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Live fast and die young

Evolution and fate of massive stars

Renzo, M.

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INTRODUCTION



Our intuition about stars is built on the everyday¹ experience of seeing the star closest to us, the Sun. Thus, people commonly expect stars to be relatively isolated, possibly orbited by a set of planets, but certainly far from other stars. However, as often in astrophysics, our best observations (in this case of the Sun) can be misleading because they target a somewhat special object: their interpretation needs to be embedded in the broader context.

This thesis deals with stars that are quite different from the Sun in two key aspects: they are typically *not alone* and much more *massive*. Most stars are not isolated, but instead orbit one or more companions, and they often live in regions of space where many neighboring stars are found close by. The presence of other stars can have a profound impact on the way a star evolves. Secondly, the appearance, evolution, and final fate of stars are primarily determined by their total mass: the most luminous stars, which are also the most massive, live a very different life compared to the Sun. Stars with initial masses larger than about 7.5 M_{\odot} (where $1 M_{\odot} = 1.9892 \cdot 10^{33}$ g is the mass of the Sun), although rare, have an extreme impact on their surroundings. They can end their lives in spectacular supernova explosions producing neutron stars, black holes, or fully destroying the star and leaving nothing behind.

1.1 Multiplicity

Most stars are thought to be born in relatively dense clusters or associations (e.g., Lada & Lada 2003; Stahler 2018). They typically have one or more companions gravitationally bound to them (e.g., Abt 1983; Sana et al. 2012; Duchêne & Kraus 2013; Almeida et al. 2017). For example, one of the most iconic asterisms in the Northern sky, the "Big Dipper" (Fig. 1.1), was used during the Hellenistic period to test the eyesight of prospective astronomy students and soldiers. It contains the visual binary consisting of the stars Mizar and Alcor, which can only be distinguished with the naked eye by people with good eyesight (Bohigian 2008). Spectroscopic observations reveal that "Mizar" is itself a quadruple system (i.e., two spectroscopic binaries orbiting each other as a visual binary), and Alcor is itself a triple system (Hoffleit & Jaschek 1991; Mamajek et al. 2010), for a total of seven stars packed in a light dot that most would mistake for one single object. These stars are not exceptional from the point of view of their multiplicity.

¹Or not so much in Amsterdam...



Fig. 1.1: Zoom-in of the visual binary Mizar-Alcor in the Big dipper (emphasized with thin dotted lines). Distinguishing two separate light sources in the biggest circle was a requirement to become an astronomer in Hellenistic times.

1.1.1 Brief historical context of the study of stellar binarity

The study of binaries has progressed hand in hand with the technological advancements. As the example of Mizar and Alcor illustrates, its origin dates back at least to ancient Greece, with the first mention of "double stars" by Ptolemy (Aitken 1935). In the early 17th century, the pioneers of the astronomical use of telescopes soon realized that a large fraction of stars appearing as single to the naked eye are actually binaries, or even triples (Aitken 1935; Verbunt 2015). It took another century to realize, through a combination of statistical and astrometric arguments (e.g., Michell 1767), that the presence of companions is not merely chance alignment, but instead, it implies a physical relationship between the stars (e.g., Herschel 1802).

With the development of the first spectrographs and the dawn of astro*physics*, i.e. the (search for) physical explanations of celestial phenomena, the study of stellar multiplicity again advanced greatly: very close binaries that could not be resolved even with telescopes became known through the detection of periodic Doppler shifts of spectral lines, as first shown in Mizar itself (Pickering 1890). With the progressive increase in telescope sizes and spectrograph technology (in particular, the decoupling of the optics of the telescope from the spectrograph itself by means of fiber optics), the sample of spectroscopic binaries available steadily increased.

In the 20th century, the development of rockets first, and satellites soon after, allowed for observations in wavelength regions not accessible from the ground. The discovery of X-ray sources beyond the solar system (Giacconi et al. 1962) was soon related to stellar binaries

where a "compact object" (i.e., white dwarf, neutron star, or black hole) was accreting mass from a companion star (e.g., Burbidge et al. 1967; Shklovsky 1967; Schreier et al. 1972; van den Heuvel & Heise 1972). Therefore, stellar binarity became the tool to study both matter and the structure of space-time in the most extreme conditions. The orbital solution for Cyg X-1 coupled to its emission of X-rays provided the first observational confirmation of the existence of black holes (Webster & Murdin 1972; Bolton 1972), a recurrent theoretical speculation since the studies of J. Michell (Michell 1784) and P.-S. Laplace (Laplace 1799, see also Montgomery et al. 2009). Before this discovery, black holes were often considered a mathematical consequence of General Relativity with no physical realization in nature.

Binaries and multiple systems also hold a forefront position in the theoretical developments of stellar astrophysics. Observations of binary systems can provide accurate stellar parameters (e.g., stellar masses and radii in double-lined eclipsing binaries, Andersen 1991, although see also Valle et al. 2018), which can be used to underpin theoretical models of stellar evolution. The "three-body problem" in classical mechanics is obviously related to the treatment of the dynamics of gas parcels under the influence of the gravitational field of two stars orbiting each other. Many famous "puzzles" (evolution of Algol-like systems, binaries at the center of planetary nebulae, formation of helium white dwarfs, formation of millisecond pulsars, etc.) require understanding of binary evolution, which was developed collectively during the 19th and 20th centuries. Some of the earliest applications of numerical simulations of stars dealt with the evolution of interacting binaries (e.g., Paczyński 1966, 1967; Kippenhahn & Weigert 1967; Paczyński 1971).

With the spectacular detection of the nearby supernova SN1987A, models for the evolution of massive binaries merging before their final explosion became highly debated (e.g., Arnett et al. 1989; Podsiadlowski et al. 1990; Podsiadlowski 1992; Menon & Heger 2017). The task of understanding how a variety of transients (SN subclasses, novae, X-ray bursts, Ca-rich gap transients, luminous red novae, etc.) arise from the different evolutionary paths of multiple stars is still an ongoing effort, further accelerated by the recent development of robotic telescopes that can scan large portions of the sky each night (see also Sec. 1.5).

More recently, the direct detection of gravitational waves from the merger of two compact objects (Ligo Scientific Collaboration and Virgo collaboration, LVC 2016c, 2018b) has raised the question of how these systems form. It is very easy for a massive binary system to avoid becoming a gravitational wave merger progenitor, because of the many pitfalls on their path to this final fate (e.g., Belczynski et al. 2016b; Tauris et al. 2017). Thus, we need to improve our understanding of massive stars, both as single and as members of a binary or more complex groupings. The third observational run from ground-based gravitational wave detectors is ongoing at the time of writing this thesis, and will reveal a population of compact object mergers that will allow for statistically significant physical constraints on the evolution of their progenitor systems (e.g., Fishbach & Holz 2017). The technological leap that has allowed for the direct detection of gravitational waves, together with advancements in time-domain astronomy can be considered, at least partially, the present-day drivers of the renewed interest for massive binary evolution.

1.2 The life of (massive) stars with a companion

Stars are often accompanied by one or more companion(s), and this is especially true for massive stars. The pre-main sequence evolution of massive stars (until the ignition of hydrogen thermonuclear burning) happens fast and it is typically enshrouded in a dusty and optically thick environment. How this process leads to stellar multiplicity is not yet well understood (e.g., Zinnecker & Yorke 2007; Sana et al. 2017). Nevertheless, a variety of observations suggest that most massive stars are born with companions (e.g., Abt 1983; Mason et al. 2009; Sana & Evans 2011; Chini et al. 2012; Kobulnicky et al. 2014; Almeida et al. 2017), and that the majority will (try to) exchange material with their companion(s) before the end of their stellar lifetime (Sana et al. 2012).

From a theoretical perspective one might wish to fully understand the evolution of single stars before studying how companion(s) can change it. In practice, however, the fact that the majority of young massive stars are found in close binary systems means that any observational constraints will likely be influenced by the presence of binaries and their products (e.g., de Mink et al. 2011, 2014). Therefore, any observationally-supported theory of massive star evolution cannot leave aside the issue of binarity.

Binary interactions can result in a variety of outcomes, depending on the masses of the two stars, their initial orbital configuration (initial separation, eccentricity, etc.), and their content in elements heavier than helium (so-called metallicity). The initial parameter space for the evolution of a binary system is further expanded by the many uncertain parameters entering into the physical modeling of each star (e.g., convective overshooting, efficiency of rotational mixing, etc.) and of their interactions (e.g., efficiency of mass transfer, tidal coupling, etc.).

Depending on the initial configuration (and, on another level, on the assumptions made to model the evolution), many different outcomes are possible. The majority of massive binaries are expected to go through a mass-transfer phase², initiated when one star expands beyond its Roche Lobe. The resulting mass transfer can be dynamically stable or unstable, depending on the responses of the radii and Roche lobes of each star to the transfer of mass and angular momentum. Dynamically unstable mass transfer can lead to a common-envelope phase (e.g., Paczynski 1976), during which the two stars share material filling equipotential surfaces enclosing both stars. The two stars typically spiral in within the common envelope, and this process can result in a merger or in the ejection of the common material and a significant reduction of the orbital separation (see Ivanova et al. 2013, for a review).

If the two stars avoid merging during their evolution, the initially more massive one will typically end its life first³, especially since the accretion of material can "rejuvenate" the

²For low mass stars, the different period distribution and radial evolution makes mass transfer less common. Nevertheless, if a phase of mass transfer happens, the physical processes are the same as those discussed here.

³However, for binaries starting with an initial mass ratio $q = M_2/M_1 \simeq 1$ and an initial period short enough that mass transfer starts before the end of the donor star's main sequence, the deaths of the two stars can happen in reversed order. This is predicted to happen in ~ 4% of all massive binaries (Pols 1994; Ch. 3).

accreting star by making its convective core grow and drag fresh fuel inwards (e.g., Hellings 1983; Braun & Langer 1995; Wellstein et al. 2001; Schneider et al. 2015).

