APPROCHE MULTI-ÉCHELLE DE LA FORMATION ET L'ÉVOLUTION DES AMAS D'ÉTOILE

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INTRODUCTION

Foreword

Looking at the four fundamental forces, gravity is probably the one that we, as a species, take the most for granted. Of course, few of us stop and meditate on the strong and nuclear forces on a daily basis, but we never experience their direct effect. We do not feel the strong nuclear force tying together the protons inside our bodies, neither do we feel the weak nuclear interaction inducing our potassium atoms to decay into calcium. The electromagnetic force is more present in our mind on a daily basis. Even more so since the arrival of the *fée électricité* in our lives and the advent of her child, the electronic age. Even though some manifestations of the electromagnetic force, such as sunlight, are taken for granted, humans keep a sense of wonder about electromagnetism. Magnets, lightning, electromagnetism *feels* magical, as humans have only understood it for a few generations.

What about gravity? Gravity is part of our mental landscape, we experience its direct effects all the time. If we drop something, it falls, if we throw something, it curves back to the ground, we know this, instinctively. The absence of gravity feels much stranger as our brains evolved under the influence of this fundamental force. Thus we rarely reflect on it.

However, it is by no means the least interesting of forces.

Gravity is the Great Herder, the maker of galaxies, the creator of stars and author of planets. It brings matter together.

0.1 From Aristotle to GPU computing: an history of physics and gravity

0.1.1 Motion

For two thousand years, Aristote physics dominated european philosophy. Rocks fell to the ground because they wanted to join their element, objects in the sky were attached to eternal rotating crystal spheres, and motion was either natural or violent, the latter needing a continuous force to exist. As the importance of projectiles grew in middle-age warfare, some improvement were made to explain trajectories, such as the impetus, a "contained source of motion" imprinted to a projectile by the thrower. Introduced by Philopon in the 6th century and relayed by Avicenne in the 11th century, it was properly formalized by Jean Buridan in the 14th century in his "Questions on Aristotle's Metaphysics". Buridan's impetus had a lot in common with momentum, in that it was proportionnal to mass and velocity, but could be circular, as shown by this description of celestial motion from Buridan:

"God, when He created the world, moved each of the celestial orbs as He pleased, and in moving them he impressed in them impetuses which moved them without his having to move them any more...And those impetuses which he impressed in the celestial bodies were not decreased or corrupted afterwards, because there was no inclination of the celestial bodies for other movements. Nor was there resistance which would be corruptive or repressive of that impetus." (Clagett, 1959)

Despite the conceptual mistake of a circular momentum, Buridan, with this text, is the first to include the motion of celestial bodies in the same framework used for everyday, terrestrial motion. The impetus is not a good model, but it is a model for everything in the universe. No more eternal crystal spheres, everything in the universe must obey the same laws. Scientific revolutions do not happen in a vacuum: Buridan and others paved the way for the intellectual landslide of the 16th and 17th century.

0.1.2 Geocentrism and heliocentrism

While the concept of motion was slowly being refined, our vision of the universe was undergoing some faster changes. The dominant system in Europe since 150AD was the Ptolemaic geocentric model: the Sun and planets went around the Earth, following convoluted trajectories made of circles within circles called epicycles. Though complex, this system was consistent with Aristotle principles of celestial spheres and was accurate to a reasonable extent. Some alternate geocentric models were proposed by arab astronomers, such as Nasir ad-Din at-Tusi and Ibn al-Shatir, as well as rejected attempts to heliocentric models.

Nicolaus Copernicus studied astronomy in Cracow and Bologna, under the influence of hard critics of the ptolemaic system. Strangely, this criticism was not fueled by observations, but by astrology. Astronomy and astrology were closely intertwined, and the chaotic structure of the ptolemaic system made astrological considerations complicated (Barker et al., 2014). In a quest for consistency and simplicity, Copernicus proposed his heliocentric system, published in *De revolutionibus orbium coelestium* in 1543, the year of his death, in which all planets went around the sun, in the correct order. However, clinging to circular orbits, Copernicus had to preserve ptolemaic workarounds such as epicycles.

The astronomical evidence was, at the time, paradoxically against him. The apparent size changes of planets could not be measured yet, as well as stars parallaxes, contradicting heliocentrism. The idea of a moving Earth implied some effect on falling bodies (known today as coriolis effect) but was just not measurable at the time. Building on this apparent counter-evidence and on the work of indian astronomer Nilakantha Somayaji, Tycho Brahe, the most renowned astronomer of his time, proposed an alternative model known as the Tychonic system in the late 16th century (Ramasubramanian, 1998). Brahe maintained the Earth as the center of the universe, circled by the sun, orbited by all other planets. The system was very efficient and was quickly adopted by the Church as in compliance with the Holy Scriptures.

However, the seed of heliocentrism was planted in european scientific minds. The idea exalted the impetuous Giordano Bruno, who pushed the decentralization of Earth to the extreme, claiming stars were other suns, harboring other planets, which themselves could sustain intelligent life. For this, his rejection of catholic dogma and his vehement refusal of retractation, Bruno was burned at the stake on the Campo de Fiori in 1600. Bruno, the fiery dialectist, despised geometry and believed the mind alone could unravel any mystery. The contrast could not be greater with the next mind on our way to the scientific revolution.

Johanes Kepler believed in geometry, in consistency and in observations. Ardent supporter of copernicism, he convinced Tycho Brahe to grant him access to his astronomical data, unsurpassed at the time. Focusing on the motion of Mars, Kepler, through trial and error, found out the planet was moving around the Sun following an ellipse. He formulated his first two laws of planetary motions. Further exploration led him to the third law. The three laws of Kepler were formulated, initiating the mathematisation of astronomy, and with it of all physics.

0.1.3 The Starry Messenger

The father of modern astronomy, and precursor of modern science, Galileo Galilei was born in Pisa in 1564. For the first part of his scientific career, Galileo got famous for his lectures on mechanics and motion. Building on Buridan and Oresme's ideas, he expressed the mathematical

form of free fall motion $d = \frac{gt^2}{2}$. Galileo also formulated what was essentially the future first law of motion from Newton.

In 1609, his passion for scientific instruments led Galileo to build his own "dutch perspective glass", or telescope, a pioneering optical device from the netherlands. Once pointed at the sky, the device triggered an avalanche of observations who would forever bury the aristotelitian view of perfect and unchanged heavens. Moving Jupiter satellites, Moon craters and mountains, millions of stars in the Milky Way, these were consigned into *Sidereus Nuncius* (Starry messenger), the first scientific publication of astronomical observations (Galileo, 1610).

