THESIS FOR THE DEGREE OF DOCTOR OF PHILOSOPHY

The Dynamics of Star Cluster Formation

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Cover: The formation and dynamical evolution of model young star cluster, background gas is modeled as an analytical potential which decrease as stars are born. See Paper II.

Printed by Chalmers Reproservice Göteborg, Sweden 2020 Para mis padres Ely y Albert, y hermanos Rosy, Chano y Pipe. Su apoyo incondicional es el pilar de cada logro mio.

Abstract

How do star clusters form? We care, since these are the birth sites of most stars, perhaps including our own Sun. There are a great variety of different theoretical models of cluster formation and our main goal in this thesis is to examine the implications of these for the dynamical evolution of a cluster's stellar population, including the ejected stars. In contrast to the majority of previous cluster formation studies, the focus of this work is on detailed modeling, using the Nbody6 code, of stellar dynamics, including binaries, with the structure, kinematics and star formation of the natal gas cloud explored with simple analytic prescriptions. In particular, we adopt the Turbulent Clump Model of pressure-truncated singular polytropic spheres, which sets global and local initial conditions of the newly formed stars. In a first paper, exploring a fiducial 3,000 solar mass clump, we investigated the effects of overall clump density, global star formation efficiency, degree of primordial mass segregation, degree of primordial binarity and binary population properties on the dynamical evolution of the cluster. Here, like most previous works, we assumed stars are formed very quickly, i.e., approximated as instantaneously, compared to the free-fall time of the clump. In our next work, after implementing a major code development to Nbody6 that allows modeling of gradual formation of stars, we investigated how the timescale of cluster formation, parameterized via the star formation efficiency per free-fall time, $\epsilon_{\rm ff}$, affects its early dynamical evolution. This is the first time that such a study, including a realistic binary population, has been carried out. We showed that star clusters that form rapidly, e.g., with $\epsilon_{\rm ff} = 1$, expand more quickly after they emerge from the gas, while slowly-formed clusters, e.g., with $\epsilon_{\rm ff} < 0.03$, evolve into a much more stable configuration during the gas rich phase. We also showed how the stellar population is affected by the timescale of formation, including the frequency of runaway/walkaway stars, stellar age gradients and primordial binary processing. We have then carried out preliminary explorations of a broad range of star-forming clump parameters, i.e., with masses from 300 to 30,000 solar masses and background cloud mass surface densities from 0.1 to 1 g cm⁻². For the largest clusters simulated, we make use of a GPU-enabled version of the code. Further improvements to the modeling that have been implemented include global elongation of the clump so that nonspherical, including very filamentary, initial conditions can be studied. Models with internal spatial and kinematic substructure for the birth locations of the stars, based on hydrodynamic simulations of supersonic turbulence, have also been studied. In parallel, we have also carried out two projects that focus on observed systems related to dynamical ejections within the Orion Nebula Cluster (ONC). First, we examined a particular set of runaway stars associated with the Orion KL massive star forming region and carried out a systematic exploration of N-body simulations to understand the properties of the dynamical ejection that produced them. Second, we have performed a census of runaway stars from the ONC using *Gaia* data, estimating the total unbound population from the cluster. We have compared these results with our cluster formation simulations leading to new constraints on the star formation rate and dynamical age of the system.

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First, I would like to thank my supervisor Jonathan Tan for all his support and patience, and also for inviting me to join on this adventure to the North. It has been an honor to work with him and to see how much a passionate and dedicated person can do. Working with him has certainly encouraged me to improve and to look more into my own future.

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Thank you very much to Chia-Jung Hsu, Rubén Fedriani, Giuliana Cosentino, Chi Yan Law, Andri Spilker, Sara Rezaei Kh. and Jan Orkiz who made the office environment a very fun place to work and especially to Sandra Treviño, my office mate, with whom I keep sharing laughs on the silly things that make academia less serious.

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List of Publications

This thesis is based on the following appended papers:

- Paper I. Juan P. Farias, Jonathan C. Tan, Sourav Chatterjee. Star Cluster Formation from Turbulent Clumps. I. The Fast Formation Limit. The Astrophysical Journal, Volume 838, page 116. (2017)
- Paper II. Juan P. Farias, Jonathan C. Tan, Sourav Chatterjee. Star Cluster Formation from Turbulent Clumps. II. Gradual Star Cluster Formation. Monthly Notices of the Royal Astronomical Society, Volume 483(4), Page 4999. (2019)
- Paper II. Juan P. Farias & Jonathan C. Tan. Star Cluster Formation from Turbulent Clumps. III. Across the Mass Spectrum. Preparing for submission to MNRAS.
- **Paper IV.** Juan P. Farias & Jonathan C. Tan. On the formation of Runaway Stars BN and x in the Orion Nebula Cluster. Astronomy & Astrophysics Letters, Volume 612. (2018)
- **Paper V.** Juan P. Farias, Jonathan C. Tan & Laurent Eyer. *Hunting for Runaways from the Orion Nebula Cluster* Accepted for publication in the Astrophysical Journal.

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Part I Introductory Chapters

Chapter 1

Introduction

A major question in Astrophysics is how and where star formation happens. Many aspects of star formation are still under active debate, and the reason of such long debate is the complexity of the process. Star formation involves a wide range of scales and the interaction of multiple physical mechanisms. However, some agreement exists that the majority of stars appear to form in "clusters" instead of in isolation (e.g. Bressert et al. 2010; Gutermuth et al. 2009; Lada & Lada 2003). Therefore, to understand star formation it is necessary to understand how star clusters form.