Most binaries with at least one massive star are disrupted when one of the stars collapses and possibly explodes in a SN (see also below): the former companion is shot out and appears as a single star for the rest of its evolution (see, e.g., Fig. 1.2). Because of mergers and binary disruptions, even apparently single stars might have experienced binary interaction (de Mink et al. 2014): ruling out the occurrence of binary-evolution processes for presently-single stars is difficult. Even populations of events that, at zeroth order, do not require involving binarity and multiplicity to explain them, have been suggested to be significantly affected by binary evolution (e.g., hydrogen-rich type II SNe, Podsiadlowski 1992; Podsiadlowski et al. 1992; Eldridge et al. 2018; Zapartas et al. 2019).

1.2.1 Supernova explosions in a binary

The impact of a SN explosion on a binary system, and in particular on the companion star, was first considered by Zwicky (1957), while the first quantitative work dates back to the seminal analysis of Blaauw (1961) and Boersma (1961).

The explosion (or possibly implosion) of one star modifies the binary orbit. In a successful SN explosion resulting in the ejection of the stellar envelope, the change in gravitational potential felt by the companion star modifies its orbit (so-called "Blaauw-kick"). Blaauw (1961) found a sufficient condition to break apart a binary system, assuming that the ejecta leaves the binary system instantaneously and that they are spherically symmetric with respect to the exploding star. Under these assumptions, the virial theorem for the binary orbit implies that if the total mass ejected M_{ej} exceeds half of the total mass of the binary $M_1 + M_2$:

$$M_{\rm ej} \ge \frac{M_1 + M_2}{2} \Rightarrow e \ge 1 \quad , \tag{1.1}$$

then a bound orbit (with eccentricity $0 \le e < 1$) will be transformed into a parabolic or hyperbolic orbit, and the newly formed compact object and the "widowed" companion star move away from each other.

However, the work from Blaauw (1961) did not consider the previous evolution of the binary system (see also Paczyński 1971; Bekenstein & Bowers 1974). The current understanding is that the majority of massive binaries will experience a phase of mass transfer before the first core collapses. The mass-transfer phase removes mass from the star that will typically die first, and by the time it reaches the onset of core-collapse, the amount of mass left in the stellar envelope that can contribute to M_{ej}

Fig. 1.2: ζ Ophiuchi is considered the result of the disruption of a binary (Hoogerwerf et al. 2001). The presence of a bow shock (red) suggests that it is moving fast. Credits: NASA/JPL Spitzer.

is limited, and the condition 1.1 can rarely be achieved in nature: the "Blaauw kick" due to the instantaneous and symmetric loss of the SN ejecta can rarely unbind massive binaries.



The assumption of spherical symmetry of the explosion was later realized to be questionable, at least in some cases. The first observational evidence suggesting to relax this hypothesis was the distribution of radio-pulsar proper motions. This revealed a population of NS moving at space velocities exceeding ~ 1000 km s^{-1} in the most extreme cases, and generally much faster than the space velocities of their progenitor massive stars (e.g., Shklovskii 1970; Gunn & Ostriker 1970; Hobbs et al. 2005; Janka 2013, 2017). To explain these velocities, the idea that asymmetries during the SN explosion (see also Sec. 1.3.3) would impart a "natal kick" to the NS at formation was proposed (e.g., Shklovskii 1970). Whether stellar deaths resulting in the formation of BHs also impart a kick to it or not is still debated (e.g., Janka 2017; Chan et al. 2018), and the question has direct relevance to the formation of BH-X ray binaries (e.g., Fragos et al. 2009; Repetto et al. 2012; Mandel 2016), the retention fraction of BHs in clusters (e.g., Pavlík et al. 2018) and gravitational-wave progenitors (e.g., O'Shaughnessy et al. 2017).

From the point of view of the binary orbit, the effect of the SN natal kick is to increase the kinetic energy of the compact object, and consequently of the total (orbital) energy:

$$E_{\rm orb}^{\rm pre-SN} = \frac{1}{2}M_1v_1^2 + \frac{1}{2}M_2v_2^2 - \frac{GM_1M_2}{a} ,$$

$$E_{\rm orb}^{\rm post-SN} = \frac{1}{2}(M_1 - M_{\rm ej})(\mathbf{v}_1 + \mathbf{v}_{\rm kick})^2 + \frac{1}{2}M_2v_2^2 - \frac{G(M_1 - M_{\rm ej})M_2}{a} ,$$
(1.2)

where E_{orb} is the total orbital energy of the binary (before and after the SN), M_{ej} is the SN ejecta mass, M_i and $v_i = |\mathbf{v}_i|$ are the (pre-explosion) masses and orbital velocities of the two stars, *a* the pre-core-collapse semimajor axis, and v_{kick} is the velocity added to the compact object by the natal kick. Eq. 1.2 implicitly assumes a circular pre-collapse orbit (e = 0) and instantaneous loss of the ejecta (so that *a* does not have the time to vary during the explosion). If, after the SN, E_{orb} becomes positive, the binary system is unbound. There is a theoretical consensus on the fact that, because of natal kicks, the vast majority of massive binaries does not survive the first stellar death, and that widowed stars rarely remain bound to the compact remnant of their former companion (e.g., De Donder et al. 1997; Eldridge et al. 2011; Kochanek et al. 2019, see also Ch. 3).

Thus, it appears that SN kicks disrupt the majority of massive binaries by giving a large velocity to the compact objects, but typically without significantly modifying the velocity of the companion star, which is shot out at its own pre-explosion orbital velocity⁴. Moreover, the occurrence of SN natal kicks also means that the compact objects formed by the first core-collapse in a binary will typically *not* retain their stellar companions: compact objects with a companion are an exception rather than the rule in massive binary evolution.

⁴The orbital velocity that is relevant for the widowed companion is not $v_{orb} = \sqrt{G(M_1 + M_2)/a}$, but rather the velocity of the physical star $v_2 = v_{orb}M1/(M1 + M2)$ (e.g., Bekenstein & Bowers 1974). The mass-dependent factor relating v_2 and v_{orb} is typically lower than one at the time of ejection, especially if mass transfer has occurred during the previous evolution.

1.2.2 Higher multiplicity, associations, and clusters

The average observed number of stellar companions to massive stars is ~ 1.5 (e.g., Eggleton & Tokovinin 2008; Moe & Di Stefano 2017), indicating that not only massive stars tend to live in binary systems, but that triple, quadruple (e.g., Leung et al. 1979) and higher multiplicity systems are also common.

These systems can be dynamically stable or not, depending on the orbital configuration, stellar masses, and evolutionary stage. The presence of multiple companions can also lead to dynamical effects on the orbits, for example, the oscillations in eccentricity and inclination of the orbit of the inner binary in a hierarchical triple (Kozai 1962; Lidov 1962; Naoz 2016), which can result in an enhancement of the rate of binary interactions. The exploration of the effects of coupling the multi-body gravitational dynamics with the evolution of stars is a present topic of research (e.g., Toonen et al. 2016; Antonini et al. 2017).

Moreover, as mentioned above, most stars are born in relatively dense associations or clusters, where gravitational interactions between a large number N (>2) of stars in a (meta-) stable configuration can occur. Again, coupling the stellar dynamics in a cluster or association to stellar evolution (radial evolution, impulsive tides, etc.) in these complex systems is also an ongoing endeavor (e.g., Portegies Zwart et al. 1997, and references therein). Given the generally chaotic nature of *N*-body interactions and the complex-



Fig. 1.3: The cluster R136 in the Large Magellanic Cloud is one of the most extreme dense stellar environment in the Local Universe, with ~ $10^5 M_{\odot}$ of stars within ~ 1 pc. Credits: Hubble/WFC3.

ity of the initial conditions for a cluster, statistical methods are usually employed to study these systems (e.g., Aarseth 2003). Occasionally, close encounters between stars will result in the dynamical ejection of one star from the association or cluster, and the ostracized star can acquire large velocities. This process is particularly relevant during the initial evolution of a cluster (especially in the first ~ 1 Myr, e.g., Oh & Kroupa 2016), when the initial dynamical relaxation of the cluster can lead to a copious amount of ejections.

Although binary systems are not *required* for this process to happen, the presence of binaries enhances the rate of ejection because of two important facts (e.g., Fujii & Portegies Zwart 2011; Banerjee et al. 2012). First, the cross-section for interacting with a binary is larger than for single stars, as can be seen considering the geometric cross section $\sigma \propto a^2 \gg R_*^2$, with *a* orbital separation of the binary and R_* the radius of the star. This argument remains valid considering the mutual gravitational pull, neglected in the geometric cross-section. The mutual attraction of the interacting bodies modifies σ , introducing a dependence on their relative velocity. Secondly, binary systems store energy in their orbit, which the

gravitational interaction can transform into kinetic energy of a third body interacting with the binary, producing fast-moving runaway stars: the kinetic energy of the ejected star comes from the change in orbital binding energy of the binary.

In the simplest case of the scattering of a star off a circular binary (N = 3), the variation in orbital energy is

$$\Delta E_{\rm orb} = \frac{G}{2} \left| \frac{M_1^f M_2^f}{a^f} - \frac{M_1^i M_2^i}{a^i} \right| \,, \tag{1.3}$$

where the superscript f and i refer to the pre- and post-scattering masses and separations of the binary. The minimum energy configuration for the binary is approached by decreasing the orbital separation $(a^f \leq a^i)$ and by pairing the two most massive stars out of the three interacting in the binary: swapping the interloper star with one binary member is typical, thus in general $M_j^f \neq M_j^i$ for j = 1, 2. This means that subsequent three-body scatterings will typically eject the least massive stars, and pair the two most massive stars in a "bully binary" (Fujii & Portegies Zwart 2011). Further interactions (and stellar ejections) shrink its orbital separation, until the binary itself can be considered a single point mass for the purpose of the cluster dynamics, and a massive tight binary can ultimately also be ejected (e.g., Fujii & Portegies Zwart 2011; Banerjee et al. 2012).