Strong advocate of copernicism, but lacking proper evidence, Galileo caused a large controversy with his *Dialogue Concerning the Two Chief World Systems* published in 1632, a pamphlet against the ptolemaic system, presenting (arguably unintentionnaly) one of its advocates as a simpleton. Despite his friendship with the pope, he had to retract his work and reject copernicism. Galileo spent the rest of his life on house arrest. Observationnal evidence at the time still on the side of geocentrism, but the extent of the backslash against Galileo showed the febrility of a Church having absorbed Ptolemy and Aristotle principle into its doctrine, in a time where the debate was shifting from theology to physics and observations.

The relativity of motion is often attributed to Galileo, as he includes it in its controversial pamphlet, stating that a traveller inside a ship sailing smoothly would not be able to tell he's moving. Thus, people could be standing on a moving Earth without feeling it. However, this thought experiment was nothing new at the time and had been a recurring theme of mechanical philosophy since Buridan. Oresme, Copernicus and Bruno had been building on the idea, expanding and improving it, developing over the centuries an implicit understanding of inertia, until Bruno actually gives it a name: $virt\hat{u}$. Galileo may have met Bruno himself, and had surely been influenced by his writings (De Angelis & Santo, 2015). Galileo's formulation was clearer, and part of a larger understanding of motion, introducing the concept of reference frame. After Copernicus decentralized the Earth, Galileo decentralized human subjectivity itself, setting the scene for the revolution to come.

0.1.4 On the shoulders of giants

Isaac Newton is without a doubt the father of modern mathematical science. Admitted in Cambridge in 1661, Newton supplemented the -still- official aristotelitian teaching with more modern authors: Copernicus, Galileo, Kepler, and most of all, Descartes. The french philospher had a profound impact on the young student, rooting his love for mathematics and deductive reasoning. However, while Descartes showed disdain for experimentation, Newton was an acute observer of the natural world.

In 1666, while in is mother's farm, having been forced out of Cambridge by the Plague, Newton began his reflexion on the motion of celestial bodies. He derived from Kepler's law that the Sun had to exert an inverse squared distance attraction on the planets. Extending the concept to the Earth, moon, and a famous apple, Newton found a way to verify his hypothesis, using data from Galileo mechanical studies on the strength of Earth attraction. The wrong estimate of Earth radius he used at the time introduced a discrepancy which put the young man off his gravitas studies for 18 years.

Edmond Halley, astronomer and friend of Newton, having heard of Newton inverse squared law, urged him in 1684 to communicate his work the Royal Society. With a new accurate measure of Earth radius and confronted to a concurrent claim to his law from Robert Hooke (Kramer, 1982), Newton capitulated to Halley's eager enthousiasm and communicated his work in the famous *Philosophi Naturalis Principia Mathematica* (Newton, 1687). Published at Halley's own expense, the Principia shook all of Europe. Newton had invented Calculus (in parallel of Leibniz) and applied it to derive the universal law of Gravitation.

$$F = G \frac{m_1 \cdot m_2}{r^2} \tag{1}$$

Where:

F Gravitational attraction between object 1 and object 2 G Gravitational constant, $6.67408.10^{-11}m^3kq^{-1}s^{-2}$ (Pavese, 2015)

 m_i Masses of object 1 and 2

r Distance between object 1 and 2

Though Newton was part of continuous line of geniuses and innovative minds building from each others, as he puts it "If I have seen further it is by standing on the shoulders of giants" (Maury, 1992), his input was truly revolutionnary. He made large advances in optics and mathematics, and created a consistent mathematical framework to compute motions, essentially founding modern science and sowing the seeds of the industrial revolution. This framework is summed up by Newton's three laws of motion (from recent translation Cohen I. B. 1999):

Law I: Every body persists in its state of being at rest or of moving uniformly straight forward, except insofar as it is compelled to change its state by force impressed.

Law II: The alteration of motion is ever proportional to the motive force impress'd; and is made in the direction of the right line in which that force is impress'd.

Law III: To every action there is always opposed an equal reaction: or the mutual actions of two bodies upon each other are always equal, and directed to contrary parts.

The second law can be mathematically formulated in more modern terms:

$$\sum \mathbf{F} = \frac{d\mathbf{p}}{dt} \tag{2}$$

Meaning the sum of all forces **F** applied to an object is equal to the time derivative of its momentum $\mathbf{p} = m.\mathbf{v}$.

0.1.5 The n=3 body problem

As the Enlightenment brought a scientific revolution in many fields, I will now limit the discussion to the development of celestial mechanics, while acknowledging input from other fields.

While the two-body problem had been solved by Newton and expanded by Bernoulli in 1710 (Barrow-Green, 1997), in the 18th century the three-body problem remained the object of much investigation and development. A general solution for the Earth-Moon-Sun system would have had applications on nautical astronomy and trans-continental navigation. Extended analytical work by d'Alembert, Clairaut, Euler and Lagrange led to the development of early families of approximate solutions or exact solutions to special cases.

From 1773 to 1793, Joseph-Louis Lagrange, helped by his invention of Lagrangian mechanics, would make a lot of advances on the three-body problem. He introduced the concept of potential and discovered libration points (later known as Lagrange points). In the same time, Pierre-Simon de Laplace proved the stability of the solar system using a newly developed perturbation theory. The solar system dynamics were being unraveled, with finely tuned perturbation computation, but the general three-body problem remained unsolved.

In 1888, Henri Poincar, greatest mathematician of his time, submitted an entry to a contest organized by the King of Sweden Oskar II. The goal was to determine a usable solution to the n-body problem, for any given n. While Poincar does not submit a complete solution, he wins the contest by presenting an in-depth exploration of the phase-space of the restricted three-body problem, which would later give rise to the Chaos theory ,see Yoccoz (2010). Poincar managed to prove that the three-body problem had no solution involving simple functions.

Contrary to popular belief, the three-body problem *has* a solution, it was derived by Karl F. Sundman in 1912 (Sundman, 1912). However, any attempt to obtain accurate trajectory predictions would face tremendous convergence time and is in practice unusable (Belorizky, 1930).

It is interesting to note that Elis Strömgren performed by-hand calculation of a three-body system, see Aarseth (2003); Strömgren (1909), prefiguring the advent of numerical orbit computation.