There is a long standing debate on whether star cluster formation is a short process that happens in about one single cloud collapse timescale, i.e., a "free-fall timescale" (Elmegreen 2000; Elmegreen 2007; Hartmann & Burkert 2007), or if it takes place over a longer duration with clouds evolving in a quasi-equilibrium state (Nakamura & Li 2007; Tan 2006). Star cluster formation, like individual star formation, is the result of a complex interaction of numerous physical processes inside molecular clouds. Star-forming regions are massive, self-gravitating systems, supported by a combination of magnetic fields and turbulent motions. Thermal pressure is not important on these scales, as gas in molecular clouds is able to cool to about 10 K. Formation of stars involves gas infall, accretion via disks, and jets and winds launched from these disks that enhance and support turbulence (Nakamura & Li 2007; Nakamura & Li 2014), i.e., part of the process of "feedback". Other forms of feedback, include when newly formed stars irradiate energy into their environments (e.g. Dale et al. 2015), launch stellar winds and ultimately when the most massive stars explode as supernovae injecting large amounts of energy into the clouds, potentially dispersing residual gas within the cluster.

It is extremely challenging to conduct a numerical simulation that accounts for all the physics involved during star cluster formation and with the necessary resolution to follow these processes accurately. Thus it can be useful and insightful to address the problem from different angles. Since the main ingredient during the transition from a molecular cloud to a star cluster is the dynamics of the gas, many studies have been focused on reproducing the outcome of star formation from hydrodynamical and magneto-hydrodynamical (MHD) simulations (e.g. Bate 2009; Dale et al. 2015; Gavagnin et al. 2017; Girichidis et al. 2012; Wu

et al. 2017). However, these kind of studies are very expensive computationally and only few simulations can be done per study. Furthermore, these simulations are still limited in their spatial resolution and typically cannot accurately follow the close orbits and interactions of stars, e.g., in typical binary systems with separations of less than 100 AU. Furthermore, star formation in typical clusters involves sparse sampling of the stellar initial mass function (IMF), especially at its upper end. It is thus a stochastic problem, which can only be addressed by an statistical approach involving analysis of many simulation realizations, which is not possible from expensive hydrodynamical simulations.

In this thesis we aim to address this problem by a statistical study of the dynamics of stars during the formation of star clusters. In order to achieve this, we accurately follow the dynamics of the stars, given simple assumptions, approximations and parameterizations for the individual star formation and the global cluster formation processes. We are then able to explore by numerical experiments the influence of these assumptions, approximations and parameterizations for the dynamical evolution of the clusters and their general properties, including for stars that escape from the clusters.

Here in Chapter 1 we introduce basic concepts of stellar dynamics that will be discussed during this thesis. In Chapter 2 we overview the physics involved in the evolution of star clusters. In Chapter 3 we describe the numerical codes used in this work and in Chapter 4 we introduce the appended papers that discuss our results.

1.1 Basic concepts

1.1.1 The virial theorem

The virial theorem applied to gas free stellar clusters, states that a system is in *virial equilibrium* if:

$$T_* = -\frac{1}{2} \sum_{i=1}^{N} \mathbf{F}_i \cdot \mathbf{r}_i$$
(1.1)

$$= -\frac{1}{2}\Omega_{\rm tot} \tag{1.2}$$

where T_* is the kinetic energy of all stars in the cluster, \mathbf{F}_i is the force felt by the *i*th particle by the other N - 1 particles, \mathbf{r}_i is the position of the *i*th star and Ω_{tot} is the total potential energy of the cluster (Aarseth 2003). However, not all systems are in virial equilibrium and it is useful to characterize a system by its relation to the virial theorem.

Virial ratio, Q, is the ratio defined by the kinetic and total potential energies of the cluster, i.e.:

$$Q = -\frac{T_*}{\Omega_{\text{tot}}}.$$
 (1.3)

Depending on this value, we call a system with: Q < 0.5, a cold system, i.e., a highly bound system with low velocity particles; Q = 0.5, a system in virial equilibrium; 0.5 < Q < 1, a hot system with high velocity particles; and Q > 1, an unbound system where a significant fraction of particles have velocities higher than the escape velocity¹.

Virial radius, $r_{\rm vir}$, is characteristic length unit commonly used in numerical simulations (Aarseth 2003; Heggie & Hut 2003). It is defined in terms of the potential energy of an isolated system by:

$$r_{\rm vir} = -\frac{GM_*^2}{2\Omega_*} \tag{1.4}$$

where M_* and Ω_* are the system mass and potential energy of the system.

1.1.2 Dynamical timescales

One of the most debated features of star cluster formation is the timescale on which it happens, and this particular issue is the most important parameter we wish to constrain. The relevant timescales regarding star cluster formation and stellar dynamics are:

Free-fall time, $t_{\rm ff}$, is a commonly adopted timescale used in star formation simulations. The free-fall time defines the time it would take to a cloud of mass M and radius R to collapse under it own weight if no other forces support it against gravity. It only depends on the volume density of the cloud (ρ) and can be calculated to be:

$$t_{\rm ff} = \sqrt{\frac{3\pi}{32G\rho}} \tag{1.5}$$

for a uniform density sphere.

Crossing time, t_{cross} , is a typical timescale used in stellar dynamics denoting the timescale needed for a typical particle to cross the system, i.e., $t_{\text{cross}} = 2R/v$ where R is the radius of the system and v is the typical speed of a star in the system. The value of v will depend on the dynamical state of the system, i.e., a hot system will have higher v than a cold system. The crossing time is generally used as a characteristic timescale, often used as the time against which to compare some other dynamical process.

A typical velocity of a stellar system is the velocity dispersion (σ) of the particles. Assuming virial equilibrium, we can define the crossing time as (see Aarseth 2003):

$$t_{\rm cross} \approx 2 \frac{r_{\rm v}}{\sigma}$$
 (1.6)

In virial equilibrium we can estimate the value of σ by $\sigma^2 \approx GM/2r_{\rm vir}$ where G is Newton's gravitational constant and M is the total mass of the cluster. Thus the crossing time can be estimated as (Aarseth 2003; Heggie & Hut 2003):

$$t_{\rm cross} \approx 2\sqrt{\frac{2r_{\rm vir}^3}{GM}}$$
 (1.7)

¹Note that this does not mean that the whole stellar system is completely unbound. In fact it can be shown that a system with Q = 1 that follows a Maxwell-Boltzmann velocity distribution would have ~65% of their particles bound (see Farias & Tan 2018) and figure 2.3.