Therefore, statistically speaking, clusters tend to eject the least massive star in a scattering event. Nevertheless, recent observational evidence supports the ejection via N body interactions of very massive stars, even with masses exceeding ~ $100 M_{\odot}$ (e.g., Lennon et al. 2018; Drew et al. 2018; Kalari et al. 2019, see also Ch. 4).

1.3 The physics of massive stars

Massive stars are rare objects, but of paramount importance for many areas of astrophysics. Like human beings are characterized by their capacity to adapt the environment to themselves, and thus have a dramatic impact on the ecosystem Earth, massive stars are also in some sense defined by the enormous impact they can have on their host galaxy. In fact, massive stars are among the main drivers of galaxy evolution through their chemical, radiative, and mechanical feedback. Therefore, massive stars are among the main drivers of the evolution of galaxies (e.g., Larson 1974; Dekel & Silk 1986; Nomoto et al. 2013; Naab & Ostriker 2017).

The minimum initial mass required for a star to be considered massive typically depends on the context: in this thesis, I consider *massive* to mean initial (zero-age main sequence) masses greater than $M_{ZAMS} \gtrsim 7.5 - 10 M_{\odot}$. This threshold corresponds to stars that evolve through hydrogen-, helium-, carbon-, and neon-core burning and ignite (at least partially) their oxygen-rich core. Each burning phase slows down the gravitational contraction of the star through the release of nuclear binding energy that compensates for the surface energy losses. As the nuclear energy released per nucleon decreases with heavier elements, the nuclear timescale of the core shortens. The onset of a new energy loss term due to thermal neutrinos (on top of the photon luminosity and mass loss processes) further speeds up the core's evolution: evolved massive stars during carbon core burning and beyond are "neutrino stars" that emit more neutrinos than photons (Fraley 1968).

By the definition assumed here, massive stars result in core structures too massive to remain dynamically stable, which ultimately collapse. The possible outcomes of this corecollapse are described in more detail in Sec. 1.3.3 and Sec. 1.3.4. In short, the collapse is expected to produce a supernova explosion (at least in some cases), and possibly form a neutron star, a black hole, or fully disintegrate the star (see Langer 2012, for a review).

The precise minimum mass to end the stellar life with a collapsing core is not known. It depends on many factors including the metallicity of the star (Poelarends et al. 2008; Doherty et al. 2017) or, in other words, the environment in which the star was born; the rotation rate of the core (e.g., MacFadyen & Woosley 1999), and last but not least, the presence of companion(s) that can modify the life and final fate of a massive star (e.g., Paczyński 1971; van den Heuvel et al. 1994; Podsiadlowski et al. 2002; Zapartas et al. 2017a; Poelarends et al. 2017, see also Sec. 1.1).

In principle, there is no upper limit to the mass of a star, although feedback during the star formation might result in an effective upper mass limit for massive stars (e.g., Figer 2005). Several stars with masses exceeding ~ 80 M_{\odot} measured through orbital dynamics in binaries exist (e.g., Bonanos et al. 2004), and stars with spectroscopically determined masses exceeding ~ 300 M_{\odot} have also been claimed (de Koter et al. 1997; Crowther et al. 2010, 2016), and finally, statistical arguments based on the analysis of the population of O-type stars in 30 Doradus suggest that the upper-mass limit for stars might reach ~ 500 M_{\odot} (Schneider et al. 2018a). The maximum mass of a star might also depend on the metal content of the parent cloud, which determines the amount of radiative cooling possible during the formation process and thus the seed self-gravitating mass that collapses. It is generally thought that stars in the primordial Universe with virtually zero metals had, on average, higher masses (e.g., Bromm et al. 1999).

1.3.1 Mass loss processes in massive star evolution

One substantial difference between massive stars and their lower-mass counterparts is the impact of mass loss on their internal structure and evolution. For a Sun-like star, which loses mass in a pressure-driven thermal wind (Parker 1958; Weber & Davis 1967), the observed mass loss rate is of order $\dot{M}_{wind,\odot} \simeq 10^{-14} M_{\odot} \text{yr}^{-1}$. This gives a characteristic timescale for mass loss

$$\tau_{\rm ML,\odot} = \frac{M}{\dot{M}_{\rm wind,\odot}} \simeq 10^{14} \,\rm yr \quad , \tag{1.4}$$

much longer than the evolutionary timescale of the Sun ($\sim 10^{10}$ yr for its main sequence lifetime). Therefore, mass loss is typically negligible when modeling the internal structure and evolution of Sun-like stars, at least until the final phases of their evolution.

In contrast, massive stars have much stronger winds, that are line-driven (e.g. Lucy & Solomon 1970; Castor et al. 1975, see also Ch. 2 and references therein). Fig. 1.4 illustrates

the process: photons in the stellar atmosphere (defined as the region of the star that is partially optically thin where the radiation field has a net radial component) are scattered by metallic ions, which results in a transfer of momentum from the photons to the ions. These then drag away hydrogen and helium via Coulomb coupling, driving the wind mass loss (e.g., Lamers & Cassinelli 1999; Puls et al. 2008).

Massive stars have high luminosities $(L \ge 10^3 L_{\odot})$, see for a recent example Schneider et al. 2018b) and surface temperatures $(T_{\rm eff} \ge 10^4 \text{ K} \text{ for most of their evolution})$, which result in large ultraviolet (UV) fluxes of photons that can therefore drive powerful stellar winds with mass loss rates spanning $10^{-9} M_{\odot} \text{yr}^{-1} \le \dot{M}_{\text{wind}} \le 10^{-4} M_{\odot} \text{yr}^{-1}$ (see Smith 2014, for a review). Although massive stars are intrinsically short-lived with lifetimes spanning few $10^6 \text{ yr} \le \tau_* \le 10^8 \text{ yr}$, the wind mass-loss timescale can become comparable or shorter than the relevant evolutionary timescale: wind mass loss cannot be realistically neglected when investigating their internal evolution.



During advanced evolutionary stages, especially for stars that successfully retain their hydrogen-rich envelope and become red supergiants (RSG), the wind mass-loss rate is observed to be much higher. On the theoretical side, the driving mechanism becomes less clear. It is likely that dust grains, instead of metallic ions, provide the bulk of the opacity and intercept

Fig. 1.4: Sketch of the line-driving mechanism producing strong stellar winds in massive stars. This is an adaptation of Fig. 1 in Höfner (2012).

outgoing photons. However, it is unclear how dust production proceeds in the envelope of RSGs. Pulsations might be required to form the dust in the first place, and observational and theoretical research on this topic is still ongoing (e.g., Beasor & Davies 2018).

Moreover, massive stars have other ways to lose mass, which can lead to even higher mass-loss rates and thus have an even more dramatic effect on their structure. As argued in Sec. 1.1, most massive stars begin their life in close binaries. The presence of a companion star in a short-period orbit might change, through external irradiation, the ionization state of the outer layers of a massive star and influence its mass-loss rate and the wind velocity structure, but this effect quickly becomes negligible with increasing separation (e.g., Gayley et al. 1997). The presence of two stars with strong wind outflows can also generate X-rays in the collision region, which can be used to detect binary systems even if only one observational epoch is available. Mass transfer in a binary system is a mass loss channel at least for the donor star, which can lead to $\dot{M}_{\rm RLOF} \gtrsim \dot{M}_{\rm wind}$, depending on the evolutionary phase during which mass transfer is initiated (i.e., on the initial orbital configuration of the binary and/or the presence of more companions).

Last, but not least, (some) evolved massive stars are observed to experience violent outbursts of mass loss of yet unknown origin. Stars showing this behavior are called Luminous Blue Variables (LBV, Hubble & Sandage 1953; Humphreys & Davidson 1994), and in the most extreme cases they can reach mass loss rates $\dot{M}_{LBV} \leq 10^{-1} - 1 M_{\odot} \text{yr}^{-1}$, cf. the P Cygni and η Carinae outbursts during the 17th and 19th century, respectively. Some observed LBVs are presently observed in binary systems, e.g., η Carinae. Recently, the role of binarity in these eruptive mass loss events has received a lot of attention because of the apparent position of LBVs relative to other massive stars (e.g., Smith & Tombleson 2015; Humphreys et al. 2016; Davidson et al. 2016; Smith 2016), which could be explained if the LBVs are binary products (e.g., Aghakhanlootakanloo et al. 2017). Another reason to consider binarity in the context of LBVs is the potential importance of opacity bumps due to helium enrichment in driving their eruptive mass loss (Jiang et al. 2018): accretor stars in a binary are expected to have a higher helium mass fraction because of the accretion of partially processed material from a companion star (Blaauw 1993).

Very early observations of SN within the first few hours after the explosion also suggest that a significant fraction of massive stars experience late outbursts of mass loss. These produce dense layers of circumstellar material close to the exploding star (e.g., Khazov et al. 2016). This material is illuminated by the SN shock precursor and this produces emission lines that disappear as soon as the SN ejecta runs into the previously ejected layers. The frequency of these outbursts and their physical origin are also actively investigated, and the current leading hypothesis for the driving mechanism is transport of energy through gravity waves from the carbon and oxygen shells to the surface (Shiode & Quataert 2014; Fuller 2017; Fuller & Ro 2018).

1.3.2 Other physical processes

Besides mass loss, other physical processes strongly influence the evolution of massive stars. While these are not the main topic of this thesis, they deserve to be mentioned briefly.

Rotation One key ingredient is rotation, which can be probed directly only for the stellar surface, by measuring the width of spectral lines. Young main-sequence massive stars can have rotational velocities reaching above 100 km s^{-1} from birth (e.g., Ebbets 1979; Ramírez-Agudelo et al. 2013; Ramírez-Agudelo et al. 2015). A companion star on a close orbit can also induce rapid rotation (or spin down a star) through tidal synchronization (de Mink et al. 2009; Mandel & de Mink 2016; de Mink & Mandel 2016a; Marchant et al. 2016). Moreover, in an interacting binary, the accretion of mass from a companion star can spin up significantly the surface of a star (e.g., Hut 1981; Cantiello et al. 2007). This is because the moment of inertia of stars is relatively small, owing to the concentration of mass in the central regions, therefore the angular momentum carried by the incoming material can easily spin up a star, or at least its surface, to break-up speed.