0.1.6 The n>3 body problem

"The Sun attracts Jupiter and the other planets, Jupiter attracts its satellites and similarly the satellites act on one another."

By this sentence from the *Principia*, Newton formulates the n-body gravitational problem, an arbitrary number of massive bodies all interacting gravitationally, for the solar system. The "n>3-body" problem didn't receive a lot of attention at first, as the unruly three-body problem was on everyone's mind, and a n>3-body problem seemed abstract, the solar system example being appropriatly dealt in approximations.

In 1764, Charles Messier resolved individual stars in Messier 4, a globular cluster, hundreds of thousands of stars grouped together. Many new clusters were to be found afterwards, extending the catalog of real-life n-body systems. However, nothing was known of their kinematics, the stars were somehow suspended motionless in the sky. This was the case until the advent of Doppler spectroscopy, which allowed astronomer to measure stars velocities (Doppler, 1842). Stellar dynamics had begun.

The n>3-body problem was still inaccessible, so scientists like James Jeans and Arthur Eddington decided to take the problem from the other hand, and took advantage of the large number of stars. Inspired by Poincaré (1906), both astronomers applied the statistical theory of gas to stellar systems, founding the field of stellar dynamics (Jeans, 1916; Eddington, 1916).

An interesting experiment was conducted by Holmberg (1941) to understand the collision of two stellar systems (galaxies). With too few points to warrant a statistical approach, and before the rise of numerical integration, Holmberg modelled two galaxies with lightbulbs and photocells, measuring the attractive force with the amount of light received in each direction, taking advantage of the inverse squared fall of luminosity with distance, akin to gravity.

0.1.7 The numerical age

The first numerical N-body computations were performed by Sebastian Von Hoerner in 1959 when visiting the University of Tübingen, on a Siemens 2002, a cutting edge calculator at the time. The very first had N=4. Then, Von Hoerner, back in Heidelberg, worked his way up to 16 stars, then 25, programming and debugging on punch cards. This story was told by Von Hoerner himself in von Hoerner (2001). He very quickly realized the importance of binary stars and their impact on computations. He was also able to confirm some theoretical prediction on cluster dynamics, and found an interesting radial density profile with a center cusp (von Hoerner, 1960, 1963).

There was two ways to increase the number of stars in simulations: buy a better computer or improve the algorithm. Sverre Aarseth got invested in the second path, which would take over his scientific life. Aarseth pioneered the use of individual time-step, changing the rate at which particles positions are updated, gravitationnal softening, allowing convergence for close approach, and polynomial prediction for force calculations (Aarseth & Hoyle, 1964). As power and optimization grew, investigations expanded, such as the interaction star-gas (van Albada, 1968b) and binary formation (van Albada, 1968a).

The 1970s brought two new important optimisation methods: KS regularization of close pairs (Aarseth, 1972) and Ahmad-Cohen neighbour scheme (Ahmad & Cohen, 1973). The number of

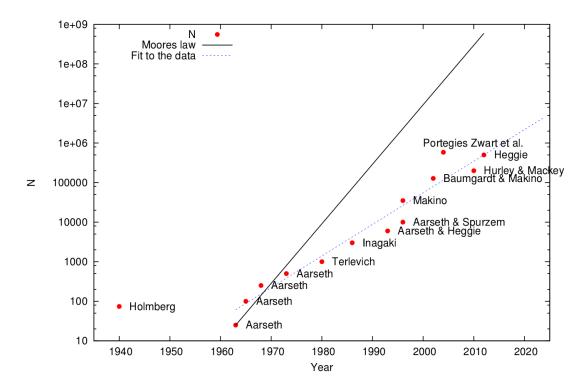


Figure 1: The evolution of the number of particles in N-body simulations. Solid line shows the Moore law. The figure was taken from Bédorf & Portegies Zwart (2012).

stars in simulations kept growing, reaching 1000 with Terlevich (1980) and materializing into the NBODY5 integrator. At this point various methods departing from a pure collisional calculation began to emerge, such as the simplified distant interaction with the Barnes & Hut (1986) tree algorithm.

To go beyond the regular improvement of computing power with time, a group of japanese researchers, among whom Junichiro Makino, designed and built special purpose hardware for many-body problems, such as n-body gravitational interaction (Ebisuzaki et al., 1990; Ito et al., 1991). These cards vastly improved the speed of nbody simulations and were a milestone on the road to the parallelization of computing. With the force calculation directly implemented in the hardware, GRAPE dominated the field for 15 years.

The latest technological leap in Nbody simulations came from graphic cards, see Bédorf & Portegies Zwart (2012) for a more detailed historical perspective. Graphical Processing Units, or GPU, were originally designed for computer games visual rendering, applying the same transformations to a lot of pixels at the same time. These made them very efficient parallel computing machines for physics. Interest in GPU computing started to grew in the 2000s (Nyland, Harris & Prins, 2004; Elsen et al., 2006; Portegies Zwart, Belleman & Geldof, 2007) until the advent of usable GPU programming languages, like CUDA, in the late 2000s. At this point GPU were more efficient than GRAPE hardware for force calculation. Keigo Nitadori and Sverre Aarseth developped a GPU-accelerated version of the latest NBODY code, NBODY6, in 2012 (Nitadori & Aarseth, 2012).

Last year, 329 years after the publication of the *Principia*, a collisional nbody simulation of one million stars was performed with a modified version of NBODY6 running on GPU (Wang et al., 2015). Computers have made it possible for humans to study systems of incredible scales in space and time, only using the universal law of gravitation. N-body numerical integrators are the culmination of centuries of scientific development on the motion of massive bodies.

0.2 Star clusters

0.2.1 But why star clusters?

The widest definition possible for a star cluster is "An area of the sky with visibly grouped stars". However, this includes binary stars and galaxies. We are interested in intermediate systems, such as open clusters, globular clusters or associations, in which stars are, if not bound, at least under direct mutual gravitational influence. Clusters are the result of bursts of star formation in Giant Molecular Clouds. All stars within a cluster were born approximately at the same time, which explains the sustained interest of the scientific community for star clusters for more than a century. They are the best laboratories of stellar physics available to us: a large population of stars sharing the same age and distance to Earth. The age of the cluster can be derived from the most massive stars in the population, as stars have lifetimes inversely correlated with their mass. Overall, integrated spectral features from all members of a star cluster can provide a wealth of information.

