones. This is a challenging task.
for GPUs, which rely on latency hiding, because we may not be able to hide the latency when one zone is reacting much longer than the rest. We are currently investigating a strategy that involves identifying those outlier zones (which will realistically only be a small fraction of the total number of zones) and performing their ODE solves on the CPU, while the GPU handles the rest.

With advances in numerical algorithms, the software contributed in this work and related software developed by the HPC community, and high-performance accelerated computing architectures, the science problems we really care about are now in reach.

ACKNOWLEDGMENTS

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SUMMARY OF THE EXPERIMENTS REPORTED

We ran three software experiments: two scaling tests and one science case. The first scaling test is the Sedov blast wave problem that comes with the Castro software, in its Exec/hydro_tests/Sedov directory. The specific test case used for our submission was placed in the Exec/hydro_tests/Sedov/scaling/sc20 subdirectory. The second scaling test was the reacting_bubble test problem that comes with the MAESTROeX software, in its Exec/test_problems/reacting_bubble directory. The specific test case used for our submission was placed in the Exec/test_problems/reacting_bubble/scaling/sc20 subdirectory. Each problem setup has a README file which explains how to compile the executable and submit the job (if running on the OLCF Summit supercomputer).

The git tag 20.04.1 for both Castro and MAESTROeX will retrieve the state of both codes at the time of the submission, and includes all problem setup files and input decks necessary to run our simulations. The specific commit hashes used to compile the executables for the runs was 947049960509f011b5b716de063bd160064ca062 for Castro and 58b75fbb03d3a51a83d102d57b4153270b17b9 for MAESTROeX, which are both slightly older than the 20.04.1 tags.

All simulations were run on OLCF’s Summit system. Fortran code was compiled with PGI version 19.10 as available through the pgi/19.10 module; host CPU code was compiled with gcc version 4.8.5 (the default system compiler in /bin); and device CPU code was compiled with nvcc version 10.1.243 as available through the cuda/10.1.243 module. The MPI implementation was the system default, Spectrum MPI version 10.3.1.02rtm0 as available through the spectrum-mpi/10.3.1.2-20200121 module.

ARTIFACT AVAILABILITY

Software Artifact Availability: All author-created software artifacts are maintained in a public repository under an OSI-approved license.

Hardware Artifact Availability: There are no author-created hardware artifacts.

Data Artifact Availability: There are no author-created data artifacts.

Proprietary Artifacts: No author-created artifacts are proprietary.

Author-Created or Modified Artifacts:

Persistent ID: https://github.com/AMReX-Astro/CASTRO; 
→ releases/tag/20.04.1; 
→ https://zenodo.org/record/3880807
Artifact name: CASTRO 20.04.1

Persistent ID: https://github.com/AMReX-Codes/amrex/
→ releases/tag/20.04; 
→ https://zenodo.org/record/3736659
Artifact name: AMReX 20.04

Persistent ID: https://github.com/starkiller-astro/Microphysics/releases/tag/20.04.1; 
→ https://zenodo.org/record/3880819
Artifact name: Microphysics 20.04.1

BASELINE EXPERIMENTAL SETUP, AND MODIFICATIONS MADE FOR THE PAPER

Relevant hardware details: IBM AC922 server nodes: 2 IBM Power9 DD2.1 CPUs, 6 NVIDIA Volta V100-SXM2 GPUs. The total CPU memory is 512 GB DDR4 RAM per node, with 16 GB of HBM2 memory on each of the GPUs. The CPU memory bandwidth per socket is 170 GB/s peak, while the GPU peak memory bandwidth is 900 GB/s. Each CPU socket has 22 SMT4 cores (though one core on each socket is reserved for the OS by the system). 3 GPUs are attached to each socket, with an NVLink connection between each GPU and its nearest CPU, as well as an NVLink connection between the three GPUs on a socket, with each NVLink connection having a peak unidirectional bandwidth of 50 GB/s. The CPU bus connecting the two sockets has a peak bandwidth of 64 GB/s. Each node has a single Mellanox ConnectX-5 HCA (100 Gb/s EDR) with 2 physical ports and 4 virtual ports. The network topology of the system as a whole is a non-blocking fat tree.

Operating systems and versions: RHEL 7.6 running Linux kernel 4.14.0-115.14.1.el7a.ppc64le

Compilers and versions: PGI 19.10; gcc 4.8.5; nvcc 10.1.243

Applications and versions: Castro 20.04.1, MAESTROeX 20.04.1, Microphysics 20.04.1, AMReX 20.04

Libraries and versions: Spectrum MPI 10.3.1.02rtm0

Key algorithms: partial differential equations; ordinary differential equations; multigrid

URL to output from scripts that gathers execution environment information.
https://pastebin.com/raw/hWmMGKBV