Obtaining information on the internal rotation of stars is more difficult. The competi-

tion between wind mass and angular momentum loss, internal transport, and possible spin-up processes determines the internal angular momentum distribution in the star. Asteroseismology (e.g., Cantiello et al. 2016; Hekker & Christensen-Dalsgaard 2017) and long Gamma Ray Bursts (GRB) might provide an indirect handle on the rotation rate of the core. From the theoretical side, the transport of angular momentum in the stellar interior and the associated mixing processes are still actively investigated (e.g., Zahn 1977; Spruit 2002; Langer 2012; Kissin & Thompson 2018; Fuller et al. 2019). There is still debate on whether shear instabilities or meridional circulation play the dominant role in rotational mixing of chemical species, and whether rotation can prevent the formation of a core-envelope structure by achieving (close to) complete mixing of the stellar gas, and so preventing chemical stratification (e.g., Maeder & Meynet 2000).

Magnetic Fields Closely related to rotation is the presence of internal and surface magnetic fields. About $\sim 10\%$ of massive stars have measurable surface magnetic fields (e.g., Schneider et al. 2016), but many more might have internal magnetic fields influencing the internal evolution and possibly their final fate. Magnetic massive stars have been observed to have a bimodal distribution in field amplitude, with a "magnetic desert" between 1 and 100 G. In general, the field topology can be much more complex than a simple dipole. These fields also couple to the wind mass loss and modify both the mass loss and angular momentum loss rates (e.g., Shore 1987; Shore & Brown 1990; Petit et al. 2017; Georgy et al. 2017).

1.3.3 Core collapse

The definition of a *massive* star adopted in this thesis requires a dynamical instability of the core structure at the end of the evolution. The majority of massive stars end their life once nuclear fusion in hydrostatic equilibrium cannot release sufficient energy to slow down the gravitational collapse. This can happen either because the composition of the core is dominated by the most tightly bound nuclei (⁵⁶Fe and ⁶²Ni), or because the conditions in the core are not sufficient to ignite further nuclear fusion (this typically happens with cores composed mainly of ¹⁶O, ²⁰Ne, and ²⁴Mg and leads to so-called "electron capture" SNe⁵). At this point the core dynamically contracts under its own weight, initiating the process of *core collapse*. That results ultimately in the formation of a neutron star (NS) or black hole (BH), possibly with an associated bright transient called a supernova (SN). Understanding which stellar progenitors produce NS or BH, how the core-collapse is inverted into an explosion, and which evolutionary processes influence this outcome is an active topic of research (O'Connor & Ott 2011; Ugliano et al. 2012; Ertl et al. 2016; Sukhbold et al. 2016, 2018; Couch et al. 2019; Müller 2019a).

Such stellar explosions have been observed by the naked eye and logged in historical records from thousands of years ago (e.g., "guest star" 185 CE or SN1054 that formed the

⁵However, it is important to underline that electron capture processes are of paramount importance for the dynamics of any type of core-collapse SN, regardless of the core composition.

iconic Crab nebula, Xi 1955; Clark & Stephenson 1977; Zhou et al. 2018). However, the study of their physics started with Baade & Zwicky (1934), who first recognized that the collapse of a stellar core would release enough gravitational binding energy to drive these explosions. The amount of energy released can be estimated assuming that the collapsing mass is about the typical NS mass $M \simeq 1.4 M_{\odot}$ (and above the Chandrasekhar limit, so that electron degeneracy pressure is insufficient to stabilize it), the typical radius of the core is $R_{\rm Fe} \simeq 1000 \,\rm km$, and it collapses to a proto-NS with radius of $R_{\rm NS} \simeq 10 \,\rm km$:

$$\Delta E_{\text{bind}} \simeq \frac{GM^2}{R_{\text{NS}}} - \frac{GM^2}{R_{\text{Fe}}} \simeq 10^{53} \,\text{erg} \quad , \tag{1.5}$$

where G is the gravitational constant. The energy released by the gravitational collapse is, in principle, more than sufficient to power SN explosions: it exceeds the total binding energy of the stellar envelope, the typical energy radiated in such explosions ($\int L_{SN}(t) dt \approx 10^{49}$ erg, with L_{SN} the luminosity during the explosion, integrated in time t over the explosion duration), and amounts to about 100 times more that the typical kinetic energy of SN explosions (1 Bethe $\equiv 10^{51}$ erg).

Nevertheless, the complex interplay between the fundamental forces involved complicates understanding how the explosion taps into this energy source. The dominant, but highly debated, class of models to explain this is the *neutrino-driven explosion paradigm* (see Janka et al. 2012, for a review). As the core collapses, the density becomes so high that a copious amount of electron captures can occur. These progressively turn the majority of the protons into neutrons and produce a very large neutrino flux. The neutrinos carry away most of the energy released by the collapse (Colgate & White 1966). As the collapse proceeds, the core splits into an inner core collapsing subsonically and an outer core which instead collapses supersonically (and thus does not have time to respond to changes within the inner core). As the density exceeds the nuclear density $\rho \gtrsim 10^{14}$ g cm⁻³ the repulsive term of the nuclear force causes a sudden stiffening of the equation of state (EOS). The inner core becomes denser than the equilibrium density of the stiffened EOS: this stops the collapse and reverses the infall velocity in the so-called "core-bounce", triggering a shock wave that is thought to, at least in some cases, successfully disrupt the star in a SN explosion.

As the shock wave propagates outwards, it loses energy by heating and photodisintegrating the infalling material from the outer core, and overcoming the ram pressure of this same infalling material. The energy loss through these mechanisms leads to a stalled shock in most numerical simulations (the shock radius remains roughly constant for ~ 100 millisec, e.g., Janka et al. 2012). An as-yet poorly understood "shock revival mechanism" must act to revive the shock and restart its radial expansion allowing it to unbind the stellar envelope and produce a SN explosion. Identifying the shock revival mechanism is a longstanding open problem in theoretical astrophysics (e.g., Arnett 1996, and references therein).

In the *neutrino-driven paradigm*, the shock revival mechanism is provided by the high neutrino emission from the ongoing electron captures and thermal neutrinos from the inner core and its immediate surroundings (the "cooling region"). A small fraction of these neutri-

nos will interact in a region behind the shock (the so-called "gain region"). This is because the stellar plasma now has densities and temperatures such that the cross-section for neutrino interactions is non-negligible (unlike during any phase of the stellar lifetime). However, this alone is not sufficient to revive the shock in numerical simulations, at least when imposing spherical symmetry on the explosion. Asymmetries (whose presence is suggested by the observed pulsar velocities, cf. Sec. 1.2.1) have recently been recognized as the key ingredient to achieve successful explosions. Several sources of asymmetry, both local and global, (co-)exist in the collapsing core of a massive star:

- The neutrinos heat the bottom of the gain region, driving convection (a steep temperature and entropy gradient can develop because of the neutrino heating). Convection implies the presence of turbulent flow and an associated turbulent pressure ($P \propto v_{turb}^2$) that can help push the shock (O'Connor & Couch 2018);
- The Standing Accretion Shock Instability (SASI, Blondin et al. 2003): when the shock stalls, small perturbations arise because of the infalling material. These perturbations (e.g., in the local velocity field) are advected downwards by convection and amplified which leads to a sloshing motion of the shock;
- The Lepton Emission Self-Sustained Asymmetry (LESA, Tamborra et al. 2014), found in 3D simulations where the neutrino emission is roughly dipolar. Its role in the explosion dynamics is not yet fully understood, but asymmetries in the neutrino flux might contribute to the initial development of kicks (e.g., Nagakura et al. 2019).

The overall effect of asymmetries is to (i) increase the amount of time spent by matter in the gain region, where the energy of the neutrinos can be harvested to push the shock and (ii) provide extra pressure terms (e.g., due to turbulence). The combination of these two effects in multi-dimensional core-collapse SN simulations results, at least in some cases, in successful explosions. Because of the deviation from spherical symmetry, the collapse of a stellar core can also generate gravitational waves, on top of copious amounts of neutrinos and photons (see Ott 2009, for a review). However, the detectability range for these events is limited to ~ 10 kpc, i.e. effectively within the Milky Way galaxy (e.g., Dimmelmeier et al. 2008; Ott 2009).

As of early 2019, the emerging picture from the 3D core-collapse SN simulations of different research groups is the following: *not only are the asymmetries after core-bounce necessary to achieve successful explosions, the pre-collapse core structure and in particular the Si/O interface is crucial* (Ott et al. 2018; Kuroda et al. 2018).

Thus, it is reasonable to expect that asymmetries that develop within the first few hundred milliseconds after core bounce determine the outcome of the core-collapse. However, these asymmetries continue to have an effect for up to a few seconds after the success or failure of the explosion is decided (Janka 2017), and in particular, they can lead to SN natal kicks (see also Sec. 1.2.1).

The asymmetric ejecta continue to influence significantly the newly formed compact object for as long as ~2 sec (Wongwathanarat et al. 2013; Janka 2017): this gravitational coupling can accelerate the compact object in the direction of the densest ejecta, which pulls the compact object like a "tug-boat" (Janka 2013). This model predicts that most of the explosive nucleosynthesis by the SN shock should happen in the direction *opposite* to the kick, where the density is lower and the shock propagates faster. Recent observations of the spatial distribution of radioactive elements synthesized by the explosion in supernova remnants support this "tug-boat" kick mechanism (e.g., Holland-Ashford et al. 2017; Grefenstette et al. 2017; Katsuda et al. 2018). Other natal kick mechanisms, e.g. solely because of asymmetries in the neutrino emission from the proto-NS (e.g., Socrates et al. 2005) have also been proposed, but the prediction of a correlation between the resulting NS magnetic field and the kick amplitude does not appear to be supported by recent observations (Katsuda et al. 2018).