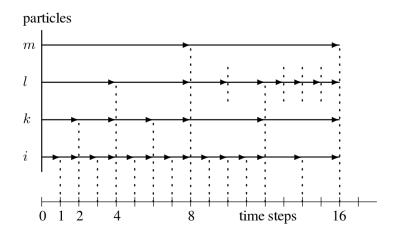


Figure 2: Illustration of block time steps on 4 particles. Particles get their positions updated for each arrow symbol, common time steps are shown as vertical dotted lines. Figure from NB6++ User Manual.

0.3 NBODY6

NBODY6 is the second youngest iteration of the NBODY family, a suite of n-body integrators created by Sverre Aarseth. It can compute the gravitational interaction between up to 128,000 stars in a collisional fashion, meaning there is no softening of the potential, at any scale. This allows for very close binaries to form and remain in the system. To achieve its impressive performances, NBODY6 relies on several optimization technique which have been developed in the 1960s and 1970s, and improved ever since. Here will be developed four major features of NBODY6, in chronological order of their implementation: block time-step, KS-regularization, Hermite scheme and Ahmad-Cohen neighbour scheme. A full description can be found in Sverre Aarseth's book (Aarseth, 2003). Inspiration for this section should be credited to the user manual of NBODY6++, written by Emil Khalisi and Rainer Spurzem.

0.3.1 Block time-step

In the first Nbody simulations, the system was integrated with an universal time-step, determined by the most accelerated star. A star in the outer regions of the cluster with a small velocity did not need to be updated that often. One of the first improvement was the introduction of individual time-step: each star is attributed its own time-step, depending on the force that is applied to it and its derivative:

$$\Delta t_i = \eta \sqrt{\frac{|\mathbf{F_i}||\mathbf{F_i^{(2)}}| + |\mathbf{F_i^{(1)}}|^2}{|\mathbf{F_i^{(1)}}||\mathbf{F_i^{(3)}}| + |\mathbf{F_i^{(2)}}|^2}}$$
(3)

With $\mathbf{F}_{i}^{(j)}$ begin the j-th derivative of the force applied to particle i and η a user-defined accuracy parameter. Such a complex formulation is the result of extensive tests and is quite robust for many special cases. Individual time-steps leads to desynchronized particles, hence the need to interpolate the positions of other particles to compute \mathbf{F}_{i} , which was achieved through fourth-order polynoms.

To limit the amount of desynchronization, block-time steps were introduced. Instead of having as many time steps as particles, one only allows quantized power of 2 of an initial time step. $\Delta t_0, \frac{\Delta t_0}{2}, \frac{\Delta t_0}{4}, \frac{\Delta t_0}{2^i}$. All time steps are then commensurate and regularly fall back on the same time steps, minimizing the amount of interpolation during the force calculations.

- ${\bf 0.3.2\quad KS-regularization}$
- 0.3.3 Hermite prediction scheme
- 0.3.4 Ahmad-Cohen neighbour scheme

0.4 Young star clusters

CHAPTER 1

The Hubble-Lemaître fragmented model

1.1 How to build a Hubble-Lemaître model

1.1.1 Initial state

The first step to obtain a HL-fragmented model is to build an uniform sphere model. The N stars, depending on the required membership, have to be distributed randomly in space inside a certain radius, producing an uniform density. This can be achieved by sampling separately the distance to the center and the angular position of each star, in a method analog as used in Aarseth, Hénon & Wielen (1974) for a Plummer model. The distance to the center should be sampled from the function:

$$f_R(X) = R_0 X^2 \tag{1.1}$$

With R_0 the bouding radius and X a random variable following a uniform probability law between 0 and 1. A direct uniform law for the radius would overpopulate the outer regions. The angles ϕ and θ , respectively azimuthal and polar angle in the physics convention, should be sampled from:

$$f_{\phi}(X_1) = 2\pi X_1 \tag{1.2}$$

$$f_{\theta}(X_2) = \arccos(X_2) \tag{1.3}$$

With X_1 following a uniform probability law between 0 and 1 and X_2 between -1 and 1. The cartesian coordinates are then found:

$$x = R\sin\theta\cos\phi\tag{1.4}$$

$$y = R\sin\theta\sin\phi\tag{1.5}$$

$$z = R\cos\theta\tag{1.6}$$

(1.7)

The N particles are then homogeneously distributed in space in a sphere of radius R_0 . The next step is to attribute velocities. Unlike other models like the Plummer model, the velocities are here straightforward. We use the well known velocity field of neighbouring galaxies: velocities are radial from the Milky Way, larger with increasing distances, taking the form:

$$\mathbf{v} = \mathbf{H}_0 \mathbf{r},\tag{1.8}$$

with H_0 being an equivalent of the well-known Hubble parameter. For historical accuracy, I added the name of Georges Lemaître when I named my model. It has now been shown that the astronomical observations of redshifted galaxies and its interpretation as the consequence of an expanding universe predated Hubble's paper (Hubble, 1929). Georges Lemaître had published his conclusion on an expanding universe two years earlier (Lemaître, 1927). The account of this can be found in Kragh & Smith (2003); van den Bergh (2011) and Freeman et al. (2015).

An appropriate H_0 to obtain a fragmented subvirial model has to be inferior to 1.4 (see next section). The model obtained from this is then evolved through a nbody integrator, which in my case is NBODY6.

1.1.2 Fragmentation

The cluster expands, driven by the initial Hubble-Lemaître velocity field. During this expansion, poissonian fluctuation in density from the uniform model starts to grow: the part of the cluster with more mass initially attract more stars, forming clumps, clumps merge, spontaneously building substructure. These clumps will be analyzed in another section. If H_0 is well chosen, the expansion stops at some point, the apex, at which the initial kinetic energy has been spent and converted to potential energy: the cluster is now larger, substructured and subvirial, about to collapse. The apex time t_a of the end of the expansion and the critical value of H_0 can be derived from Newton's second law applied to an expanding spherical shell of matter.

