Toward simulating Black Widow binaries with CASTRO

Platon I. Karpov [*] [†]
Department of Physics and Astronomy
Stony Brook University
Stony Brook, New York 11794
plkarpov@ucsc.edu

Maria Barrios Sazo
Department of Physics and Astronomy
Stony Brook University
Stony Brook, New York 11794
maria.barriossazo@stonybrook.edu

Michael Zingale
Department of Physics and Astronomy
Stony Brook University
Stony Brook, New York 11794
michael.zingale@stonybrook.edu

Weiqun Zhang
Center for Computational Sciences and Engineering
Lawrence Berkeley National Laboratory
Berkeley, CA 94720
weiqunzhang@lbl.gov

Alan C. Calder
Department of Physics and Astronomy
Institute for Advanced Computational Sciences
Stony Brook University
Stony Brook, New York 11794
alan.calder@stonybrook.edu

ABSTRACT

We present results and lessons learned from a 2015-2016 Blue Waters Student Internship. The project was to perform preliminary simulations of an astrophysics application, Black Widow binary systems, with the adaptive-mesh simulation code Castro. The process involved updating the code as needed to run on Blue Waters, constructing initial conditions, and performing scaling tests exploring Castro's hybrid message passing/threaded architecture.

CCS Concepts

•**Applied computing → Astronomy;**

Keywords

pulsars:general – stars:evolution – stars:neutron – radiative transfer – methods:numerical

1. INTRODUCTION

Black Widow Pulsar Systems.

Black Widow Pulsar systems (BWPs), also known as Black Widow binaries, are binary star systems consisting of a millisecond pulsar (MSP) along with a substellar mass companion star that is being ablated by the pulsar's wind. Pulsars are highly-magnetic rotating neutron stars (NSs) that emit beamed electromagnetic radiation, and MSPs are extremely rapidly rotating pulsars that have been spun up by accreting angular momentum from a close binary companion and are sometimes referred to as "recycled" pulsars. Observed BWPs mostly reside in globular clusters [?] and the systems have orbital periods of less than about 10 hours. An example of a system clearly demonstrating ablation is B1957+20 [?], and at least 27 systems are currently known with more being found as searches continue.

BWP systems may be the final stage in the evolution of the low mass X-ray binaries (see, e.g. [?]), which are NSs accreting from a low mass companion overflowing its Roche lobe. However, [?] argue that some ablating secondaries require a companion exchange in a dense environment. In any event, the low-mass companions are indeed ablating: about half the known BWPs exhibit a radio eclipse at low frequencies (e.g., [?]) due to a low density plasma cloud surrounding the secondary. The shape of the low frequency attenuation suggests a comet-like shape to the plasma cloud. In the case of PSR B1957+20, in addition to the radio eclipse, a plasma tail counter to the proper motion is observed in X-rays [?]. Eventually, the companion will be completely ablated away.

An interesting aspect of BWPs is that the pulsars seem to be relatively massive, possibly due to accretion of substantial amounts of the companions. Very few of these have been analyzed with corresponding optical observations that allow estimation of system masses, but those that have are intriguing. In at least five cases, NS masses have been estimated:

- B1957+20 [?] $M = 2.4 \pm 0.3\ M_\odot$, the original BWP.
- PSR J1311-3430 [?] $M = 2.55 \pm 0.50\ M_\odot$.
- PSR J1544+4937 [?] $M = 2.06 \pm 0.56\ M_\odot$.
- PSR 2FGL J1653.6-0159 [?] $M > f(M_2)/\sin^3 i \gtrsim 1.96$ $M_\odot$. The largest measured companion mass function, $f(M_2)$, to date.
- PSR J1227-4859 [?] $M = 2.2 \pm 0.8 M_\odot$, a related system, a "redback" pulsar.

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[*] 2015-2016 Blue Waters Intern.

[†] Now at the Department of Astronomy & Astrophysics, UC Santa Cruz, Santa Cruz, CA 95064

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Uncertainties in the size and shape of the ablating companion, however, preclude an exact determination of the pulsar's mass. If the companion is point-like, the inferred mass is small. If the companion is able to fill its Roche Lobe, allowing its mass to spill onto the pulsar, the inferred mass would be much larger. Improving estimates will require sophisticated radiation hydrodynamics simulations of the ablation of the companion to thereby inform interpretation of the observations. The work proposed for this Blue Waters Internship represents the fist steps along this path.

Proposed BWP Work for the Blue Waters Internship:.