This last equation is particularly useful in numerical simulations since a typical N-body code uses units such that G = 1, M = 1 and $r_{\text{vir}} = 1$ and thus $t_{\text{cross}} = 2\sqrt{2}$.

Relaxation time, t_{relax} , is the timescale on which a typical star in the system will lose any memory of its initial energy and angular momentum through interactions with other stars. It can also be defined as the typical timescale that a system needs to reach dynamical equilibrium or to come back to equilibrium after being disturbed. A useful approximation of this timescale is derived in Binney & Tremaine (2008) as:

$$t_{\rm relax} \approx \frac{0.1N}{\ln N} \times t_{\rm cross}.$$
 (1.8)

This relation only depends on the number of particles in the system, and it is very important to understand the difference between a *collisional* and *collisionless* regime.

For galaxies with $N \approx 10^{11}$ stars with an age of approximately 10 Gyr and a few hundred crossing times old, the relaxation time-scale for the whole system is much longer than the age of the Universe, and it is possible to neglect the contribution from close encounters, i.e., these are *collisionless* systems.

On the other hand a globular cluster (GC) with $N \approx 10^5$ members and a relaxation time of $t_{\text{relax}} \approx 100$ Myr, close encounters may be important over the lifetime of the cluster of ~ 10 Gyr and we can not ignore close encounters, i.e., these are *collisional* systems.

In general a system is called collisional when its lifetime or the time range that we are interested in is much greater than t_{relax} , and collisionless when the time-scale of interest is much smaller than t_{relax} . In this thesis we focus on highly collisional systems, so we need to follow their evolution accordingly.

1.2 The stellar population

Initial mass function (IMF), is the distribution function of individual masses of stars at birth during a given star formation event. Introduced by Salpeter (1955). A common form of this function is:

$$\xi(m) = \frac{dN}{dm} \propto m^{-\alpha}, \tag{1.9}$$

where m is the mass of a star and N the number of stars with masses in the range m + dm. Salpeter (1955) derived a slope of $\alpha = 2.35$ for stellar masses in the range $0.4 - 10 M_{\odot}$, however it has been found that this value overestimates the number of low mass stars, where this slope has been found to be shallower, and many variations have been proposed over the years (e.g. Chabrier 2003; Kroupa et al. 1990; Miller & Scalo 1979). In these works, it has been shown that the IMF slope varies in different mass ranges. Kroupa et al. (2001) has proposed a three part power law, usually referred to as the canonical IMF, equivalent to equation 1.9 with the slopes:

$$\alpha = \begin{cases} 0.3 & ,0.01 \le m/M_{\odot} < 0.08, \\ 1.3 & ,0.08 \le m/M_{\odot} < 0.5, \\ 2.3 & ,m/M_{\odot} \ge 0.5 \end{cases}$$
(1.10)

This form of the IMF is adopted in this thesis to sample the initial stellar masses in our star cluster simulations.

Stellar binaries are pairs of stars orbiting each other. Stellar binaries are very important for stellar dynamics as they can store large amounts of energy in their orbits, and they can exchange this energy with nearby stars. The nature of the interchange of energy will depend on the relation between their internal binding energy and their environment. The internal mechanical energy of a binary is given by:

$$E_{\rm bin} = -G \frac{m_1 m_2}{2a}, \tag{1.11}$$

where m_1 and m_2 are the masses of the components and a is the semi-major axis of their orbit. If a binary is located in an environment where the mean stellar mass is \bar{m} and the velocity dispersion is σ , then we call the binary hard if $|E_{\text{bin}}| \gg \bar{m}\sigma^2$, soft if $|E_{\text{bin}}| \ll \bar{m}\sigma^2$ and intermediate if $|E_{\text{bin}}| \sim \bar{m}\sigma^2$.

Their interaction with their environment is given by the Heggie-Hills law: hard binaries get harder, and soft binaries get softer with time (Heggie 1975; Hills 1975). What this means is that a hard binary will decrease (on average) its internal energy on each interaction. For instance, if a single star approaches, the perturber star will absorb kinetic energy from the binary and it will leave the interaction with a higher velocity than it approached. The opposite happens to soft binaries that gain internal energy as they interact, eventually becoming positive and the binary is dissolved. An approaching perturber will give kinetic energy to the binary and so, it will leave the interaction with a smaller velocity. There is no rule for intermediate stars, and only numerical simulations can determine their individual behaviour in a given environment.

In general, energy exchanged for hardening a binary is much bigger than when a binary is softened (or disrupted). Therefore, in star clusters, binaries behave like sources of energy that can prevent the collapse of the internal, central, dense "core" regions of star clusters, thus keeping their central densities relatively flat (see, e.g., Chatterjee et al. 2013).

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Chapter 2

The Birth and Death of Star Clusters

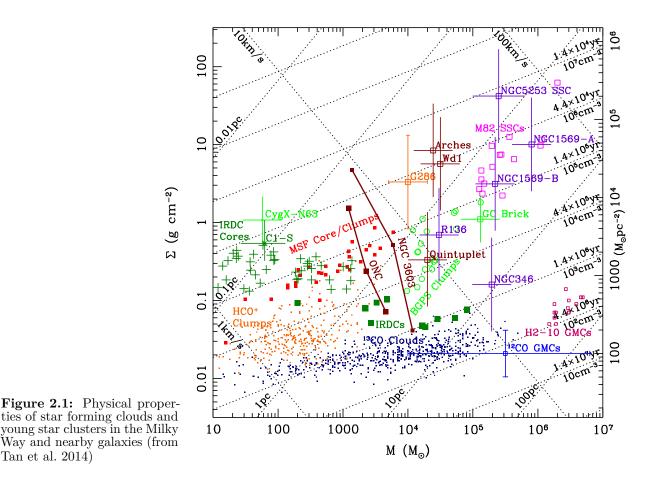
While it is generally agreed that the majority of stars form in clusters instead of in an isolated, dispersed manner (e.g. Bressert et al. 2010; Gutermuth et al. 2009; Lada & Lada 2003), there is no general consensus for how this comes about. It is also agreed from the above studies that most young clusters dissolve into the Galactic field population fairly quickly, or, more accurately, most of their stars become unbound from the cluster, leaving behind a much smaller remnant bound central core.