We start from a uniform sphere of radius R_0 , total mass M. We consider spherical shells as mass elements, situated at distance r from the origin. As previously said, they are attributed a radial velocity following (for the shell at $r = R_0$) $\vec{v}_0 = H_0 \vec{R}_0 = H_0 R_0 \vec{u}_r$. We want to follow the radial motion of the last shell of mass m, situated at R from the origin. Newton's second law gives:

$$m\frac{dv}{dt} = -\frac{GMm}{R^2} \tag{1.9}$$

By multiplying on both sides by v and integrating between a given time and t = 0, one finds:

$$v^{2}(t) - v_{0}^{2} = 2GM\left(\frac{1}{R} - \frac{1}{R_{0}}\right)$$
(1.10)

Which becomes, by taking $\nu = v/v0$, x = R/R0 and $E_* = \frac{2GM}{R_0v_0^2}$, which is a dimensionless measure of the total energy of the system:

$$\nu^2 = 1 + E_* \left(\frac{1}{x} - 1\right). \tag{1.11}$$

The evolution of the system has 3 outcomes, depending on the value of E_* :

- $E_* < 1$ The velocity is always strictly positive as the system expands $(x > \infty)$. The system is unbound.
- $E_* = 1$ The velocity approaches zero as the system expands. The expansion "stops at an infinite radius". The system is marginally bound.
- $E_* > 1$ The velocity reaches zero for a finite radius, the system is bound and will collapses back on itself once the expansion stops.

Using Hénon units, G=1 and M=1, and we choose $R_0=1$. Which gives a critical value E_* to have a bound system: $E_*=\frac{2}{\mathrm{H}_0^2}<1$. This means to have a bound system, which stops

expanding at some point, one must have $H_0 < \sqrt{2}$. We only consider in the following the case in which $E_* < 1$. We have the expression

$$\nu = \sqrt{1 + E_* \left(\frac{1}{x} - 1\right)} \tag{1.12}$$

Taking the time derivative gives:

$$\frac{d\nu}{dt} = -\frac{E_*}{2x^2} \left[1 + E_* \left(\frac{1}{x} - 1 \right) \right]^{-\frac{1}{2}} \frac{dx}{dt} \tag{1.13}$$

Combining this with (1.9), one obtains:

$$\frac{dx}{dt} = H_0 \sqrt{1 + E_* \left(\frac{1}{x} - 1\right)} \tag{1.14}$$

which can be rewritten, using $\tilde{H_0} = H_0 \sqrt{E_* - 1}$ and $x_t = \frac{E_*}{E_* - 1}$

$$\frac{dx}{dt} = \tilde{H_0}\sqrt{\frac{x_t}{x} - 1} \tag{1.15}$$

 x_a being the extent of the maximum expansion as we assumed a bound system. The subscript a is for apex. If we choose the notation $u = \frac{x}{x_a}$:

$$\sqrt{\frac{u}{u-1}}\frac{du}{dt} = \frac{\tilde{H}_0}{x_a} \tag{1.16}$$

We know that x varies from 1 to x_a , thus u varies from $1/x_a$ to 1. We can then make the change of variable $u = \sin^2 \theta$ and separate the variables:

$$\sqrt{\frac{\sin^2 \theta}{1 - \sin^2 \theta}} 2 \sin \theta \cos \theta d\theta = \frac{\tilde{H_0}}{x_a} dt \tag{1.17}$$

which becomes after simplifications:

$$[1 - \cos(2\theta)]d\theta = \frac{\tilde{H}_0}{x_a}dt. \tag{1.18}$$

We now integrate the expression from t=0 to t, the time at which the expansions stops and x reaches x_a (wich implies $u_a=1$ and $\theta_a=\pi/2$):

$$\int_{\theta_0}^{\pi/2} [1 - \cos(2\theta)] d\theta = \int_0^t \frac{\tilde{\mathbf{H}}_0}{x_a} dt$$
 (1.19)

$$\frac{\pi}{2} - \theta_0 + \frac{\sin(2\theta_0)}{2} = \frac{\tilde{H}_0}{x_a} t \tag{1.20}$$

$$\pi - 2\theta_0 + \frac{2}{\sqrt{x_a}}\sqrt{1 - \frac{1}{x_a}} = 2\frac{\tilde{H_0}}{x_a}t\tag{1.21}$$

which boils down to the expression of the time at which the expansion stops:

$$t_a = \frac{E_* \left(\frac{\pi}{2} - \theta_0\right) + \sqrt{E_* - 1}}{H_0(E_* - 1)^{-\frac{3}{2}}}.$$
 (1.22)

Recalling the quantities:

$$E_* = \frac{2GM}{R_0 v_0^2};$$
 $x_a = \frac{E_*}{E_* - 1};$ $\theta_0 = \sin^{-1}\left(\frac{1}{\sqrt{x_a}}\right)$ (1.23)

See figure 1.1 for the value of t_a as a function of H_0

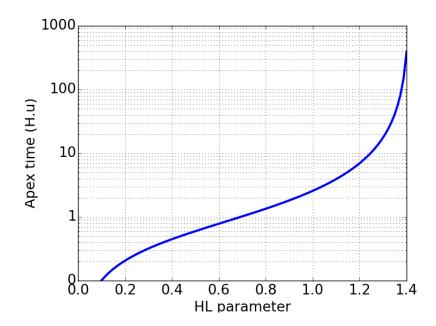


Figure 1.1: Theoretical values of the apex time, at which the system stops expanding, as a function of initial HL parameter, which tunes the strength of the initial expansion.

1.2 Perturbation theory

1.3 Analysis of the fragmented system

1.3.1 Clump finding algorithm

The study of substructures requires an efficient clump-identification algorithm (or, halo-finding in cosmology). By clump we mean here a local overdensity of stars. Several methods are commonly used such as the HOP algorithm (Eisenstein & Hut, 1998; Skory et al., 2010) which relies on attributing local densities to each particle and separating the clumps through density thresholds. The HOP algorithm is very robust on large cosmological data sets. However, our calculations have comparatively coarse statistics and noisy density fields. This issue, coupled with the large number of free parameters of the HOP algorithm, makes the method less appealing. Instead

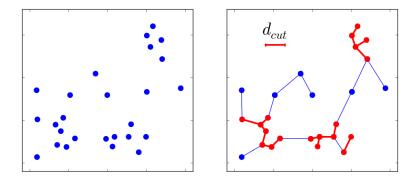


Figure 1.2: Illustration of a Minimum Spanning Tree and its use to isolate subgroups, using a cutting length d_{cut} .