The proposed work for the internship was for the intern to perform preliminary simulations of BWPs with the adaptive-mesh astrophysical simulation code Castro [?, ?, ?][1] Initial simulations were to assume two-dimensional axisymmetry with a strong radiation field coming from the boundary to understand how the energy deposition disrupts the star, with full three-dimensional studies eventually following. Meaningful scaling tests required three-dimensional simulations, however, so full three-dimensional simulations were performed for the internship.

The radiation hydrodynamics module for Castro consists of radiation transport in the flux-limited diffusion (FLD) approximation, which is not sufficient for the BWP problem because the absence of the directional information in FLD makes it insufficient for modeling the ablation of the stellar companion. Preliminary simulations exploring the dynamics of BWP systems, however, are intended to yield important information about the relevant hydrodynamic and radiation hydrodynamic time scales and allow construction of initial models.

Further development of the radiation hydrodynamics module in Castro was expected to occur during the performance period of the internship by a then-unnamed graduate student in collaboration with Castro developers at the Lawrence Berkeley National Laboratory. The core solvers in Castro (an interface to the algebraic multigrid solvers in the hypre package [?]) support a more general system, and expected development for the project includes implementing an M_1 approximation, like that used in [?], to better describe the radiation. In contrast to FLD, the M_1 approximation includes an angular dependence enabling it to "cast a shadow"—it doesn't artificially diffuse where it shouldn't. This improvement will allow for accurate simulation of ablation, but the time required for this development was known to be far longer than the performance period of this internship.

The intern, Karpov, was expected to contribute to all aspects of the preliminary problem, including exercising Castro at scale on Blue Waters, constructing the model star and initial conditions, performing the preliminary simulations, and as possible contributing to the development of the M_1 transport module. During the internship, a graduate student (Barrios Sazo) became involved and began working on the project along with the intern.

2. BLACK WIDOW BINARIES

2.1 Setup

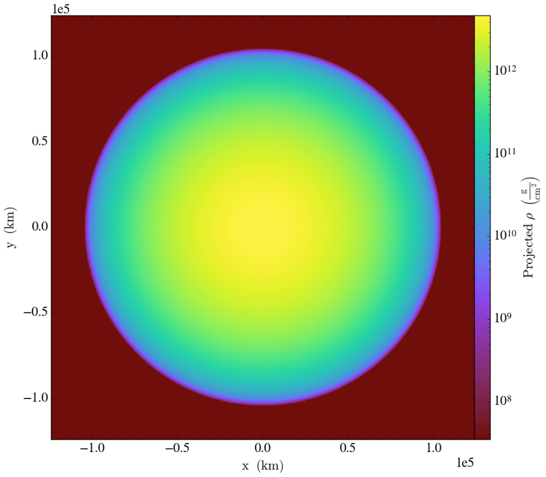

Figure 1: Rendering of the G type companion star to be ablated. The initial conditions included constructing this three-dimensional hydrostatic model.

Our model consists of a Solar-like companion star with radially varying density, being exposed to a "wind" of constant radiation coming from a single direction, as if from the accompanying neutron star (Fig. 1). As simulation time progresses, the ablation process would be visible as the wind interacts with the star.

2.2 Results

The XE node of Blue Waters contains 4 non-uniform memory access (NUMA) domains, hence we focused on this optimal configuration of runs performed with 4 MPI-ranks and 8 OpenMP threads per rank, to utilize all 32 cores on each node. When we tested this setup with the runs of 5120 cores and 256^3 resolution for the BWP model, we found it to have the best performance out of any other MPI-OpenMP hybrid configuration, as shown in Fig. 2.

This model was expanded onto a wider range of cores (1280, 2560, 10240, 20480, 40960, and 81920). In Fig. 3 we can observe the effects of message passing (MPI) and threaded (OpenMP) parallelism within the hybrid architecture for our BWP simulations with Castro. The figure only compares the results of the MPI-only runs to MPI-OpenMP hybrid runs with optimal thread configuration, as stated above[2]. In the case of 40960 and 89120 cores, the time required for I/O exceeded the maximum wall-clock time allowed in the message passing only case so we were only able to make the comparison out to 20480 cores. The addition of threads was observed to increase the calculation time at each step up to 20480 cores (Fig. 3(a)). The I/O time for each checkpoint, however, was significantly decreased with the addition of threads (Fig. 3(b)). We found an optimal combination of the two effects, providing the best total simulation time (Fig. 3(b)).

Even though this scenario might seem as the most optimized for our BWP simulation, further studies showed a deviation from this model. Castro utilizes the BoxLib adaptive mesh library, and the main metric is the number of boxes

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[1] Castro is freely available from https://github.com/BoxLib-Codes/Castro.