In this thesis we are addressing the question of how the physics of star formation affects the dynamical evolution of young star clusters during their formation, as well as in their later evolution. While we are focused on stellar dynamics, the evolution of star clusters involves a set of physical process that rise and fall in relevance during the cluster's life. In this chapter we overview the life cycle of a star cluster and the physics involved at each stage. We discuss the relevant metrics that are outcomes of star formation, which have potential consequences for the long term evolution of star clusters.

2.1 Molecular clouds

Most star clusters form from the densest parts of Giant Molecular Clouds (GMCs) (McKee & Ostriker 2007), which are defined to have masses $> 10^4 \,\mathrm{M_{\odot}}$. They are also observed to have mass surface densities $\Sigma \sim 0.01 \,\mathrm{g \ cm^{-2}}$ (see Figure 2.1). Star clusters are formed within ~ 1 to 10 parsec structures, termed star-forming *clumps*. Within clumps, star-forming *cores* host the formation of individual stars or small multiple systems, such as binaries.

Overall, most GMCs appear to be gravitationally bound (McKee & Ostriker 2007; Tan et al. 2012). This is likely to be true for star-forming clumps also, including those traced as Infrared Dark Clouds (Kainulainen & Tan 2012). The stability of clumps is a competition between gravity and several internal pressures such as thermal, magnetic, as well as turbulent stochastic motions. However, the relative importance of magnetic fields and turbulence is still a matter of intense debate, in part because of the difficulty of accurately measuring magnetic



field strengths in molecular clouds (see, e.g., Li et al. 2014a; Pillai et al. 2015). Cores within clumps need to become dense enough to become gravitationally unstable and undergo star formation. However, when gas is adiabatically compressed thermal pressure increases stopping the collapse. It is necessary that gas is also able to cool down. This is possible due to the fact that molecular clouds contain several efficient cooling mechanisms, including dust and different molecular species, especially CO, that are able to emit energy in the form of radiation. The amount of energy radiated will depend on the internal chemical structure of the gas, but in general the equilibrium between cooling and external pressures causes local overdensities to become dense in approximate isothermal equilibrium. Only when the gas reaches very high densities, at number densities of $n(H_2) > 10^{10} \text{ cm}^{-3}$ (Mac-Low et al. 2004), does it become opaque to cooling radiation so that it starts behaving adiabatically. At this point, thermal pressure starts to support the core against gravity and formation of a "first hydrostatic core" as the first stage of star formation takes place.

2.2 Star cluster formation

As soon as a protostar forms it is also acting gravitationally with surrounding sources. It is in this stage that stellar dynamics starts to become important and the outcome of individual star formation affects the early evolution of the embedded star cluster. Star-forming cores can fragment and form binaries or small systems. Binaries are extremely important as they can store large amounts of energy in their orbits. They can either absorb or release energy into

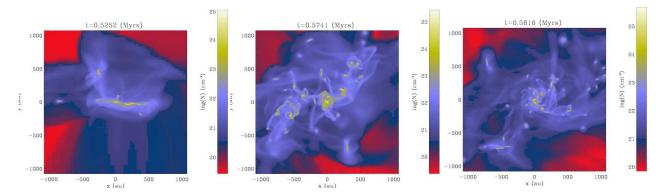


Figure 2.2: An example of fragmentation on a magneto-hydrodynamical simulation of the collapse of a turbulent magnetized cloud (from Hennebelle et al. 2011).

the environment depending on if they are hard or soft binaries (Heggie 1975; Hills 1975) (see Section 1.2). Observations shows that a large fraction of stars in the field are binary systems (Duquennoy & Mayor 1991; Fischer & Marcy 1992). However, the dynamical formation of binaries by capture is very inefficient, and the majority of observed binaries must have been formed initially as binaries (Goodman & Hut 1993; Goodwin 2010), i.e., as "primordial binaries" formed from a core. Binaries and small systems are formed through core fragmentation (Goodwin et al. 2006). Fragmentation happens in several modes, e.g., disk fragmentation and turbulent fragmentation, and depends on several factors such as the equation of state of the gas, the strength of magnetic fields, the amount of angular momentum, etc. The general idea is that as a core collapses it increases its rotation velocity by conservation of angular momentum and instabilities within the core cause it to fragment. However, magnetic fields can efficiently transport angular momentum (Li et al. 2014b), so the question of rotational evolution and disk formation is still debated.

An important outcome of star formation is the initial mass function of stars (IMF). The IMF has been shown to be quite invariant on a variety of environments, and its actual universality under debate (see Bastian et al. 2010). Stars of different masses can interact with other stars causing some of them to leave the cluster at high speeds, e.g. two stars can form a binary system and the excess of energy is lost ejecting a third star. This effect would be suppressed for instance, if all stars had the same mass (see Pfalzner & Kaczmarek 2013).

Dynamical ejections can be particularly important during the early phases of star cluster formation and evolution. Star clusters are generally at their densest in these stages. Other factors are important for the relative numbers and energy of ejected stars, such as multiplicity and mass segregation (Oh & Kroupa 2016). Both of these are potentially dependent on the star formation process, i.e., can have "primordial" values. However both can also be modified during the evolution of the cluster.

In the case of mass segregation, it has been argued that massive stars need higher densities and gas rich environments to form, and therefore should be born in the central areas of molecular clumps (Bonnell et al. 2001). However mass segregation can also develop dynamically, since more massive stars are more affected by dynamical friction than low-mass stars, so that they decay to the center of star clusters naturally. In fact, it has been shown that mass segregation timescales are quite short, and distinguishing between primordial or developed mass segregation is a very difficult task. While some efforts have been made to distinguish between primordial or developed mass segregation (e.g. Baumgardt et al. 2008; Moeckel & Bonnell 2009; Parker et al. 2014) unfortunately most of these studies assumed that all stars are formed instantly and thus ignore the crucial star cluster formation stage.

