Simulations of Dense Stellar Systems with the AMUSE Software Toolkit

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Abstract. We describe AMUSE, the Astrophysical Multipurpose Software Environment, a programming framework designed to manage multi-scale, multi-physics simulations in a hierarchical, extensible, and internally consistent way. Constructed as a collection of individual modules, AMUSE allows computational tools for different physical domains to be easily combined into a single task. It facilitates the coupling of modules written in different languages by providing inter-language tools and a standard programming interface that represents a balance between generality and computational efficiency. The framework currently incorporates the domains of stellar dynamics, stellar evolution, gas dynamics, and radiative transfer. We present some applications of the framework and outline plans for future development of the package.

1. Introduction

Many areas of computational astrophysics entail simultaneous solution of systems of equations spanning multiple physical domains. These domains may themselves span broad ranges in length and time scales, and separate domains may be tightly coupled on the scales of interest. The combination of many competing physical processes and large dynamic range, together with the sheer size of the computation, represents a major theoretical challenge for computational astrophysics. As simulations and data analysis become increasingly complex, computational scientists face an increasing need for flexible frameworks capable of integrating new and existing scientific codes and allowing scientists to easily build their simulation workflow.

The targets of interest here, young massive star clusters and galactic nuclei, are dense stellar environments in which gravitational dynamics, radiative processes, stellar physics, and gas dynamics all play important roles. Spatial and temporal scales range from $10^3$ m and $10^{-3}$ s on the small end to $10^{20}$ m and $10^{17}$ s at the other extreme. Close encounters and physical collisions among stars and binaries are commonplace, and large and small scales are intimately coupled by stellar mass loss, binary heating, stellar collisions, dynamical mass segregation, and core collapse. The number of stars can exceed $10^6$ in many cases. Combining all these elements within a large-scale simulation of such a system poses significant software development problems.

The present generation of cluster simulation packages—often generically referred to as “kitchen-sink” codes—have been very successful in modeling the long-term dynamical evolution of star clusters, from a few megayears after formation to their eventual dissolution possibly gigayears later in the galactic tidal field. These packages in-
clude both N-body (Aarseth 2003; Portegies Zwart et al. 2001) and Monte Carlo codes (Fregeau & Rasio 2007; Giersz et al. 2008). All contain sophisticated and comprehensive treatments of stellar dynamics and binary/multiple interactions—a reflection of their historical development—but these are generally coupled with much more approximate treatments of other physical aspects of the system. For example, stellar evolution is typically calculated as a look-up from precomputed results (Hurley et al. 2000), while binary evolution consists of a set of rules of varying accuracy, implemented on top of the stellar evolution subsystem.

Other aspects of the simulation, such as stellar collisions, are treated even more approximately. Stars are modeled as “sticky spheres” which merge when they come into contact, preserving virtually none of the underlying stellar physics. Still other physical processes, such as global gas dynamics and the effects of stellar winds and radiation, which are now regarded as critical components as we push our simulations back into the star-formation phase, are not included at all. An additional limitation of most kitchen sink codes is that specific implementations of each physical process are hard-coded into the simulation, so adoption of a particular package implies a particular choice of dynamical integrator, stellar modeling, binary evolution, and so on.

We submit that the monolithic design and consequent internal complexity of existing codes are limiting their future development, making alternate treatments of existing physics hard to implement and new physical processes even more difficult to deploy. We expect that these codes will encounter more and greater structural challenges as the demands of greater realism and more comprehensive content mount.

In this paper we describe AMUSE, the Astrophysical Multipurpose Software Environment, a modular simulation framework designed to address the shortcomings just described. The individual modules in AMUSE contain dedicated and efficient implementations of specific pieces of the calculation, and are linked by a high-level scripting language to ensure flexibility and facilitate management. Modules can contain wrapped legacy code or new code developed specifically for the project. All have a standard interface exposing only necessary functionality, allowing them to be easily mixed and replaced as needed. We use the term “community code” to refer collectively to public domain codes encompassed by the AMUSE framework. Section 2 discusses the structure of AMUSE in more detail; Section 3 presents some simple applications of the framework.

2. The AMUSE Software Framework

The global structure of the AMUSE environment is illustrated in Figure 1. In the AMUSE programming model, each piece of physics (advance the stellar or hydrodynamics to a specified time, evolve a star, collide two stars, etc.) is implemented as a module with a standard interface onto the rest of the system, but the details are private to each module. For example, all stellar modules include accessor functions that provide information on the mass and radius of a specified star, but the details of what a “star” is (an analytic formula, an entry in a look-up table, or a set of 1- or 2-D arrays describing the run of density, temperature, composition, etc.) are internal to the module and are normally invisible to the user. Objects within each module are identified by a global ID, and it is the responsibility of the module implementation to provide the required accessor functions for a specified ID.
The high-level “glue” language for AMUSE is Python, chosen for its rich feature set, ease of programming and rapid prototyping, object-oriented capabilities, large user base in the astronomical community, and extensive user-written software. The design of AMUSE places no restrictions on the choice of language for any given module, except that it must support the parallel Message Passing Interface (MPI). In a typical application, the top-level loop (the flow control layer in Figure 1) of a simulation is written entirely in Python, allowing monitoring, analysis, graphics, grid management, and other Python tools to be employed. The modular design and the use of private internal data minimizes both the computational overhead of the Python code segments and data flow between modules. The relatively low speed of the language does not significantly impact performance, because in practice virtually all of the computational load is carried by the (high-performance) modules.