[2] Other configurations had been tested (eg. 8, 16 MPI-ranks with 4, 2 OpenMP threads per rank respectively), and they showed the same trends, but worse performance overall.

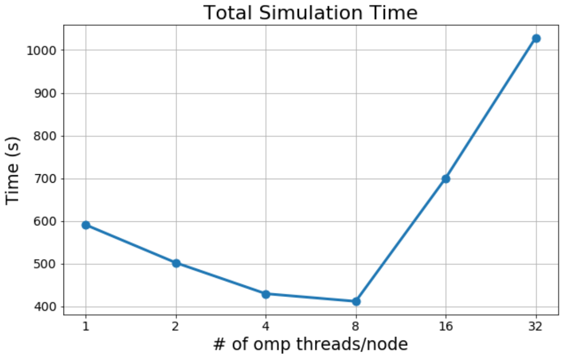


Figure 2: An example of MPI-OpenMP hybrid for a run on 5120 cores and 256^3 resolution.

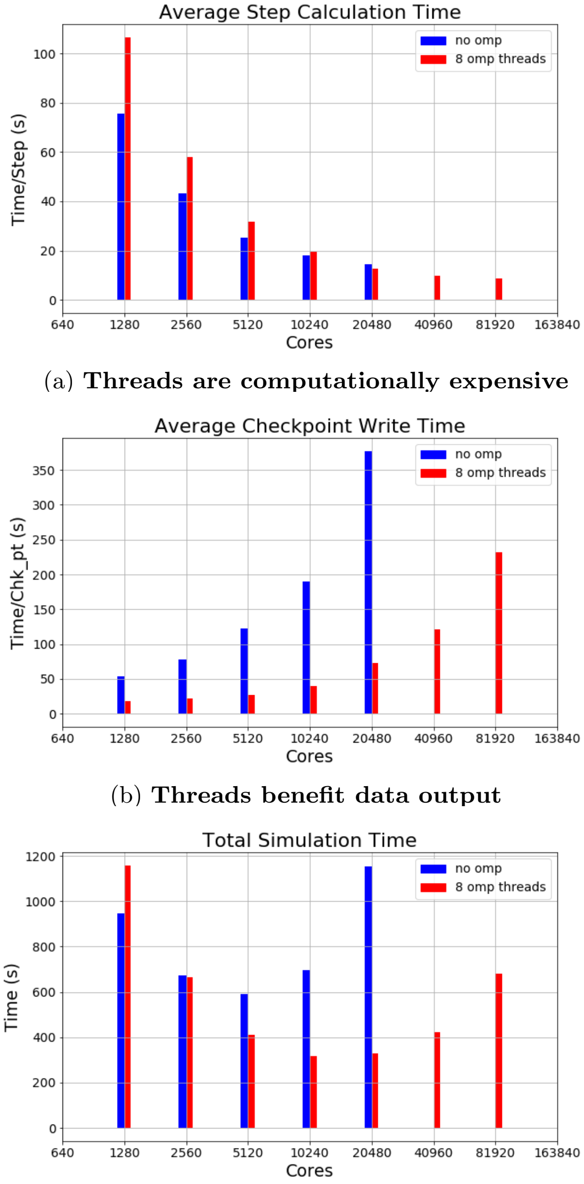
per MPI task. Too few, and a particular job is work-starved and does not perform well. Fig. 3(c) shows that running with 8 threads at higher core count slows down in its total simulation time. Further, Fig. 4 presents the result that Castro demands more threads as we increase the number of cores in order to keep up with the performance. That being said, the total simulation time appears to stagnate at the core counts above 10240, with 8 threads per rank setup.

Given the limited amount of computing time (20,000 node hours), the further study of ablation processes onto the companion were not possible. The MPI-OpenMP hybrid performance study left no computing time to evolve computationally expensive Black Widow binary system enough to see significant effects of ablation due to radiation.

2.3 Lessons Learned

The study presented here was initiated as a project for an intern in the Blue Waters Student Internship Program for 2015-2016 (Karpov). The problem of BWPs is of interest to the nuclear astrophysics research group at Stony Brook, including the mentor (Calder) and the Castro expert (Zingale). And, as mentioned above, during the course of the internship, a graduate student (Barrios Sazo) began working on the problem as well. Also, one of the developers of the radiation hydrodynamics module (Zhang) kindly assisted as well. Thus the results presented in this paper show the combined effort of a team, and discussion of contributions of members and the education of each during the process is warranted.