It is also uncertain what are the primordial properties of binaries, as well as their initial fractions. If wide binaries are formed, then they are likely to be destroyed during the dense, early phase. However they can also form dynamically during the later expansion of the cluster (e.g. Kouwenhoven et al. 2010), in the stage discussed in the next section. Most of what we know about binary populations comes from observations of binaries in the field, i.e., when any dynamical processing is finished.

After stars are formed, they can be kept in a dense state by the background gas that is still present. Star formation is a highly inefficient process and only 20% to 50% of the initial gas is observed to be transformed into stars, at least in local young clusters in the Milky Way (Lada & Lada 2003). It is uncertain how long the residual gas stays within star cluster boundaries. However, while it is present it can be an important contribution to the potential well of the star cluster, and thus keep stars in a dense environment with high velocity dispersions.

When the first massive stars are born they can dissipate the surrounding gas via radiation pressures, ionization and strong stellar winds. Gas will start to dissipate and ultimately, the first supernovae explosion may remove any remaining gas from the cluster.

2.3 Surviving gas expulsion

After the gas is gone, the evolution of the star cluster is only determined by the gravitational interaction of its members, together with stellar evolution processes, which include some gas removal from stars, e.g., by winds. However, the transition from an embedded star cluster to naked bound entity is thought to be a violent process that might disperse most of young star clusters. The low global star formation efficiencies imply that the gas not used by star formation will be the main component of the potential well that keep the cluster bound. The violent removal of the gas results in most of the stars suddenly having higher velocities than the escape velocity and therefore are unbound to the system. In the classical picture of this scenario, the only way for star clusters to remain bound is having relatively high SFE (> 20%) or removing the gas on timescales much greater than their crossing time (Baumgardt & Kroupa 2007).

However, recent studies have shown that this transition may not be as destructive as originally thought. Many of the assumptions on star cluster formation that these classical models use are far from reality, and in fact these assumptions have a great influence on the survival and early evolution of star clusters.

Star clusters are likely to be out of equilibrium at formation, e.g., either sub- or super-virial. Then, they need time to reach equilibrium and relevant global parameters oscillate during several crossing times. The result is that survival rate, if gas expulsion is explosive, will depend on how these parameters end up when gas is expelled. The two relevant parameters are the stellar to gas mass fraction in the central regions of the cluster, e.g. within the half mass radius, and the stellar virial ratio, both measured when gas expulsion beings.

The central stellar fraction may also be an outcome of star cluster formation. Star formation may happen faster in denser parts of the star forming clump where the free-fall time is shorter (Parmentier & Pfalzner 2013). Furthermore, stars do not form in spherical distributions. Star forming clumps usually show filamentary structures on several scales. It has been shown that

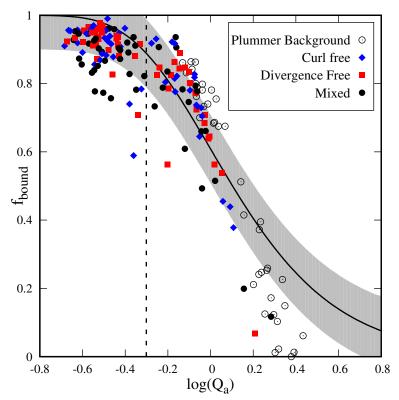


Figure 2.3: The bound fraction as a function of stellar virial ratio at gas expulsion time for star clusters with different levels of stellar and gaseous structure and SFE of 20% (from Farias & Tan 2018).

just by the introduction of substructure in numerical simulations, there is an increase in the central stellar fraction considerably via merging of substructures (Farias et al. 2015; Smith et al. 2011, 2013).

Most importantly, it has been shown that the stellar virial ratio at the time of final gas expulsion is the only necessary parameter to estimate the minimum amount of mass that a star cluster will retain (Lee & Goodwin 2016), even in the most complex stellar and gaseous distributions (Farias & Tan 2018), as can be seen in Figure 2.3.

2.4 Gas-free evolution

Even if a star cluster survives gas expulsion, the process will likely expand it considerably. It is important that the cluster remain dense after gas expulsion so its internal binding energy is large. If it is not dense enough it could be easily destroyed by tidal forces from nearby molecular clouds and/or from the host galaxy.

In the best scenario, if the star cluster remains dense after emerging from its parent clump, internal dynamical processing may also expand the cluster. Star clusters are collisional systems, which means that close encounters between stars determine the internal evolution and structure of the entity. Strong dynamical interactions between stars, especially multiples, typically end up in one or more stars being ejected with high velocities. High densities enhance these interactions in energy and frequency, therefore they are most likely to happen in the center of the cluster. These ejections remove binding energy from the cluster in the form of kinetic energy of the ejected stars and therefore the cluster expands. The timescale at which a star cluster evaporates completely is ~ $100t_{relax} \approx (10N/\log N)t_{cross}$ (Binney & Tremaine 2008). For a small star cluster of 100 members, this means $1000t_{cross}$ which is in general a relatively long

timescale, especially compared to expected formation timescales.

At this stage, the most massive stars have already exploded as supernovae – and may have been the ones that removed any residual gas from the cluster – but at later stages, the mass loss from other intermediate- and lower-mass stars starts to play a role in the evolution of the star cluster. Stellar evolution becomes a secondary source of dynamical ejections. If one of the stars that explode as a supernova happens to be a binary system, the sudden mass loss will modify the binary orbit and it could even cause the ejection of both star and remnant in opposite directions. Even the remnants of single massive stars can be ejected spontaneously when exploding as supernovae, since these explosions are not necessarily symmetrical and the supernovae remnant (neutron star or black hole) can be ejected in a random direction at very high speeds, i.e., a few hundred km/s.

Thus, once a star cluster is born its subsequent evolution will depend on its environment and the ability of the cluster to remain dense. Clusters will tend to keep losing mass by stellar evolution, dynamical evaporation and tidal stripping.

We have briefly overviewed the life cycle of star clusters and the physics involved. We have seen that the evolution and survivability is the combination and interplay of several physical processes. However, most of the factors that determine the dynamical evolution of star clusters are determined by the physics and the outcome of star formation. Many theories exist on how stars are formed and there is a long standing debate on what the outcome of star formation is and how star clusters are born. All these different theories have direct and indirect implications in the evolution of star clusters and in this thesis we will explore some of them. We will aim to identify the observables that could constrain some of these theories using a statistical approach.