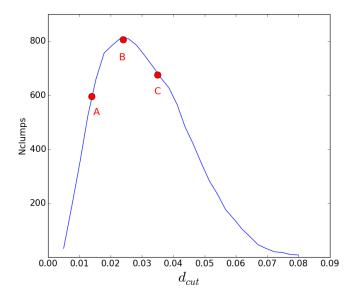


Figure 1.3:

we follow Maschberger et al. (2010) who adapted the minimum spanning tree (MST; see e.g. Allison et al. 2009; Olczak, Spurzem & Henning 2011) technique to the detection of clumps. A spanning tree is a set of edges connecting a group of particles but without closed loops; the MST seeks to minimise the total length of the edges. One may then construct the MST for the whole system, and then delete all edges larger than a chosen cutting length, d_{cut} . The sub-sets that are still connected are labeled as clumps. This process is illustrated in Fig 1.2. In practice a minimum sub-set size N_d is also chosen so as to avoid many small-N subgroups: experience led us to choose $N_d = 12$ for the minimum number of stars per clump.

With N_d fixed, the length d_{cut} is then the only free parameter left. There is some freedom in choosing an appropriate value. Maschberger et al. (2010) fixed the value of d_{cut} by visual inspection of clumps. We instead identified clumps in a fragmented system for a range of values for d_{cut} and settled for the value which optimised the number of identifications. This is shown on Fig. ?? for an N = 80k fully-fragmented Hubble model. For small d_{cut} 's, the number of detected clumps at first increases rapidly. The rise is due to the length d_{cut} initially being small compared with the typical volume spawned by N_d or more nearest-neighbours. Beyond a certain value, a transition to another regime occurs, whereby the algorithm starts to connect previously separated clumps, counting them as one. The number of clumps thereafter begins to decrease. The value $d_{cut} \approx 0.025$ H.u optimises the outcome of the clump-search. This is a generic feature of the MST algorithm and we have adopted the same strategy throughout, adapting the value of d_{cut} to the number N of stars used.

On Fig. 1.4, a sub-set of the model is shown where we have identified stars that belong to clumps with filled symbols. The three panels on that figure are each for a different value of d_{cut} , increasing from top to bottom. For the smallest value d_{cut} =0.015 H.u, clumps look somewhat truncated as we are still in the under-sampling regime and only their cores registered as clumps. The second, optimal, value d_{cut} =0.025 H.u produces visually well-isolated clumps. Finally, the third and largest value is so that clumps begin to merge together: this is shown by the unique clump identified in the bottom panel (filled blue squares).

The procedure developed here gives results in agreement with other clump-identification algorithms developed using the MST (see e.g. Gutermuth et al. 2009; Kirk & Myers 2011).

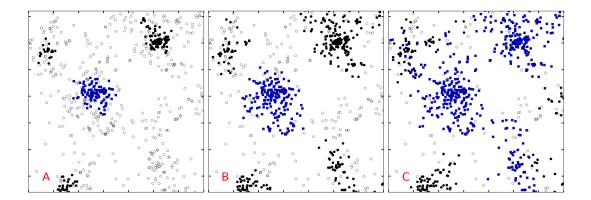


Figure 1.4:

CHAPTER 2

Dynamical evolution

2.1 Bla

The Hubble expansion comes to a halt at a time τ when $\theta(\tau) = \pi/2$ in Eq. (??). The system as a whole is then in a sub-virial state. We wish to explore briefly the violent relaxation that follows and the equilibrium that ensues. In the present section, simulations will use the fully fragmented state of Hubble models as initial conditions for the subsequent dynamical evolution. Observationnal clues point to collapsing and violently relaxing clusters. For example, ? find IC348, a young (2-6 Myr) cluster, to be both super-virial and with a convergent velocity field, consistent with infalling motion. Dry collapse with no gas is an idealized situation: clearly if there was residual gas between the clumps and it was evacuated through stellar feedback, both the clump merger rate and the depth of the potential achieved during relaxation would be affected. As a limiting case, rapid gas removal may lead to total dissolution (see for instance ? and ?). In the current situation, all clumps will merge.

The numerical integration were done once more with the Nbody6 integrator with the same computational units. For comparison purposes, we also performed simulations of cold uniform sphere, a configuration which has been extensively used in the past (e.g.,?????) and one that minimises the level of fragmentation and mass segregation in the on-set of collapse. Table 2.1 lists the simulations performed. We focus here on models with a mass function from $0.35M_{\odot}$ to $20M_{\odot}$ and 15000 stars, a compromise value for rich open clusters that should allow us to identify clearly collisional effects and trends with time, and ease comparison with the recent study by Caputo et al. (2014) where most calculations are performed with that sampling. We let both Hubble-fragmented- and uniform sphere evolve up to 40 H.u.

2.1.1 Scaling to physical units

Before discussing the results, it is useful to translate the units of computation to physical scales. This is important if we want to discuss the state of the systems using one and the same physical

Table 2.1: Summary of collapse simulations and their characteristics. These simulations started from a subvirial state: cold uniform sphere or fully fragmented Hubble model; each were evolved up to t = 40 H.u

Name	N	Mass range	Model
Rh100	15000	[0.3 - 100]	Hubble
Rh20	15000	[0.35-20]	Hubble
Ru100	15000	[0.3 - 100]	Uniform
Ru20	15000	[0.35-20]	Uniform

Table 2.2: Number of initially ejected stars in two collapse calculations

Run	Ejected stars	Ejected mass
Ru20	4227	27%
Rh20	1932	12%

time, such that the hypothesis of no stellar evolution holds good. This complicates the analysis, because all the time-scales defined in §3.1 are based on the hypothesis of equilibrium, and we start-off out of equilibrium. To make things clearer, let us resize the configurations so that the half-mass radius $r_h=1$ pc initially, with a total system mass of $M=15\times 10^3\,M_\odot$ for a volume density $\rho=M/(8\pi/3r_h^3)\simeq 10^3M_\odot/pc^3$, well within values typically inferred from observations. We then compute a free-fall time for the uniform-density model of $t_{ff}=\pi/2\left(r_h^3/GM\right)^{1/2}\approx (\pi/24)^{1/2}\times 10^5$ years; the initial crossing time would then be $t_{cr}=2r_h/\sigma_{1d}=4\sqrt{6}/\pi\,t_{ff}$ where we invoked the virial theorem to compute $\sigma_{1d}^2=1/3\times GM/2/r_h$. (The crossing time is larger than t_{ff} because all the mass goes into the origin during free-fall.) In practice the more useful crossing time has to be computed from the equilibrium state achieved. If we once more invoke the virial theorem and note that at constant mass and energy the equilibrium state would reach a size $r_h^{eq}\approx r_h^{(0)}/2$ or half the initial radius, then one computes $t_{cr}^{eq}\approx t_{cr}^{(0)}/2\sqrt{2}=2\sqrt{3}/\pi t_{ff}\approx 1.10\,t_{ff}$. Direct computation of the problem of a collapsing sphere give $t_{ff}\approx 1.36$ H.u. We therefore use the conversion factor

$$\frac{t}{10^5 \, {\rm years}} = (4/3)/(\pi/24)^{1/2} \simeq 3.7 \, t_{Henon} \, .$$