Both the proper motion of radio pulsars and the morphology of supernova remnants suggest that at least *some* NSs receive large natal kicks. However, it remains unknown whether BH formation can also occur with significant kicks (e.g., if the asymmetric ejecta ultimately fall back onto the compact object, Chan et al. 2018). Another open question is whether there is a relation between the pre-collapse core structure and the amplitude of the natal kick (e.g., Katz 1975; Arzoumanian et al. 2002; Podsiadlowski et al. 2002; Verbunt & Cator 2017). This possible relation needs to be further investigated to explain jointly both the large proper motions of single NSs and the observation of binary NSs (e.g., Tauris et al. 2017; Vigna-Gómez et al. 2018), either as binary pulsars, or in transients such as short-gamma ray bursts, and gravitational wave mergers (LVC 2017e).

1.3.4 The fate of the most massive stars: pair instability

Extremely massive stars have a different predicted final fate than the core-collapse described in Sec. 1.3.3. Their cores become dynamically unstable before energy generation by nuclear fusion becomes impossible (e.g., Fowler & Hoyle 1964; Barkat et al. 1967; Rakavy & Shaviv 1967; Fraley 1968). While core-collapse SNe are not yet well understood despite the large number of observations, the opposite is true for the death of these extremely massive stars. The theoretical picture of the process is well established, but a clear observational counterpart is still lacking because of the rarity of stars this massive at low metallicity in the local Universe. So far, only candidate events have been reported (e.g., Woosley et al. 2007; Gal-Yam et al. 2009; Arcavi et al. 2017a; Terreran et al. 2017; Lunnan et al. 2018; Gomez et al. 2019, see also Ch. 7), but their interpretation remains ambiguous.

The most massive stars are supported by radiation pressure. If their helium-core mass exceeds $M_{\text{He}} \gtrsim 30 M_{\odot}$ (corresponding roughly to $M_{\text{ZAMS}} \gtrsim 70 M_{\odot}$), evolution leads to temperatures and densities such that electron-positron (e^{\pm}) pairs are produced via photon-photon interactions, $\gamma \gamma \rightarrow e^+e^-$ (cf. Fig. 1.5). The e^{\pm} pairs then annihilate producing neutrino-pairs which freely stream out of the core, or producing a new pair of photons which will typically have lower energy than the photons that produced the e^{\pm} pair to begin with. The effect of this

is to reduce radiation pressure support and leads to a *local* instability as the star readjusts to its new structure.



Fig. 1.5: Temperature and density diagram colored with the value of Γ_1 – 4/3. Stellar layers that have $\Gamma_1 < 4/3$ (red) are *locally* unstable because of the runaway conversion of photons into e^{\pm} pairs. The Γ_1 is obtained from MESA's EOS using pyMESA (Farmer & Bauer 2018) assuming the chemical composition at the beginning of the collapse of a PISN model.

The production of a e^{\pm} pair requires a photon energy (E_{γ}) larger than the rest mass of the electron, i.e. $E_{\gamma} \gtrsim m_e c^2 \simeq$ 0.511 MeV, corresponding to a temperature of $T_{\rm PP} \simeq 6 \times 10^9$ K. Since stars are in local thermal equilibrium in their interior, the photons follow a Planck distribution. Thus, even at temperatures lower than $T_{\rm PP}$ there is a tail of high energy photons which can produce e^{\pm} pairs and *pair-production* alone does not necessarily produce an instability. A lower mass star can reach tempera-

tures sufficient for e^{\pm} production, but it does not trigger a global dynamical readjustment of its structure. This is because for a low-mass star the region that is hot enough for pairproduction is too dense for runaway pair production. At high densities, the mean free path for photon-photon encounters $(\lambda_{\gamma\gamma})$ increases above the mean free path for the interaction of photons with electrons $(\lambda_{\gamma e})$, thus the runaway e^{\pm} production cannot take place. The requirement for $\lambda_{\gamma\gamma} \leq \lambda_{\gamma e}$ can be translated in a temperature and density-dependent threshold for pair-production to drive a *local* instability. This determines the shape of the lower boundary of the instability region shown in Fig. 1.5.

For densities $\rho \gtrsim 10^{5.7}$ g cm⁻³, e^{\pm} pairs rapidly fill the continuum energy levels available (Fraley 1968). Consequently, the photon energy required to produce a pair will increase as the e^{\pm} chemical potential μ_e increases. Production of e^{\pm} stops because the bulk of the photons can no longer meet the energy requirements to produce e^{\pm} pairs (Zeldovich & Novikov 1999). The upper temperature limit for the occurrence of a *local* pair-instability, corresponds roughly to $\log_{10}(T/K) \gtrsim 9.5$. At these energies e^{\pm} pairs are non-relativistic, typically the photon energy E_{γ} only slightly exceeds the rest energy of the pair $2m_ec^2$. Due to the temperature dependence of neutrino production, a large amount of e^{\pm} are rapidly produced. Electron gas pressure from e^{\pm} will then have a stabilizing effect on the stellar structure (Kippenhahn et al. 2013).

Figure 1.6 depicts the various phases of the stellar *global* readjustment from the *local* instability that occurs due to the production of e^{\pm} pairs.





Step 1. The core is supported by radiation pressure. At the first onset of the instability, the core typically consists of a mixture dominated by oxygen, neon, and sodium. As the core evolves, it contracts and increases its temperature. The most central region is typically too dense for pair-production to result in an instability, especially for the least massive stars experiencing this evolution. Thus, the instability can start off-center. As the temperature increases, so does the rate of e^{\pm} production. This removes pressure support from photons, causing a runaway thermal contraction of the core and consequent increase in the temperature and e^{\pm} production rate.

Step 2. The net effect of the pair-instability is a softening of the EOS (by decreasing the adiabatic index $\Gamma_1 \equiv \partial \log(P)/\partial \log(\rho)$ below the stability threshold 4/3), which leads to a collapse of the unstable layer on a thermal timescale. For $T \gtrsim 6 \cdot 10^8$ K, the dominant energy loss for the star is thermal neutrinos, (e.g., Rakavy & Shaviv 1967), thus the relevant thermal timescale is the neutrino mediated Kelvin-Helmholtz timescale:

$$\tau_{\rm KH}^{\nu} \propto \frac{GM^2}{RL_{\nu}} \quad , \tag{1.6}$$

where the proportionality constant depends on the details of the geometry, M is the total mass, R is the radius and $L_{\nu} \gg L$ is the neutrino luminosity which exceeds the photon luminosity L. As the unstable layers contract, the temperature keeps increasing and pair-production accelerates.

Step 3. The increase in temperature triggers a thermonuclear explosion. This is fuelled by primarily ${}^{16}\text{O}+{}^{16}\text{O}$ burning, at least during the first pulse. The energy released depends on the temperature and density at which the ignition happens, and on the amount of fuel available in the unstable region. Subsequent pulses will also burn magnesium, sulfur, silicon, as well as any remaining oxygen.

Step 4a. For sufficiently massive cores, the thermonuclear explosion releases more energy than the total binding energy of the star and the thermonuclear explosion successfully unbinds the entire star in a PISN, leaving no compact remnant (e.g., Bond et al. 1984).

Step 4b. For slightly less massive cores (see Ch. 7), the energy released from the thermonuclear burning is insufficient to unbind the whole star. Instead, the energy injection expands the core which then cools and shuts down the nuclear burning. The expansion launches a wave through the star, which steepens into a shock at the surface and can lead to a mass-loss episode.

Step 4c. For much higher helium-core masses instead, the thermonuclear explosion happens at such low density that all the nuclear binding energy released by fusion is used to photodisintegrate newly-formed heavy nuclei, instead of going into kinetic energy of the

stellar gas (e.g., Bond et al. 1984; Heger et al. 2003). Thus, models reaching this photodisintegration limit are also expected to produce BHs, possibly without an associated transient, because of the collapse of the inner layers.

Step 5. After the adiabatic expansion and possibly the ejection of mass at step 4b., the core cools through thermal neutrino losses (or photons, in cases when the core has cooled too much for significant neutrino production) and contracts. As the contraction proceeds a new layer may enter the instability region triggering a new pulse. The star can then loop through the steps 1-4b-5 several times.

Step 6. Eventually, because of the mass loss, the entropy losses due to the neutrinos, and the consumption of nuclear fuel each time the star goes through step 3., the core structure is stabilized. The evolution then proceeds through burning the remaining nuclear fuel in the core (if any) and finally the core collapses.

The pair-instability evolution of the most massive stars shapes the mass distribution of the most massive stellar BHs (depending on the physical process that governs the trifurcation between steps 4a., 4b., and 4c. in Fig. 1.6 and the amount of mass lost at step 4b.), and creates a PISN BH mass gap above a certain threshold, where PISNe fully disrupt the stars leaving no compact object behind it. The recent detection of BHs with $M \ge 30 M_{\odot}$ (LVC 2018b, and references therein), together with the increase in the samples of superluminous SNe which might, at least in some cases, be explained by these explosions, has greatly revived the interest in this topic.

1.4 Researching massive stars

The study of the internal structure and evolution of stars is a multi-scale problem which requires to combine a variety of ingredients: e.g., atomic physics, radiative transfer, neutrino cooling, thermonuclear burning, hydrodynamics in highly stratified media. All these processes interact with each other in a non-linear way on a wide range of timescales, from subhour dynamical timescales to millions and billions of years for nuclear timescales. The range of lengthscales that are relevant also spans several orders of magnitude, from sub-centimeter (e.g., the width of a carbon flame in a super-asymptotic giant branch star, Timmes & Woosley 1992) to several thousand solar radii for RSGs. The complexity of the problem often requires varying levels of simplification to make it tractable.

To prevent (or amend) theoretical, modeling, and/or computational mistakes, the approach from "first principles" must be constrained by observations⁶. Generally speaking, these can be of two kinds: (i) individual events or sources and (ii) population constraints.

⁶In this perspective, stellar physics is no different from other subfields of theoretical and computational astrophysics.