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Chapter ${\mathcal 3}$

Numerical Methods

3.1 The N-body Code: Nbody6

In this thesis aim to follow accurately the dynamical evolution of star clusters over millions of years, mainly focussing on the gravitational interaction between their members. This treatment includes an accurate modeling of stellar binaries with a wide range of period distributions, including periods as short as ~ 1 day. This achievement is enabled by use of the Nbody6++ (Wang et al. 2015), a multiprocessor optimized version of the extensively developed code Nbody6, the first version of which is almost 50 years old, and which is still under active development. Here we will briefly describe its main features, as well as the modification done by ourselves in order to accomplish our goals. A complete description of the code can be found in Aarseth (2003).

Nbody6 is a sixth order Hermite integrator that calculates the forces between the particles directly with no approximations. The resulting acceleration vector of the forces acting on a given particle i by the rest of the N-1 particles is given by:

$$\ddot{\mathbf{r}}_{i} = \sum_{\mathbf{j}\neq \mathbf{i}} \frac{Gm_{\mathbf{j}}(\mathbf{r}_{\mathbf{i}} - \mathbf{r}_{\mathbf{j}})}{|\mathbf{r}_{\mathbf{i}} - \mathbf{r}_{\mathbf{j}}|^{3}}, \qquad (3.1)$$

where m_j is the mass of the *j*th particle and **r** is the position. The equations of motion given by equation 3.1 need to be solved for each particle. Therefore there are 3N differential equations to be solved. For $N \leq 3$ it is possible to be done analytically, however for greater numbers is only possible to do numerically. There are multiple numerical schemes to solve equation 3.1, from which Nbody6 uses the Hermite scheme, which solves the equations of motion using a Taylor expansion series up to 4th order. Here we briefly describe the scheme.

3.1.1 Hermite Scheme

In the Hermite scheme, accelerations \mathbf{a}_0 are given explicitly by equation 3.1 and their derivatives $\dot{\mathbf{a}}_0$ are calculated by:

$$\dot{\mathbf{a}}_{0} = \sum_{\mathbf{j}\neq\mathbf{i}} Gm_{\mathbf{j}} \left[\frac{\mathbf{V}_{\mathbf{ij}}}{R_{\mathbf{ij}}^{3}} - \frac{3(\mathbf{V}_{\mathbf{ij}} \cdot \mathbf{R}_{\mathbf{ij}})\mathbf{R}_{\mathbf{ij}}}{R_{\mathbf{ij}}^{5}} \right] , \qquad (3.2)$$

where G is the gravitational constant, $\mathbf{R}_{ij} = \mathbf{r}_i - \mathbf{r}_j$, $\mathbf{V}_{ij} = \mathbf{v}_i - \mathbf{v}_j$, $R_{ij} = |\mathbf{R}_{ij}|$, $V_j = |\mathbf{V}_j|$. Then a first (low order) prediction of the position and velocity of the particle *i* at $t = t_1$ is calculated (with $t_1 = t_0 + \Delta t$ and Δt as particle timestep) according to:

$$\mathbf{x}_{p}(t) = \frac{1}{6}(t-t_{0})^{3}\dot{\mathbf{a}}_{0} + \frac{1}{2}(t-t_{0})^{2}\mathbf{a}_{0} + (t-t_{0})\mathbf{v} + \mathbf{x} , \qquad (3.3)$$

$$\mathbf{v}_{p}(t) = \frac{1}{2}(t-t_{0})^{2}\dot{\mathbf{a}}_{0} + (t-t_{0})\mathbf{a}_{0} + \mathbf{v} , \qquad (3.4)$$

where the subscript p stands for "predicted". This is done for all particles in the cluster. Thus, using again equations 3.1 and 3.2 with the new positions of the particles we obtain the accelerations and their derivatives at $t = t_1$ denoted \mathbf{a}_1 and $\dot{\mathbf{a}}_1$. However, \mathbf{a}_1 and $\dot{\mathbf{a}}_1$ can also be obtained using the Taylor series with higher derivatives of \mathbf{a} at $t = t_0$:

$$\mathbf{a}_{1} = \frac{1}{6}(t-t_{0})^{3}\mathbf{a}_{0}^{(3)} + \frac{1}{2}(t-t_{0})^{2}\mathbf{a}_{0}^{(2)} + (t-t_{0})\dot{\mathbf{a}}_{0} + \mathbf{a}_{0} , \qquad (3.5)$$

$$\dot{\mathbf{a}}_{1} = \frac{1}{2}(t-t_{0})^{2}\mathbf{a}_{0}^{(3)} + (t-t_{0})\mathbf{a}_{0}^{(2)} + \dot{\mathbf{a}}_{0} .$$
(3.6)

Now, since we already know \mathbf{a}_1 and $\dot{\mathbf{a}}_1$ from the low order prediction, we can use that result to obtain the higher derivatives of \mathbf{a} , at $t = t_0$, i.e., $\mathbf{a}^{(2)}$ and $\mathbf{a}^{(3)}$:

$$\frac{1}{2}\mathbf{a}^{(2)} = -3\frac{\mathbf{a}_0 - \mathbf{a}_1}{(t - t_0)^2} - \frac{2\dot{\mathbf{a}}_0 + \dot{\mathbf{a}}_1}{(t - t_0)}$$
(3.7)

$$\frac{1}{6}\mathbf{a}^{(3)} = 2\frac{\mathbf{a}_0 - \mathbf{a}_1}{(t - t_0)^3} - \frac{\dot{\mathbf{a}}_0 + \dot{\mathbf{a}}_1}{(t - t_0)^2} .$$
(3.8)