The concept and value of modular software frameworks for program integration are familiar to most computational scientists. Perhaps less obvious is the use of MPI as the communication tool among modules. In the initial implementation of AMUSE, individual modules written in Fortran 77, Fortran 90, Fortran 95, C, and C++ were interfaced with Python using f2py or swig. This approach works well for simple

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1. See [http://www.mcs.anl.gov/mpi](http://www.mcs.anl.gov/mpi)

2. See [http://www.scipy.org/F2Py](http://www.scipy.org/F2Py) and [http://www.swig.org](http://www.swig.org).
demonstration programs (see Portegies Zwart et al. [2009]), but it has a number of serious technical drawbacks when deployed in a parallel, high-performance environment. It (1) imposes namespace restrictions that cause conflicts between independent modules, (2) makes it impossible to instantiate multiple independent copies of a given module, and, perhaps most importantly, (3) rules out incorporation of parallel modules into the AMUSE framework.

All of these problems can be eliminated by replacing the standard swig/f2py interface by an explicitly parallel structure in which MPI is used throughout the AMUSE system for communication between all modules (serial or parallel). Like Python, MPI is easily available, well documented, and widely used in the astronomical community. As a practical matter, the process of generating the necessary interface code is completely automated, using a syntax similar to that found in swig, so ease of implementation is not a significant consideration for the applications programmer. The result is that serial and parallel modules are indistinguishable one another, as seen from the flow control level (Figure 1), making them easy to combine, largely transparently to the user. In addition, the top-level script can run modules concurrently, should the structure of the problem allow it.

Currently, AMUSE contains at least two (and in most cases substantially more) independent modules for each physical process supported, allowing “plug and play” interchangeability between implementations. This and encourages approach enables direct comparison and calibration of different implementations of the same physical processes, and facilitates experimentation in constructing new models. For the current list of available modules and their properties, and to download and install AMUSE, see the project web site, http://amusecode.org.

Figure 2 illustrates schematically the AMUSE programming environment in a star cluster simulation typical of those carried out by current kitchen-sink codes. The python script acts as a scheduler for the stellar dynamical and stellar evolution modules and takes appropriate action when unscheduled events (such as collisions or supernovae) occur. In most cases there is no need for communication between modules beyond the data transferred through the standard interface. However, additional information may be needed in some circumstances—for example, the collision and stellar evolution modules may need to exchange detailed structural data before and after a physical stellar collision. At present all such exchanges are implemented as two MPI transfers (red arrows) through and under the control of the top-level Python layer. So far, we have not found this approach to contribute significantly to the total cost of a simulation. Should these data transfers become too expensive, direct module-to-module communication can be implemented.

N-body experts will notice that binary and multiple interactions (including two-body encounters) are treated by the scheduler at the same level as actual physical collisions. In the AMUSE model, the dynamical integrator follows only the centers of mass of binaries and multiples, which are regarded as unperturbed until a close encounter occurs. Encounters are flagged by the dynamics module, integrated to completion in isolation by the multiples module, and the products are then reinserted into the dynamics module. This approach is unusual for N-body codes, in which binaries and multiples are generally integrated simultaneously with the rest of the dynamics, and represents perhaps the greatest departure of AMUSE from traditional N-body practice. (See, however, the “gorilla” code described by Tanikawa & Fukushige [2009].) However, this is precisely the way in which multiples are handled in the leading Monte Carlo codes. To
the best of our knowledge, it has never been demonstrated that the neglect of weak perturbations on binaries introduces any bias into the large-scale dynamics of the system. Secular evolution of a binary due to occasional wide encounters can be modeled by integrating the orbit-averaged equations for the binary elements as the center of mass moves.

3. Applications of AMUSE

AMUSE has been applied to a number of “proof of concept” problems involving interactions between the large-scale dynamical modules and the stellar evolution and multiples modules. We describe two of them here. For a more sophisticated simulation carried out using AMUSE, see the contribution by Portegies Zwart et al. elsewhere in these proceedings.

Figure 3 is drawn from a study of mass loss from star clusters carried out by Whitehead et al. (2012, in preparation). The goals of the investigation are (1) to demonstrate that AMUSE can reproduce existing results for large simulations, (2) to quantify the run-to-run variations in simulations differing only in the random seed used to generate their initial conditions, and (3) to determine the effect of the choice of stellar evolution model on cluster lifetimes. All runs are performed using 16k or 32k particles initialized from King (1966) model distributions, with power-law \( \frac{dN}{dM} \propto M^\alpha \) stellar mass
spectra, and tidal radii corresponding to one of the Chernoff & Weinberg (1990) families (where increasing family number indicates larger galactocentric distance). In all cases, the AMUSE ph4 dynamical module is used. This C++ integrator includes an MPI parallel fourth-order Hermite integration scheme (Makino & Aarseth 1992) with block time steps and GPU acceleration. The ph4 module is coupled with one of several stellar evolution modules: the simple scheme adopted by Chernoff & Weinberg (1990, CW in the figure, written in Python), the look-up formula presented by Eggleton et al. (1989, EFT89/C), the SeBa package drawn from Starlab’s kira integrator (Portegies Zwart et al. 2001, SeBa/C++), and the two-dimensional SSE interpolation scheme of Hurley et al. (2000, SSE/Fortran-77).