Specific star, supernova, or compact object stellar populations, SN distributions in space and type

Fig. 1.7: Schematic representation of the links between the two kinds of simulations presented in this thesis, and the two different categories of observations generally available in astrophysics. Computational astrophysics is the process of establishing and revising those links and refining the theoretical models and their simulated realizations. The top row shows the two codes used in this thesis, while the bottom presents examples of observations relevant to massive-star research.

Typically, individual sources (e.g., one specific SN explosion, such as SN1987A, or a particularly well-observed star, such as ζ Ophiuchi in Fig. 1.2) provide a more direct handle on the physical processes. However, the interpretation of such observations can be misleading because of peculiar conditions in the presentation of the specific phenomenon or in its detection.

The second kind of observational constraint, those from the distribution of properties of ensembles of sources, can mitigate this problem. Moreover, because of their intrinsic rarity, or because of their duration exceeding human lifetimes, some processes can almost only be meaningfully connected to observations through the analysis of populations of sources. Finally, if the observed sources span different astrophysical environments (e.g., different types of host galaxies, metallicity), populations can reveal trends that constrain the physical interpretation of phenomena.

Most of this thesis presents results of numerical models using two complementary com-

putational approaches described below. Only Ch. 4 deals directly with the analysis of observational data from the *Gaia* mission and *Hubble Space Telescope* (HST) archival astrometry.

1.4.1 Evolution of the internal structure: MESA

The stellar structure equations are a set of stiff, non-linear, coupled, differential equations. They can be numerically solved to simulate the evolution of a star from the onset of corehydrogen burning to the final fate of the star (e.g., Cox & Giuli 1968; Kippenhahn et al. 2013). Because of the computational cost, such calculations are typically carried out using one-dimensional implicit Lagrangian codes. "Lagrangian" means that the equations are discretized using a grid made in an extensive variable of the system rather than a grid in space. Stellar evolution codes typically use as coordinate the mass M(r) of a sphere with radius r inside the star. "One-dimensional" means that the code imposes a geometry on the stars, which are modeled as spherically symmetric. Even for single stars, any degree of rotation introduces a preferential direction along the rotation axis, breaking this assumption. The presence of a binary companion, which changes the gravitational potential to a Roche geometry, also breaks this assumption for the majority of massive stars. However, deviations from spherical symmetry are moderate for relatively slow rotational velocity and influence mostly the outer layers in the case of the Roche geometry of a binary. Corrections to account for some of these effects, at least in a parametric way, are sometimes included (e.g., Heger et al. 2003).

Chapters 2, 5, 6, 7, and 8 (and their appendices) present calculations performed with the open-source stellar evolution code MESA⁷ (Paxton et al. 2011, 2013, 2015, 2018, 2019), which also has a binary evolution module (Paxton et al. 2013) allowing for the simulation of two interacting stars, and includes also a hydrodynamic Riemann solver HLLC (Toro et al. 1994; Paxton et al. 2018) to follow dynamical phases of the stellar evolution and capture possible shock waves traveling through a star. We employ the latter capability when simulating (pulsational) pair instability in Ch. 5–8.

The computational cost of these models varies by orders of magnitude depending on the spatial and temporal resolution, the number of isotopes included in the treatment of nuclear reactions, and the stiffness of the evolutionary phase simulated. Typical applications with presently-available computational resources require at least a few thousand mesh points for the spatial resolution. These are not uniformly distributed, but instead, adaptive mesh controls allow the user to increase the resolution around the steepest variations in the star. The temporal resolution is also adaptive, to allow for the treatment of slow and rapid phases of evolution (e.g., core hydrogen burning and the crossing of the Hertzsprung gap, respectively) with the same computational technique. The smallest number of isotopes that is typically used is ~ 20 to track at least the main α -elements for the bulk of the energy generation. Such a setup would typically result in run-times of tens of hours to days using ~ 10 cores. However, some applications might require much higher spatial and/or temporal resolution, or to include a larger number of isotopes, see for example Ch. 2 and Appendix. A.2.

⁷http://mesa.sourceforge.net/index.html



1.4.2 Population Synthesis:

For the typical setup described above, modeling the entire evolution of one star by directly integrating the stellar structure equations takes several hours. Including binary evolution processes typically increases the computational time. This makes the exploration of the vast parameter space of binary evolution extremely expensive (varying both stellar masses, their initial separation, possibly the initial eccentricity, and on top of these, all the free parameters entering in the algorithmic representation of physical processes).

Nevertheless, building large synthetic stellar populations is necessary to make statistical comparisons with real observed populations, predict rates of events, explore systematic trends (e.g., with metallicity, distance to their host galaxy, etc.), and quantify the likelihood of a specific observation in a given theoretical framework. Moreover, population synthesis allows for the identification of the dominant evolutionary paths producing a specific phenomenon. Broadly speaking, population synthesis techniques achieve these goals by weighting the outcome of sets of pre-computed simulations with theoretically-motivated or empirical distributions in the initial parameter space.

While population synthesis can in principle be done with any set of models (pre-computed or obtained "on the fly"), a common technique is to use a rapid *semi-analytic* approach for stellar and binary evolution, relying on fitting formulae for pre-computed single star models and analytic algorithms developed to represent binary interactions. Ch. 3 is based on calculations using the binary_c code⁸ (Izzard et al. 2004b, 2006, 2009; de Mink et al. 2013; Schneider et al. 2015; Izzard et al. 2018). It uses algorithms originally developed by Tout et al. (1997) and the fitting formulae of Hurley et al. (2000) to the single star models from Pols et al. (1998), which were computed solving the stellar structure equations with a Lagrangian stellar evolution code. Binary interactions are modeled in binary_c based on the analytic algorithm developed by Hurley et al. (2002).

This semi-analytic approach reduces the computational time of the entire evolution of a star or binary system to much less than a second on one single core, and therefore allows one to create large synthetic populations with $10^5 - 10^6$ stars in about the same time MESA takes to model one star. The price of this extreme speedup is a reduction in the physical accuracy of these models: for example each star is always assumed to be in gravothermal equilibrium. However, gravothermal equilibrium can be broken during binary interactions (e.g., because an accreting star is receiving mass faster than its envelope thermal timescale). Moreover, the physics is represented by a large number of parametrized algorithms for which the parameters are poorly constrained (for example, the fraction of the transferred mass that remains bound to the accretor star during mass transfer).

However, the extreme speed of population synthesis simulations allows for testing of the robustness of the results against parameter variations both in the input distributions and phys-

⁸https://www.ast.cam.ac.uk/ rgi/binary_c.html.

ical algorithms. Even if the predictive power of a single synthetic population is limited, an ensemble of populations exploring the parameter space can be useful. Two outcomes are possible: either the simulated population is insensitive to a given parameter, at least within the algorithmic framework adopted, which suggest that the physical process represented by such parameter does not influence significantly the results, or vice-versa, the simulated population shows variations as a function of a given parameter. The latter case allows for direct constraints on the specific parameter considered by comparing simulated results with the observations. This approach is still limited to the algorithmic representation of the physics adopted in the code, and while exploring variations of each parameter one-by-one is straightforward, considering potential degeneracies between the physical processes associated to each parameter is still complicated. Population synthesis techniques to address these problems are presently being developed (e.g., Stevenson et al. 2017; Taylor & Gerosa 2018; Andrews et al. 2018; Broekgaarden et al. 2019).

1.5 Existing, ongoing, and upcoming observations

Many different classes of observations are useful to improve our understanding of massive stars, spanning across all wavelengths of the electromagnetic spectrum, and also observations of neutrinos and gravitational waves. The observations can target either the stars themselves, the transients produced by massive stars, and/or the compact objects they leave behind. Recent technological progress for each of these classes of observations is increasing the number of constraints and improving the coverage of massive-stars phenomenology in the accessible Universe. Again, a full review is beyond the scope of this introduction, and I will limit the discussion to observations that are of direct relevance for this thesis.

The first class of observations consists of those targeting the stars themselves. Because of the rarity of massive stars, this is typically done with surveys, either photometric (e.g., OGLE, Udalski et al. 2008) or spectroscopic (e.g., VFTS, Evans et al. 2010). Observations of specific massive stars also exist (e.g., Ramiaramanantsoa et al. 2018). Observing directly resolved massive stars and binaries is necessarily limited to a local volume of the Universe. Moreover, typically massive stars show most of their spectral lines in the UV range, most of which is only accessible from space. In 2019, the ULLYSSES legacy program devoted to young stars has been approved, scheduling 1000 orbits of *HST* to generate a library of UV spectra that will include many massive stars with different metallicities.

The *Gaia* space telescope is currently providing accurate astrometric constraints on stars in the Galaxy, and by the final data release it will give a complete sample of stars with G-band magnitude (\simeq V-band magnitude) below 20.5. This will include the majority of the massive stars in the Galaxy, and potentially provide orbital solution for each detectable binary system. While *Gaia* is not designed to specifically target massive stars⁹, having precise distances will

⁹For example, the spectrograph onboard the satellite covers the wavelenght region 845-872 nm, where no lines are expected in the spectrum of O- and early B-type stars: *Gaia* cannot directly provide radial velocities for massive stars.

constrain the luminosity (and therefore mass) estimates. More importantly, the kinematics of massive stars in the galaxy can shed light on the lives and deaths of massive stars and their former companions (e.g., Eldridge et al. 2011, and Ch. 3), and on the early dynamics of dense stellar environments (e.g., Drew et al. 2018; Lennon et al. 2018; Kalari et al. 2019, and Ch. 4).

Because of their high luminosity, massive stars also dominate the optical and UV spectra of unresolved young populations of stars. Studying the integrated light from young clusters or star-forming galaxies can also provide direct constraints on how the most massive stars evolve. The integrated light of stellar population often allows observers to probe, albeit in an indirect way, the evolution of stars in the early Universe. This approach will continue in the near future with infrared (IR) instruments such as the James Webb Space Telescope (*JWST*) and WFIRST: although massive stars are not especially bright in the IR, cosmological redshift can shift into this wavelength range the UV range where massive stars outshine other sources.