The equilibrium crossing time is then $t_{cr}^{eq} = 1.1 \, t_{ff} = 3/2 \, t_{Henon} \approx 0.4 \times 10^5$ years. The time-conversion factor adopted is conservative and does not factor in the stars that may escape during virialisation. Thus by running up to 40 H.u we ensure that the systems evolve for at least 25 crossing times and $\sim 10^6$ years, short before the lifetime of massive stars. With N=15000 and a mass range of $m_{max}/\langle m \rangle = 20$ we find from (??) and (??) a two-body relaxation time of $t_{rel} \approx 80 \, t_{cr}$ (120 t_{Henon} , or 3 Myrs) and mass-segregation timescale of $t_{ms} \approx 4 \, t_{cr}$ (6 t_{Henon} , or 1.6×10^5 years).

2.1.2 Collapse and virialisation

The constant diffusion of kinetic energy by two-body interaction means that no stellar system ever reaches a steady equilibrium. However we can contrast the time-evolution of two configurations and draw conclusions about their observable properties.

With this in mind we turn to Fig. ?? in which we show the evolution of the half-mass radius for the cold uniform model (labeled Ru20; thick red curve), and the Hubble model (labeled Rh20; thin blue curve). Both systems have the same bounding radius initially, contract to a small radius when $t \simeq 1.4$ units and then rebound at time $t \simeq 2$ units. When all the stars are included in the calculation for r_h , we find that the radius increases at near-constant speed after the collapse. That trend does not appear to be slowing down which indicates that a fraction of the stars are escaping. The first batch of escapers is driven by the violent relaxation, however the trend continues beyond t = 10 units, corresponding to $t > t_{ms}$ which implies two-body scattering and effective energy exchange between the stars. Note how the uniform model has a much deeper collapse and rebounds much more violently, shedding a fraction twice as large of its stars (Table 2.2). The half-mass radius r_h increases steadily in both models, from the bounce at $t \approx 2$, until the end of the simulation (values in H.u):

```
r_h Uniform 0.11 \rightarrow 0.63 (×5);

r_h Hubble 0.34 \rightarrow 0.49 (×1.4).
```

Clearly the gentler collapse of the fragmented model has led to a more extended post-collapse configuration and reduced two-body evolution. Observe how the uniform model Ru20 is ejecting

more stars than the Hubble model: if we repeat the calculation for the Hubble run Rh20 but now include only the bound stars¹, the curve of r_h obtained and shown as dash is shifted down but keeps essentially the same slope ≈ 0.004 . By contrast, the calculation for the bound stars of run Ru20 yields a much shallower slope than for the whole system: the slope drops from 0.015 to about 0.007. Irrespective of how the half-mass radius is calculated, the conclusion remains the same and agrees overall with the remark by ? that boosting the kinetic energy of the collapsing initial configuration softens the collapse; this was shown in a different context by ? and confirms these older findings. Here, the fragmented model has finite kinetic energy due to the clumps' internal motion. The important new feature brought by the fragmented initial conditions is that the mass profile of the virialised configuration evolves much less over time in comparison.

At the bounce, the half-mass radius of the Hubble model is ≈ 4 times larger than that of the of the initially uniform sphere at rest (Fig. 10). The half-mass radii overlap at time $t \approx 15 \, H.u.$ (solid curves) or $t \approx 50 \, H.u.$ (dashed curves). Is the same trend applicable to all Lagrangian radii? To answer this question we plot on Fig. 11 the ten-percentile mass radii for the two models. The results are displayed for the two situations including all the stars (top row) or bound stars only (middle row). It is striking that the curves show very little evolution at all mass fractions for the case of the Hubble model (see right-hand panels on the figure), whereas all mass shells either contract or expand in time for the uniform one. We have noted how this model undergoes two-body relaxation on a timescale of $t \approx 10 \, H.u$: the innermost 10% mass shell shows an indication of core-collapse at $t \simeq 5 H.u.$. We note here that the two sets of curves reach very similar values at the end of the calculations ($t = 40 \, H.u$). A key difference between the two models, therefore, is that the final configuration of the Hubble model is almost identical to what it was at the bounce; the same simply does not hold in the case of a uniform-density collapse. Furthermore, the Hubble calculation shows no hint of two-body relaxation or corecollapse. This raises the possibility that the system properties in the final configuration remain better correlated with those at the on-set of (global) collapse (we return to this point in §7).

? and ? noted how a finite amount of kinetic energy in the *initial* configuration alters the depth of the bounce during collapse. The ratio of half-mass radius at the bounce, to its initial value, is then $r_h/r_h(0) \simeq Q_o + N^{-1/3}$, where Q_o is the virial ratio of the initial configuration (see Fig. 5 of Caputo et al. 2014). We computed the kinetic energy of the Hubble configuration and found that the internal motion of the clumps means that $Q_o(Hubble) \simeq 0.02$ for a Salpeter mass function with upper truncation value of $20M_{\odot}$. With N=15k stars, the ratio $r_h/r_h(0) \simeq 0.041$ when $Q_o = 0$ shifts to $r_h/r_h(0) \simeq 0.061$ when $Q_o = 0.02$, or a factor close to 3/2. To account for the difference in kinetic energy of the initial configurations, we may therefore rescale the uniform model such that positions are $\times 3/2$ and the time unit is $\times (3/2)^{3/2} \simeq 1.84$. The new configuration would evolve in time in exactly the same way after mapping positions and time to their rescaled values. The result is shown as the bottom row on Fig. 11. Note that we have blown up the vertical axis to ease comparison between uniform- and Hubble models with bound stars only included. The rescaled uniform model is now slightly more extended than before, but overal the final two configurations (at $t = 40 \, H.u.$) are as close as before rescaling. This demonstrates that the outcome of the uniform collapse and its comparison with the Hubble model is not sensitive to a small amount of initial kinetic energy. We note that while the ratio Q_0 is a free parameter in many setups for collapse calculations, that parameter is fixed internally in the Hubble approach.