![Figure 3](image_url)

**Figure 3.** AMUSE simulations of mass loss in tidally limited star clusters. (a) Comparison of the evolution of different Chernoff & Weinberg (1990) families. All models began as tidally limited $W_0 = 3$ King models at one of four galactocentric radii, with a power-law $dN/dM \propto M^{-2.5}$ stellar mass function. Solid (colored) lines represent the median behavior of 55 simulations performed for each family; grey-shaded regions represent the full range of the results. (b) Effect of varying the prescription for stellar evolution in otherwise identical simulations. From left to right at the lower right of the figure, the curves correspond to the EFT89, SeBa, CW, and SSE stellar evolution modules.

The results shown in Figure 3(a), using the SeBa stellar evolution module are in good agreement with the N-body and Fokker–Planck simulations reported by Takahashi & Portegies Zwart (2000). We find similarly good agreement in most of the other cases studied. We note in passing that the AMUSE runs are slightly faster than the corresponding calculations performed using Starlab. Since the ph4 internals are somewhat similar to those in kira, and in particular employ similar GPU acceleration, we attribute this to the fact that ph4 spends less time checking for and handling binary interactions. The grey-shaded areas in the figure show the entire range of results for 55 models initialized from the same system parameters, allowing us to measure the spread in the numerical results. Most of this spread in fact arises from variations in the initial stellar masses, rather than variations in their positions or velocities—the mass of the most massive star has a large effect on the lifetime of the system.

Figure 3(b) shows four runs carried out using identical initial conditions but with four different stellar evolution modules—a simple task using AMUSE, entailing changes
in just two lines of the driving script. We find that the choice of module—not an option with kitchen-sink codes, and one not normally thought of as a critical choice—can have a large impact on the lifetime of the system. In this example, the AMUSE capacity for easy code comparison provides valuable insights into the systematic errors inherent in our calculations. Such a comparison is not easy to make using traditional monolithic codes because of the difficulty in implementing even a simple algorithmic change within those frameworks.

Figure 4. AMUSE simulation of the collapse of an initially homogeneous spherical system with a Kroupa (2002) stellar mass function. The half-mass radii of the indicated mass groups are shown. The bottom four lines after the collapse represent the top four mass groups, their half-mass radii decreasing with mass, indicating strong mass segregation.

Figure 4 shows an AMUSE simulation that provides a stringent test of how the framework handles binaries and close encounters. The initial conditions consist of a cold homogeneous sphere of \( N = 10^4 \) particles with a Kroupa (2002) mass distribution. The scientific interest of this simulation lies in the fact that this system experiences mass segregation on a dynamical time scale, as was previously noted by Vesperini et al. (2006, 2009) and Allison et al. (2009). The segregation is clearly evident in the figure, which shows the time evolution of the half-mass radii of the particle sets making up the bottom 10 percent, 10–20 percent, 20–30 percent, etc., of the cumulative mass distribution. No segregation is evident before the “bounce” at \( t \sim 1.5 \) initial dynamical times, while immediately afterward the highest mass groups are clearly ordered by radius.

Allison et al. (2009) suggested that this unexpected result might be due to enhanced relaxation around the high density bounce, but this would only be possible if the system were still quite cold at this time, and our simulations suggest this is not the case. Instead, it appears that the system fragments as it collapses, as described by Aarseth et al. (1988), and that the fragments mass segregate quite early in the collapse.
Significant segregation within the clumps is already established by \( t \sim 1 \), well before the bounce, and is preserved when the clumps subsequently merge, as described by McMillan et al. (2007).

Our simulations test the binary handling abilities of AMUSE because the deep collapse—by a factor of \( N^{1/3} \) or \( N^{2/5} \), depending on the details of the initial conditions—leads to many close encounters and results in binary formation and interaction among the most massive stars in the system. The late expansion of the low-mass stars is driven by heating due to these binaries. In side-by-side tests we find no statistically significant differences between AMUSE and Starlab, in either the overall behavior of the system (e.g., Figure 4) or in the integration errors incurred.

We interpret these results as encouraging signs that AMUSE has crossed the threshold where it now incorporates all of the key functionality found in the leading kitchen-sink codes. Upcoming development of the framework will focus on (1) improved handling at the python level of interactions among community modules, including feedback between the multiples, collisions, and stellar/binary evolution modules, and (2) full integration of the new collisional dynamical modules with the global gas dynamics and radiative transport subsystems.

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