The Hermite interpolation then finishes the timestep correcting the low order prediction of the positions and velocities to a higher order:

$$\mathbf{x}(t) = \mathbf{x}_p(t) + \frac{1}{24}(t-t_0)^4 \mathbf{a}_0^{(2)} + \frac{1}{120}(t-t_0)^5 \mathbf{a}^{(3)} , \qquad (3.9)$$

$$\mathbf{v}(t) = \mathbf{v}_p(t) + \frac{1}{6}(t - t_0)^3 \mathbf{a}_0^{(2)} + \frac{1}{24}(t - t_0)^4 \mathbf{a}_0^{(3)} .$$
 (3.10)

3.1.2 Block Timestep Scheme

Particles in the system feel very different accelerations and the timestep needed to accurately follow their motion depends on the strength of the acceleration. Therefore, individual timesteps are needed. Nbody6 uses the *block timestep scheme* in which timesteps are sorted into a hierarchy of levels starting from a maximum timestep Δt_1 according to the rule:

$$\Delta t_n = \Delta t_1 / 2^{n-1}. \tag{3.11}$$

At the beginning of the calculation a reasonable timestep for each particle is specified. This reasonable timestep has been found by empirical experiments to be (see Aarseth 2003):

$$\Delta t_{i} = \sqrt{\frac{\eta |\mathbf{a}| |\mathbf{a}^{(2)}| + |\dot{\mathbf{a}}|^{2}}{|\dot{\mathbf{a}}| |\mathbf{a}^{(3)}| + |\mathbf{a}^{(2)}|^{2}}},$$
(3.12)

where η is a free parameter, which by experience is usually taken to be in the range $\eta = 0.01 - 0.04$. Then the nearest level is chosen according to Eq. 3.11. At any general time Eq. 3.11 is evaluated and any of these three cases apply when comparing with the previous timestep Δt_p : If $\Delta t_p > \Delta t_i$ then the timestep is reduced by a factor of 2; if $2\Delta t_p < \Delta t_i$ the timestep is increased by factor 2; otherwise there is no change. A detailed discussion about the implementation and special situations can be found in Aarseth (2003).

3.1.3 Neighbour scheme

In order to save computational time, the code adopts the Ahmad-Cohen neighbour scheme (Ahmad & Cohen 1973; Makino & Aarseth 1992). The basic idea is that the contribution to the acceleration given by distant particles does not need to be updated as frequently as close *neighbour* particles. As a difference of similar approaches like the Tree scheme (Barnes & Hut 1986), where the calculation of distant particles is done using their center of mass, in the neighbour scheme the forces are still calculated individually and therefore the method is not an approximation, but rather an optimization. The optimization is based on the fact that distant particles have smaller angular speeds and their force contribution does not change so fast as neighbouring particles.

3.1.4 Regularizations

Even with only single particles, the methods described above are not enough to efficiently handle all the length and time scales involved in the evolution of a realistic star cluster. However, the main problems are caused by binary systems with very short periods, on the order of days, that will likely keep their short separation during the whole duration of the calculation. In addition, small stable multiple systems, normally composed of a binary perturbed by another binary or single star, and very close encounters between stars, may slow down the simulations even with individual timesteps and the neighbour scheme. Nbody6 uses several methods to deal with these special cases called *regularizations*. Close encounters and binaries are handled with the Kustaanheimo-Stiefel (KS) regularization (Kustaanheimo & Stiefel 1965), which uses a coordinate transformation in order to avoid singularities. The KS scheme has been expanded to the isolated and perturbed 3- (Aarseth et al. 1974) and 4-body problem as well as higher order hierarchies (Mikkola 1997; Mikkola & Aarseth 1993, 1996, 1998; Mikkola & Aarseth 1989).

3.1.5 Gradual formation

In this thesis we study star cluster formation from the beginning, that is, during the stage of the cluster where stars are being created. Unfortunately, this is a feature not currently implemented in Nbody6. However, during a regular Nbody6 run, particles are being created and removed all the time. Each time regularization starts, the particles involved in the regularization are

removed from the calculation and replaced by a center of mass particle that interacts with the rest of the cluster, while the regularized particles are integrated in isolation. Also, high velocity escapers are normally removed entirely from the calculation. Therefore, there is no reason that stop us from adding particles arbitrarily during the run-time. Through careful investigation of the code, we have introduced our own routines in order to achieve this feature. We are able couple a time evolving background gas potential with the creation of single and KS regularized binaries until the gas is exhausted.

This feature then enables us to study a regime only explored so far by state-of-the-art hybrid N-boody/hydrodynamical codes. However, because of the complexity of the N-body problem, these codes normally have not implemented regularizations of binaries or higher-order multiples. Also, they normally use approximations like the Tree scheme (Barnes & Hut 1986). We expect that the important feature we have developed, allowing gradual star formation, can enable Nbody6 to be coupled with hydrodynamical codes in frameworks like the Astrophysical Multipurpose Software Envirionment (AMUSE) (Pelupessy et al. 2013; Portegies Zwart et al. 2009). Still, coupling Nbody6 with hydro codes would be computationally expensive, and the pure N-body approach presented here, is the first necessary step to obtain a general statistical understanding of stellar dynamics during star cluster formation.

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Chapter 4

Introduction to papers

In this thesis, we explore the effects of several fundamental parameters of star cluster formation theories, such as the initial mass surface densities of the gas clumps, the frequency of the primordial binary population, the degree of primordial mass segregation, and, of particular importance, the timescale of star cluster formation. We have developed novel techniques for modeling star cluster formation, while accurately following stellar dynamics. Ejected, so-called "runaway" or "walkaway", stars are an important population that can help us understand star cluster formation. While we follow the global evolution and structure of the bound cluster, it can quickly erase its initial state and rearrange to a near equilibrium configuration. The ejected stars are sensitive to other aspects of the history of the forming cluster, including the number density and multiplicity of the cluster members. In this thesis, we present three independent, but closely related, works. First, we present, in two papers the star cluster formation model that we use in our main work, as well as it implications. Then, we present a study that analyzes how a particular observed runaway system in the Orion Nebula Cluster may have been created by exploring the parameter space of possible binary-binary interactions. Third, we exploit the capabilities of *Gaia* by searching for runaway stars in the ONC in an attempt of characterize its unbound population. We use the results of this work to contrast the results of the theoretical models presented in the first part of this thesis.