2.2 Global mass segregation

To investigate the state of mass segregation in our models, we follow the analysis of Caputo, de Vries & Portegies Zwart (2014). The masses are sorted by decreasing values, then subdivided into ten equal-mass bins. This means that the first bin contains the most massive stars. The

¹See Appendix A for details of the selection procedure.

number of stars in each bin increases as we shift to the following bins, since their mean mass decreases, and so on until we have binned all the stars. The half-mass radius r_h computed for each bin is then plotted as function of time. In this way the mass segregation unfolds over time: if the stars were not segregated by mass, all radii r_h would overlap. If two sub-populations share the same spatial distribution, their respective r_h will overlap.

Figure ?? graphs the results for initially uniform-density- and fragmented Hubble models. The layout of the figure is the same as for Fig. 11. The violent relaxation phase leads to mass loss for both models and the much more rapid expansion of the half-mass radii of low-mass stars is an indication that most escapers have a lower value of mass. Fig. ??(c) and (d) graphs r_h for the bound stars of each sub-population. Clearly the initially uniform-density model is more compact early on, but note how the heavy stars sink rapidly to the centre, more so than for the case of the Hubble model. The spread of half-mass radii increases with time for both models, however two-body relaxation in the uniform-collapse calculation is much stronger, so that by the end of the simulations the half-mass radii of the low-mass stars of the respective models are essentially identical. Since the low-mass stars carry the bulk of the mass, that means that the two models achieve the same or similar mean surface density by the end of the run. At that time, the heavy stars in the uniform-collapse calculation are clearly more concentrated than in the Hubble run (compare the radii out to $\sim 40\%$ most massive stars). A direct consequence of this is that the color gradients of the core region of a cluster are much reduced when the assembly history proceeds hierarchically, in comparison with the monolithic collapse. It will be interesting and possibly important in future to compare such models with actual data for young clusters.

Another interesting remark is that the kinematics of the stars within the system half-mass radius is much different between the two models. For the Hubble calculation, the system half-mass radius, ≈ 0.43 H.u, at t=40 (cf. Fig. 11[d]) coincides with the half-mass radius of the 30-40% bin stellar sub-population. All bins up to that range show little or no time-evolution, around the end of the run, which we interpret as efficient retention of these stars by the relaxed cluster. In the case of the uniform-collapse run, the system half-mass radius reaches ≈ 0.33 H.u., which is significantly larger than the radius for the 30-40% stellar sub-population. For that model, only the bins 0-10% and 10-20% are flat, and all the others increase almost linearly with time. Thus a fair fraction of bright stars deep in the cluster show systematic outward streaming motion, along with low-mass ones. This brings up the possibility to measure this signature motion through relatively bright stars, originating well inside the cluster half-mass radius. Recall that only post-bounce bound stars where selected to compute r_h on Fig. ??(c) and (d); the expansion is therefore not driven by chance events (e.g., Fig. ??[a]), but rather through two-body relaxation. On the down side the bright tracers would be short-lived, and this may prove a strong constraint for observational detection.

Given the early dynamical evolution associated with substructured stellar clusters, some observed dense objects may yet be out of equilibrium (see §??). We wish to investigate the out-of-equilibrium state of our models just after the collapse. To ease the comparison between the two systems, the same rescaling procedure as for Fig ?? was applied to the uniform model, only this time the scaling was chosen so that the two clusters have comparable densities after the bounce. Lengths were multiplied by 4; the time-axis is then scaled up by a factor $(4)^{3/2} = 8$. The result can be seen in panel (e); panel (f) shows a smoothed and zoomed in Hubble model for comparison.

We compare the values of the different half-mass radii of the various population before the dynamical mass segregation sets in. This process is clearly visible as the drop of the half-mass radius of the most massive stars during the evolution. We are interested in the segregation which originates from the collapse and is present before this dynamical evolution. Table 2.3 sums up the values of the half-mass radii taken at $t \sim 5$ for both models, both corresponding to the same unevolved post-collapse state (see arrows on panels [e] and [f] on Fig ??). With on the order

Table 2.3: Values of half-mass radii and their ratio to that of the most massive stars. The results are for the rescaled bound uniform model (rescaled Ru20b) and the bound Hubble model (Rh20b), after the collapse, and before dynamical mass segregation sets in.

Uniform (rescaled)	0-10%	10-20%	20-30%	30-40%	40-50%	50-60%	60-70%	70-80%	80-90%	90-1
Radius	0.20	0.245	0.282	0.273	0.294	0.325	0.326	0.328	0.335	0.34
Ratio	1.0	1.23	1.41	1.37	1.47	1.63	1.63	1.64	1.68	1.70
Hubble	0-10%	10-20%	20-30%	30-40%	40-50%	50-60%	60-70%	70-80%	80-90%	90-1
Radius	0.18	0.21	0.286	0.293	0.316	0.321	0.333	0.338	0.342	0.34
Ratio	1.00	1.16	1.58	1.63	1.76	1.78	1.85	1.88	1.90	1.91

of ~ 100 stars per bin or more, one estimates roughly a ten-percent standard deviation from random sampling. To measure the relative segregation between populations, the table also lists the ratios of each half-mass radius to the one for the most massive stars. Both models appear mass segregated (since these ratios are significantly greater than unity). The Hubble model is more segregated, on the whole, albeit in a different way compared to the uniform model. The segregation in that one is more regular and spreads over more mass bins. In the Hubble model, the segregation is much enhanced for the first two mass bins. Such differences in the degree and nature of segregation can be explained by the clumps structure before the collapse. We showed in §?? the clumps were mass segregated with the most massive members being preferentially located at their center. The low membership and mass of most clumps implies that segregation mostly affects the very top of the stellar mass function. This segregation, predominant among massive stars, is then found in the resulting centrally concentrated system, after the collapse, and visible on Fig. ??. The inheritance of mass segregation was studied by ? for the case of merging Plummer spheres. ? furthermore showed that mass segregation in the system as a whole is enhanced for more filamentary fractal initial condition (lower dimension, D; see their Fig. 5). Here our results confirm this observation. Mass segregation is a sensitive function of the initial clumpiness of the system and has immediate bearing on the dynamics of the virialised configuration, since all massive stars are more concentrated in the core.

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