The intern came to this project with experience from a computational physics class, PHY 277 at Stony Brook University, that included experience with Linux workstations and programming, but little experience with supercomputing. Accordingly, the first lessons learned were associated with using a supercomputer such as Blue Waters: the difference between login and compute nodes, the difference between local scratch space, home directories, and mass storage, and the process of submitting jobs for execution through a queuing system. Next came lessons associated with large simulation codes: understanding the software architecture, constructing a new problem setup consisting of routines for constructing the initial conditions and setting parameters, identifying, installing as needed, and linking to requisite libraries, assessing parallel performance through scaling studies, and the necessity of platform-specific tuning for hybrid message passing/threaded architectures, and finally processing and visualizing the results, which included experience



(a) **Threads are computationally expensive**

(b) **Threads benefit data output**

(c) **Final results**

Figure 3: (a), (b), and (c) provide the performance analysis of MPI+OpenMP hybrid (resolution is 256^3). For the case of no OpenMP used for 40960 and 81920 cores, checkpoint output exceeded the maximum wall-times provided. Hence they can be noted as surpassing the limit of 1200s.

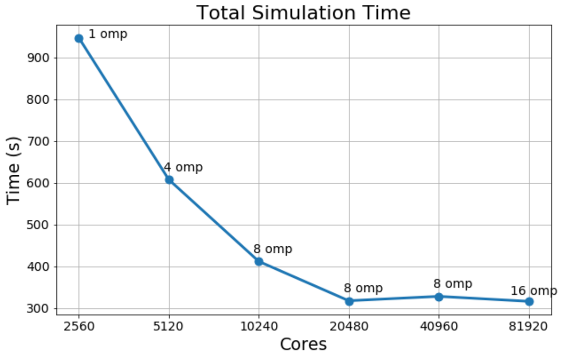


Figure 4: Higher number of cores demands higher number of threads to achieve superior performance. The data points shown are of the lowest total simulation time for a fixed core count, but varying OpenMP threads. All of the simulations were conducted at resolution of 256^3.

with developing scripts. In addition, the intern learned valuable lessons concerning the science of BWPs and numerical methods for radiation transfer. Finally, the intern gained experience with the arduous process of writing a scientific paper with collaborators.

The graduate student (Barrios Sazo), despite serving as a teaching assistant during most of the course of this work, was able to spend considerable time on developing the code for the BWP problem. Her contributions included working with the intern on constructing the routines for problem setup, which includes understanding the physics and numerical approaches and thereby constructing physically meaningful initial conditions.

Lessons learned by the graduate student principally follow from her experience in taking the lead on constructing the hydrostatic star for the initial conditions. She began by exploring examples of problem setups provided in the code distribution, and a lesson here was in the importance of good software practices to make code readily re-usable. Then she learned about how to probe the simulation for problems- in this case, when a crash occurred, was it due to the radiation module or the hydrostatic star? This process gave her valuable experience with a multi-physics application. Similarly, she began by constructing two-dimensional initial conditions and then addressed the three-dimensional case. The lesson here was how to start with a simpler case in order to gain insight into the parameters of the problem and then take on the full three-dimensional case. Also, the graduate student gained valuable experience in working with the undergraduate and faculty as part of a team on the project. Lessons learned here include the importance of communication, particularly discussing ideas, and good software practices, e.g. version control.

The collaborating member of the research group (Zingale) brought expertise with Castro to the project as he is one of the principal developers. He guided the intern and graduate student with use of the code and the development of the BWP problem setup. He also provided guidance in assessing the performance and scaling, a good example being the suggestion of exploring how the choice of solver in the hypre package affects the performance. Such insight was invaluable to the intern's experience. Similarly, guidance from the Castro developer (Zhang) was critical to the success of this project. Finally, the mentor, Calder, assisted as best he could with all aspects of this study and gained experience both the the science of BWP systems and Castro.

3. CONCLUSIONS

We conclude that the Blue Waters Internship was an invaluable opportunity that greatly enriched the intern's undergraduate experience. As of this writing, he is beginning a graduate program in Astrophysics and plans on pursuing a large-scale computational astrophysics problem for his dissertation research. The internship offered experience in all aspects of running a modern code at scale on one of World's largest platforms, from the rote details of job submission and data storage to strategies for parallelism and meaningfully testing scaling.

We also conclude that while this project began with just the intern, the formation of a team made it far more successful than it would have been otherwise, to the benefit of all parties involved. What started as a project for one student wound up benefiting a research group.

4. ACKNOWLEDGMENTS

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