The spectral and photometric observations are complemented with time-domain surveys. Many transient phenomena in the sky are directly or indirectly related to the evolution and death of massive stars (e.g., stellar mergers, LBV outbursts, SNe, long GRB, etc.). The availability of larger CCDs is progressively allowing for deeper surveys with faster cadence such as the Zwicky Transient Facility (ZTF Bellm 2014) and Large Synoptic Survey Telescope (LSST Science Collaboration et al. 2009), which can reveal rare, dim, and/or unusual transients that can, in turn, shed light on specific evolutionary paths of massive (binary and multiple) stars. Although not a survey instrument, *JWST* will also allow for the observation of the explosive transients associated with the first (population III) stars formed in the Universe. However, the stars themselves will not be directly observable (e.g., Whalen et al. 2013).

Another kind of transient deserves a separate mention: the gravitational-wave merger of two compact objects. These are related to massive-star and massive-binary evolution, although establishing the connection between the observed mergers and their progenitor systems is a complex task. One major complication is the long delay between the formation of the compact objects and their merger, which is typically of the order of Gyr (e.g., Peters 1964; Dominik et al. 2012; Belczynski et al. 2018). During the gravitational-wave inspiral the majority of the stars belonging to the same population as the progenitors of the compact objects will have either disappeared or become undetectable. Even the host galaxy can evolve significantly, leaving us with only the gravitational-wave signal to reconstruct the progenitor system. Nevertheless, when two compact objects successfully merge, the gravitational waves allow us to probe the evolution of massive binaries, triples, or dense stellar clusters indirectly through the compact objects they produce.

The fact that for detectable gravitational waves $r \gg \lambda$, where *r* is the distance to the source and λ is the wavelength, means that their amplitude scales with r^{-1} (cf. r^{-2} for electromagnetic waves): a larger volume of the Universe is accessible for observations through gravitational waves compared to electromagnetic observations. On the 1st of April 2019, the LIGO and Virgo detectors have begun the third observing run, which is predicted to reveal ~ 10 - 100 binary black hole mergers (Fishbach & Holz 2017; Talbot & Thrane 2018;

Stevenson et al. 2019). This will provide an order of magnitude increase in the sample of stellar-mass BHs with dynamically measured masses known to date. Future space-based interferometers (LISA, pulsar timing arrays) will probe lower gravitational-wave frequencies, and underground detectors (Einstein telescope, KAGRA) will improve the sensitivity of gravitational-wave interferometers. The effort for electromagnetic followup observations of gravitational-wave merger events is also driving the design and development of faster and deeper time-domain electromagnetic surveys (e.g., LSST, ZTF, BlackGEM, GROWTH).

The study of compact objects through X-ray, radio, and γ -rays can also give constraints on their progenitor stars and possibly their interaction with companion(s). In particular, binary systems with a compact object accreting from a stellar companion provide a valuable observational anchor point for an evolutionary path possibly leading to a gravitational wave merger. Radio proper-motions of pulsars also give direct constraints on the explosion physics, and SN natal kicks, as discussed in Sec. 1.2.1.

Neutrino detectors can also constrain massive-star physics: the detection of neutrinos associated with the explosion of SN1987A is the prime example (Bionta et al. 1987, see also Arnett et al. 1989). Massive stars contribute significantly to the neutrino background of the Galaxy, both because of their neutrino cooling emission during late evolutionary phases, and because of the gigantic neutrino flux produced by core-collapse and pair-instability events, e.g., Wright et al. 2017.

1.6 Thesis summary

This thesis investigates several aspects of the evolution of massive stars and binaries, with particular attention to the final fate of the star, and the implications of the stellar death for potential companions. A common theme connecting all the chapters is "objects or matter which massive stars and clusters eject or lose during their evolution": surface layers lost due to stellar winds (Ch. 2), binary companions ejected at collapse (Ch. 3), cluster members ostracized from the cluster (Ch. 4), and explosive mass loss events driven by the pair-instability (Ch. 5, Ch. 6, Ch. 7, and Ch. 8).

Chapter 2 presents a numerical experiment to quantify the systematic uncertainty of massive star models because of the treatment of wind mass loss. Using a grid of non-rotating, solar metallicity, single massive stars computed varying the algorithmic treatment of wind mass loss, we find that systematic uncertainties prevent us from determining the final mass of a star. However, the appearance of the star at the end of its evolution does not vary as much as the total mass. Moreover, we find that the *functional* dependence of the mass loss rate on the stellar properties $\dot{M} \equiv \dot{M}(L, T_{\text{eff}}, Z, ...)$ produces significant variations in the pre-collapse core structure, with potential implications for studies of the SN explosion mechanism, which might start from biased assumptions about the initial conditions. Chapter 3 presents a suite of binary population synthesis simulations computed to characterize the population of "widowed" stars separated from their companions at the first stellar death in the binary. We find that 86^{+11}_{-22} % of all the massive binaries are disrupted at the first collapse of a binary member. The uncertainty in this disruption fraction is dominated by what is assumed for the SN natal kicks. However, most disrupted binaries eject the surviving companion with a low velocity of the order of a few km s⁻¹: the SN natal kicks govern the disruption of the binaries, but in most cases do not affect significantly the speed of the companion star, which is ejected with its pre-explosion orbital velocity. We propose to use the mass function of massive runaways from the disruption of binaries to put statistical constraints on the amplitude of BH kicks.

The results from Ch. 3 can also be used to investigate the origin of the observed population of massive runaway stars, which consists of ~ 10% of the observed population of O-type stars. It is commonly expected that the majority of these runaways come from the disruption of binaries (Hoogerwerf et al. 2001). However, assuming a constant star formation history, none of our simulations can reproduce such a high fraction. This suggests that either (i) processes other than SNe in binaries dominate the production of runaways, or (ii) observations tend to overestimate the runaway fraction because of biased samples, or (iii) a key ingredient of the orbital evolution of binaries is missing in state-of-the-art population synthesis simulations, or a combination of these options (see also Sec. 1.7.1).

The main contamination to the sample of "widowed" stars are stars ejected as the result of dynamical interactions in a cluster. In Ch. 4 we study the kinematics of one of the most massive stars known to date, the WNh5 star VFTS682 ($M \ge 140 M_{\odot}$). Proper motions from the second *Gaia* data release suggest that this star is moving away from the nearby cluster R136 (Fig. 1.3), albeit with large errorbars. Archival *HST* proper motions independently corroborate the *Gaia* result, and other stars with masses exceeding 100 M_{\odot} are compatible with having been ejected from the cluster (Lennon et al. 2018). Finally, numerical N-body simulations from various groups (e.g., Fujii & Portegies Zwart 2011; Banerjee et al. 2012) support the possibility of such an extremely massive star being ejected, especially if even more massive stars exist in the cluster (e.g., Crowther et al. 2010, 2016). The coherent picture arising from multiple independent observations and theoretical work lead us to tentatively suggest that VFTS682 was indeed ejected from R136 with a velocity relative to the cluster of ~ 38 ± 17 km s⁻¹, which would make VFTS682 the most massive runaway star known to date.

Stars as massive as VFTS682 might end their life encountering the pair instability, depending on the amount of mass they lose. Ch. 5-8 are dedicated to the study of pair-instability evolution, in the context of gravitational wave and electromagnetic transient observations. These chapters are based on the analysis of hydrodynamical stellar structure and evolution simulations of single naked helium cores.

In Ch. 5 we investigate the radial expansion of pulsational pair-instability models, the

orbital consequences of these violent mass ejections, and the impact on the BH (chirp) mass distribution. We find that the pulsations can lead to significant radial expansion, and therefore possibly an enhanced rate of binary interactions. We also find that, assuming simple distribution functions for the progenitor stars, the occurrence of pulsations leads to a double-peaked (chirp) mass distribution of BHs. Finally, the mass ejection events can also create a significant eccentricity in a binary, but the eccentricity is completely washed out by gravitational wave emission before entering the band of planned space-based gravitational wave detectors.

We tested the robustness of our pulsational pair-instability models against physical and computational assumptions in Ch. 6. We find that our models have a predictive power unusual for stellar astrophysics: the maximum BH mass below the pair-instability gap is ~ 45 M_{\odot} and it is relative insensitive to variations in the metallicity and uncertain algorithmic or physical ingredients (e.g., treatment of winds, neutrino cooling rates, numerical resolution). Thus, the maximum BH mass below the PISN mass gap might provide a "standard siren" for cosmological applications, even if the rate of occurrence of the most massive BH might vary as a function of the input parameters. The uncertainty that has the highest impact on the maximum BH mass below the gap is the rate of the ¹²C(α, γ)¹⁶O reaction: the maximum BH mass detected through gravitational waves can put an upper limit on this highly uncertain reaction rate.

Chapter 7 focuses on the matter ejected by these stars, rather than on the matter remaining bound. We find that pair-instability evolution starts mildly, without really affecting the surface properties of the star or its surroundings. These weak pulses are in principle only detectable through variations in the neutrino flux produced by these stars. Increasing the core mass, models start expanding radially by large amounts, and finally, they eject mass. The number of observable pulses a given model experiences depends on which observable outcome of the pulse is considered of interest. The amount of (helium-rich) mass lost due to pair-instability pulses is a steep function of the helium core mass, $10^{-6} M_{\odot} \leq M_{\text{CSM}} \leq 20 M_{\odot}$ with the largest values for the more massive stars considered. The initial ejecta velocity is typically about ~ 10^3 km s⁻¹ which suggests a possible connection with (some) SN Ibn if the final collapse of these models is accompanied by a (possibly weak) explosion.

Finally, Ch. 8 deals with one specific long-standing problem in stellar astrophysics, the treatment of convection. The pulsational pair-instability proceeds on short timescales, for which the key assumption of steady-state convection breaks down. We compare in Ch. 8 two different approximate models for the convective acceleration, and find that the amount of mass lost to pulses at the lowest-mass end of the helium core mass range for pair instability is sensitive to the treatment of convection before and during the pulses. This, however, does not invalidate the main result of Ch. 6, since the maximum BH mass obtained in both cases is the same.