Star Cluster Formation from Turbulent Clumps. I. The fast formation limit

In this paper, we set the basis for our overall project of cluster formation modeling. We present a simple form of the model in the extreme limit of fast, i.e., instantaneous, star cluster formation. Even though this model appears unrealistic, it has been the commonly adopted assumption of most previous dynamical studies exploring the early evolution of star clusters. Also, most previous studies have used initial conditions in which the stellar population is already in dynamical equilibrium. In contrast, we draw our initial conditions from observations of starless clumps and theory describing their internal structure, i.e., the Turbulent Clump Model, from which we then form star clusters. We found that in this scenario, star clusters

expand very quickly, meaning that in order to explain the current structure and sizes of observed star clusters, dense initial conditions are necessary. Also, the periods that star clusters remain dense are very short (less than a crossing time), thus not giving enough time to produce significant dynamical ejections. In fact, not a single runaway massive star was produced. This work suggests that star cluster formation must happen in a less extreme fashion, that we will explore in the subsequent papers of this series.

Star Cluster Formation from Turbulent Clumps. II. Gradual star cluster formation

In this paper, we relax the assumption of instantaneous star cluster formation explored in Paper I (and in most of studies to date). We explore a range of star cluster formation timescales, parameterized by the star formation efficiency per free-fall time. We model the natal gas of the young cluster using a time evolving background potential, based on the Turbulent Clump Model. As the stars are created, the background potential gradually vanishes assuming a global star formation efficiency. Using this simple prescription, we study the dynamic of the stars during the formation of the cluster, and found that the longer formation timescales give enough time for the cluster to get close to virial equilibrium before gas is completely exhausted/ejected. Star clusters formed in a slow fashion are much more stable against expansion than the ones forming fast. In these models, we are able to form a significant fraction of massive runaway stars even in low density environments. In general, the models presented in this paper, appear to require lower densities to reproduce parameters that could only be explained appealing to highly dense initial environments. However, several assumptions need to be relaxed and studied to understand the real extent of these results.

Star Cluster Formation from Turbulent Clumps. III. Across the Mass Spectrum

Star clusers forms in a wide range of scales and masses, where the different physical processes involved in star cluster formation have different relative importance depending of their own timescales and environmental regimes. It is not clear how our previous results would scale to other possible environments on which star clusters are observed to be born. In this work, we extend our models to a wide range of parent clump masses and densities and explore how the different environments affect the dynamical processing of the primordial stellar population, e.g. binary properties, mass segregation and production of high velocity stars. And also how these different initial conditions affect the later evolution of these systems. In this models, clumps of higher mass are of lower initial volume density, but their dynamical evolution leads to higher bound fractions and causes them to form much higher density cluster cores and maintain these densities for longer periods. This results in systematic differences in the evolution of binary properties and the rates of creation of dynamical ejection runaways. Herem, we discuss the implications of these results for observed star clusters.

On the formation of runaway stars BN and x in the Orion Nebula Cluster

Star clusters formed in a slow fashion are much more stable against expansion than the ones forming fast. The Orion Nebula Cluster (ONC) is the closest region of massive star formation. It hosts a massive young star, BN ($\sim 10 M_{\odot}$), that is moving with a velocity of

 ~ 30 km/s in the frame of reference of the ONC. Recent observations have show that two known nearby objects, source x (~ $3 M_{\odot}$) and source I (~ $7M_{\odot}$), are moving away from the same location than BN and the three objects may have been part of the same ejection event about 500 years ago. However, this implies that the most massive star in the system was ejected with very high velocity, which seems questionable. We thus performed a large, $> 10^7$, set of "few-body" simulations testing this scenario, and have found that the event as described is nearly impossible to happen with the observed velocities. We conclude that to make this scenario plausible, requires source I to in fact be more massive than the $\sim 7 \, M_{\odot}$ that has been adopted by some authors in their previous works. This may be possible, since source I is heavily embedded in dusty molecular gas. The results are of wider interest, since this region is the closest example of massive star formation and is one of the most well studied locations of the sky, including one of the richest sites for detection of interstellar molecules. The violent nature of the interaction, including potential gas interactions and shocks, likely has a bearing on why this region appears so luminous in the infrared and is so chemically rich. After this work was published, new high resolution ALMA observations of Source I have obtained a mass of $15 \,\mathrm{M_{\odot}}^1$ very close to the optimal mass suggested in this work. Our results and these new observations suggest that the dynamical ejection scenario involving source I, source x and the BN object can not be discarded.

Hunting for runaway star from the Orion Nebula Cluster

As mentioned before, characterizing the unbound population of star clusters can provide strong constraints on the formation and early environment of star clusters. Identifying such constraints is one of the long term goals of the work presented here. One of the best targets for contrasting theoretical models with observations is the ONC, that given its close distance, large efforts have been made on characterizing its stellar population, structure and kinematics. However characterizing its unbound population is a challenging problem given that they are well mixed with the field population and also that the region that they may cover is unknown and not well mapped. In this paper, we made an attempt to identify new runaway/walkaway candidates from the ONC that may have traveled large distances from their origin. Using the unprecedented accuracy of *Gaia* we have examined a 45° area around the ONC and selected a sample of $\sim 17,000$ sources whose 2D trajectory overlap with the one of the ONC. We further classified those sources combining photometry and astrometry thresholds aiming to identify sources with well constrained orbits and that also show signs of being Young Stellar Objects. e.g. using *Gaia*, 2MASS and WISE photometry when available. We have selected a handful of 25 sources not previously identified as members of the ONC as the strongest candidates. We use the results of this work to complemented with literature members, to construct a high velocity distribution of the ONC members and compare with our previous simulations, finding good agreements with our models with the densest initial conditions.

 $^{^1 \}rm{see}$ A. Ginsburg , J. Bally, C. Goddi, R. Plambeck and M. Wright (2018). A Keplerian Disk around Orion SrCI, $a\sim 15~\rm{M}_\odot~YSO.$ ApJ 861(2), p. 119.