1.7 Outlook

This section outlines possible future research directions to build upon the results presented in the following chapters, and it should become clearer after reading the rest of this thesis.

1.7.1 Is there a "massive runaway origin" problem?

The classical work of Blaauw (1961) analyzed O- and B-type stars and called those in the tail of the spatial velocity distribution "runaway stars". Since then, the term has also be used to designate fast-moving pulsars and X-ray binaries, for which the observational selection effects are generally different. Here, I limit the discussion to non-degenerate massive stars, but complementary information about the processes governing the evolution and explosion of the progenitor systems can be obtained by looking at compact objects.

Blaauw (1961) found that these runaway stars were on average more massive than kinematically normal stars, and typically single (see also Bekenstein & Bowers 1974). The sample completeness at the time did not allow to quantify the relative population of runaways per each spectral type.

The fraction of O-type stars that have since been classified as runaways is significant, sometimes as high as $\sim 10 - 20\%$, although the literature is not uniform in the kinematic criteria adopted to call a star a runaway (see also below).

As briefly explained in Sec. 1.2, there are two known mechanisms to accelerate massive stars and make them runaways: the disruption of a binary system by a SN explosion (Blaauw 1961) and the dynamical ejection from a cluster (Poveda et al. 1967). One long-standing question is what is the relative efficiency between these two mechanisms or, in other words, which produces more runaway stars (e.g., in the Galaxy, or in a particular association).

The seminal work of Hoogerwerf et al. (2001) addressed this question and, albeit based on a limited sample of runaways that could be associated with observed pulsars, they concluded that 2/3 of the massive O-type runaways should have a binary origin.

One of the main results of Ch. 3 is that the disruption of massive binary systems by a stellar explosion cannot reproduce the observed runaway fraction among O-type stars: regardless of the parameter variations considered, and assuming a constant star formation rate, the runaway fraction we obtain is $0.5^{+2.1}_{-0.5}$ %. Other population synthesis results obtained using either semi-analytic models for the stellar and binary evolution (e.g., De Donder et al. 1997; Kochanek et al. 2019) or stellar structure and evolution codes (Eldridge et al. 2011) agree with this conclusion. Therefore, the observed runaway fraction among O-type stars and the conclusions that most should have a binary origin appear to be inconsistent with the predictions of binary evolution theory. While the solution of this apparent problem is not known, it is already possible to list caveats that might solve it or make it disappear:

• First of all, the short lifetime of massive stars make the runaway fraction sensitive to the details of the star formation history. It is possible that the assumption of a constant

star formation history is not appropriate to model populations including a large fraction of runaways;

- The literature is not uniform in the effective definition of runaway star. Some authors consider any massive star far above the Galactic plane to be a runaway, even without a direct measurement of their velocity (e.g., Leonard 1991). Sometimes, only one component of the stellar velocity is accessible, either the one along the line of sight (radial velocity, e.g., Evans et al. 2010), or the projection on the sky (proper motion, see e.g., Ch. 4). Finally, the minimum velocity cut is sometimes obtained from fitting functions to a distribution, or arbitrarily defined somewhere between 25 km s⁻¹ $\leq v_{min} \leq 40$ km s⁻¹ (see also Ch. 3), but most importantly the frame of reference adopted to infer the velocity is not consistently chosen (Galactic frame, parent cluster center of mass, heliocentric, etc..);
- Many observational biases favor the detection of fast and isolated massive stars, while they disfavor finding slow massive stars that would only contribute to the normalization of the runaway fraction. For example, the motion of the runaways is likely to bring them out of the Galactic plane, and out of their dusty formation regions, making them more easily visible (e.g., Maíz Apellániz et al. 2018);
- The result from Hoogerwerf et al. (2001) was more recently questioned by the reanalysis of Jilinski et al. (2010). The latter authors found that some of the stars considered to be runaways by Hoogerwerf et al. (2001) are instead members of a binary system, and thus the large radial velocity measured by Hoogerwerf et al. (2001) was due to the orbit, rather than a spatial velocity. If it is not correct that 2/3 of the massive runaways should come from binaries, the problem regarding their origin can be solved by invoking a larger contribution from dynamical ejections;
- Last but not least, results from the second *Gaia* data release suggest that dynamical interactions are very efficient at ejecting even their most massive members (Drew et al. 2018; Lennon et al. 2018; Kalari et al. 2019, see also Ch. 4), although more systematic studies are needed to quantify the efficiency of dynamical ejections.

If no combination of these factors can solve the apparent discrepancy between the observed kinematics of massive stars and binary evolution theory, and no other mechanism to accelerate massive stars is found, then the most natural possibility is that our current understanding of massive binaries neglects some angular momentum loss process in the orbital evolution. This would have important consequences also for byproducts other than runaways, such as X-ray binaries and gravitational wave sources.

If instead a combination of these factors can solve the discrepancy, it will become clearer once the full astrometric dataset from the *Gaia* satellite is available. Although *Gaia* will not provide radial velocities for massive stars (cf. Sec. 1.5), it will make it possible to identify potential clusters and association from which fast-moving massive stars might originate

(Bekenstein & Bowers 1974). These should be possible to find since the lifetime of massive stars is short enough that they cannot get so far from their birth location (see also Ch. 3), and they define a physically meaningful frame of reference to calculate the peculiar velocity of each massive star considered. Moreover, the age of the most likely parent association would give a direct constraint on the ejection mechanisms.

Coupling *Gaia* to spectroscopic follow up (e.g., *Gaia*/ESO survey in the southern hemisphere, e.g. Gilmore et al. 2012) will also allow for the distinction of stars that have been ejected from a binary from those ejected from a cluster. The former are predicted to accrete mass from the companion before the binary is disputed, which should leave observable signatures on the star ejected (although see also McEvoy et al. 2017 for caveats). Conversely, stars that have been ejected from clusters are not expected to carry signatures of previous binary interactions: the cross-section for dynamical interactions increases with the orbital separation, therefore wider binaries will interact more and more often eject one of their member stars.

The combination of precise astrometry and spectral characterization might also allow one to find all the slow-moving walkaway stars ejected from binaries, which constitute one of the most common outcomes of massive binary evolution. Such a population would be ideal to study the physics of mass accretion on non-degenerate stars (and its orbital consequences), and constrain binary evolution processes using a population of common outcomes rather than more exotic and rare byproducts. Identifying a sufficient number of post-mass transfer widowed stars that have been separated by a compact object might allow to put statistical constraints on the amplitude of BH kicks without ever seeing the BHs or the events associated with their formation (Ch. 3).

1.7.2 Mass loss events and detailed simulations

A large portion of this thesis is dedicated to some of the possible mass loss processes that a massive star can encounter in its life. As mentioned in Sec. 1.3.1 and more extensively in Ch. 2, even the less extreme form of massive-star mass loss (in terms of \dot{M}), the stellar wind, has been a longstanding problem in stellar astrophysics.

On top of the computational advances that will make studying the line-driving mechanism more tractable, one interesting way forward that is being taken recently is to combine observations of the stars themselves with constraints from their immediate surroundings or environment. For example, infrared signals from bow shocks surrounding runaway stars (cf. Fig. 1.2) can be used to constrain the wind momentum (e.g., Gull & Sofia 1979; Kobulnicky et al. 2019), X-rays from an accreting compact object can be used to study the wind structure around the donor star of X-ray binaries (e.g., El Mellah & Casse 2017), and interactions of the SN shock with pre-existing shells of material around the star can be used to probe late mass loss events (e.g., Morozova et al. 2017). We discuss these possibilities more extensively in Ch. 2. Following the general idea to couple together observations of the stars with constraints from their surroundings, Beasor & Davies (2018) recently analyzed the mass-loss rate of massive RSGs. By narrowing their targets to stars in clusters, these authors were able to constrain not only their mass-loss rate, but also to relate it to the mass of the stars themselves. By investigating two different clusters with different turn-off masses they were able to see how the wind mass loss rate of red supergiants might evolve in time. In this case, progress was made by combining the constraints from the cluster membership (loosely speaking "the surroundings") with infrared observations of the stars.

The other mass loss process central to this thesis are pulsational pair-instability driven mass ejections. As discussed in Sec. 1.3.4, and more extensively in Ch. 5-8, there has been a recent surge in interest about the evolution of very massive stars through the pair-instability, driven by the detection of very massive BHs through gravitational-wave mergers, and the present and upcoming efforts in time-domain astronomy.

Nevertheless, all the theoretical predictions available are based on calculations of the evolution of single massive stars (Woosley et al. 2007; Chatzopoulos & Wheeler 2012a; Yoshida et al. 2016; Woosley 2017; Leung et al. 2019) or possibly single naked helium cores, sometimes interpreted as a proxy for post-mass transfer donors, (e.g., Woosley 2019, see also Ch. 5–8). Simulations of post-merger structures up to the onset of the instability are also available (see, e.g., Vigna-Gómez et al. 2019), but these simulations do not compute the pair-instability evolution itself. Nevertheless, real progenitor systems of gravitational-wave merger events are most likely to evolve in binaries, which opens up a variety of evolutionary scenarios, both for the donor and the accretor star. In particular, to the best of my knowledge, no study has yet investigated the evolution of the accretor star in binary systems through pulsational pair-instability. The increase of its total mass during the mass transfer also drives an increase in its helium core mass (e.g., Neo et al. 1977; Schneider et al. 2016). It is possible that in very massive binary systems where both stars are initially at the edge of the pair-instability regime, the donor star avoids this fate by losing mass, and only the accretor experiences pulsations.

Useful predictions accounting for binary effects in post-processing can be made starting from single-star models (see for example Ch. 5). However, the self-consistent simulation of binary evolution and how it can modify the internal structure of a star before and during the pulses is an effort that will aid using observations from the third observing run of LIGO/Virgo to better understand the physics of the most massive stars and the formation of BHs.