A systematic study of super-Eddington envelopes in massive stars

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ABSTRACT

Proximity to the Eddington luminosity has been attributed as the cause of several observed effects in massive stars. Computationally, if the luminosity carried through radiation exceeds the local Eddington luminosity in the low-density envelopes of massive stars, it can result in numerical difficulties, inhibiting further computation of stellar models. This problem is exacerbated by the fact that very few massive stars are observed beyond the Humphreys-Davidson limit, the same region in the Hertzsprung–Russell diagram where the aforementioned numerical issues relating to the Eddington luminosity occur in stellar models. Thus 1D stellar evolution codes have to use pragmatic solutions to evolve massive stars through this computationally difficult phase. In this work, we quantify the impact of these solutions on the evolutionary properties of massive stars. Using the stellar evolution code MESA with commonly used input parameters for massive stellar models, we compute the evolution of stars in the initial mass range of 10−110 M⊙ at one-tenth of solar metallicity. We find that numerical difficulties in stellar models with initial masses greater than or equal to 30 M⊙ cause these models to fail before the end of core helium burning. Recomputing these models using the same physical inputs but three different numerical methods to treat the numerical instability, we find that the maximum radial expansion achieved by stars can vary by up to 2000 R⊙ while the remnant mass of the stars can vary by up to 14 M⊙ between the sets. These differences can have implications on studies such as binary population synthesis.

Key words: stars: massive – supergiants – stars: evolution – stars: black holes – gravitational waves

1 INTRODUCTION

Stars more massive than about 9 M⊙ are key to several astrophysical processes. During their lives, they enrich their surroundings with ionising flux and nuclear processed material while altering the dynamics of their host systems. At the end of their lives, these massive stars again expel copious amount of radiation and metal-rich matter in the form of supernovae, leaving behind compact remnants: neutron stars and black holes. Furthermore, mergers of these compact remnants result in gravitational wave (Abbott et al. 2016, 2017) emission and can also lead to the formation of rare elements (Kasen et al. 2017). Therefore, a better understanding of how these stars evolve is crucial in comprehending their contribution to the evolution of star clusters and galaxies.

The evolution of massive stars is typically modelled using one-dimensional (1D) stellar evolution codes. In the last few decades, these stellar evolution codes have progressed a lot and so has our understanding of massive stars. Together with the advances in our observing capabilities (Evans et al. 2011; Simón-Díaz et al. 2015; Wade et al. 2014; Abbott et al. 2016), the development of sophisticated numerical methods for simulating physical processes and newer input data in the form of opacity tables and nuclear reaction rates has led to the development of modern and improved stellar structure and evolution codes (Langer 2012; Ekström et al. 2020).

Even with these new capabilities, 1D modeling of massive stars is limited by a number of approximations. Several evolutionary properties of massive stars such as the mass-loss rates (Smith 2014; Renzo et al. 2017), nuclear reaction rates (Heger et al. 2002; Fields et al. 2018) and rotation (Heger et al. 2000; Maeder 2009) remain uncertain. The high mass of these stars makes it feasible for sophisticated physical process to operate in these stars but their short lives makes it difficult to obtain observational constraints.

One such process is the treatment of convective transport of energy through the Mixing Length Theory (MLT: Böhm-Vitense 1958). In this theory, energy is transported through fluid elements supported by buoyancy forces. These elements travel over a radial distance known as the mixing length after which they dissolve in their surroundings. MLT assumes hydrostatic equilibrium in stars, meaning no acceleration of particles and depends only on local conditions (i.e., local values of pressure, density etc.), without taking into account other parts of the star. Time-dependency and non-local treatments are included through ad-hoc methods such as convective overshoot, semiconvection and diffusion (e.g., Renzini 1987; Kippenhahn et al. 2012).
The simplicity of MLT makes it a popular choice for many stellar evolution codes. However, in the low-density envelopes of massive stars, convection as given by MLT is inefficient. Changes in the elemental opacity as the star evolves can cause the radiative luminosity to exceed the Eddington-luminosity and lead to the formation of density and gas pressure inversions in the sub-surface layers. The presence of density inversions has been attributed as the source of several instabilities such as the dynamical instability (Stothers & Chinn 1993), the convective instability (Langer 1997), and the strange-mode instability (Saio et al. 1998, 2013) in massive stars. Observationally, these have been linked to stellar variability phenomena such as stochastic low-frequency photometric variability (Pedersen et al. 2019; Bowman 2020), spectroscopic macroturbulence (Simón-Díaz & Herrero 2014; Simón-Díaz et al. 2017) and episodic mass ejection behaviour in luminous blue variables (LBVs: Bestenlehner et al. 2014; Gräfener 2021).

From a numerical perspective, the presence of density inversions in the inflated envelopes of supergiant stars requires 1D stellar evolution codes to take prohibitively short time-steps (of the order of hours and minutes) leading to convergence issues (Maeder 1987; Aloni et al. 1993; Paxton et al. 2013). Evolving stars past these numerical difficulties in the supergiant phase has been a long standing challenge for the 1D stellar evolution approach. As shown in Agrawal et al. in prep (hereafter Paper I), stellar evolution codes often resort to numerous pragmatic methods to evolve stars such as enhancing the convective efficiency (e.g. Ekström et al. 2012) or limiting temperature gradients such that the density gradient is always positive (e.g. Chen et al. 2015). While these methods help evolve stars through numerically difficult phases of evolution, they can also modify their surface behaviour, such as the radius evolution and mass-loss rates.

The different methods used by 1D codes and their interplay with other physical parameters of massive stars can alter the dynamics of stellar evolution, thereby adding a potential bias to any study aiming to determine the properties of these input parameters from the evolution of a star. While other uncertainties in the evolution of massive stars have received considerable attention in a number of studies, the role of density inversions has not been explored to the same extent.

In Paper I, the comparison of stellar models from five different codes revealed large differences in the evolutionary behavior of stars more massive than 40 $M_\odot$ around solar metallicity (at Z = 0.014). The maximum radial expansion predicted by different stellar models varied by more than 1000 $R_\odot$ and the predictions of remnant mass varied by 20 $M_\odot$. However, the stellar models also had different physical inputs beside the treatment of density inversions arising due to the Eddington luminosity, making it difficult to untangle the impact of this process from other inputs. There is therefore a need for a systematic study of the impact of these methods within a single code and single set of assumptions.

In this work, we perform a study of the impact of density inversions on the evolution of massive stars up to 110 $M_\odot$ using consistent input parameters. Since Paper I focused only on solar metallicity stars, we choose a metallicity ten times lower than solar here to demonstrate the impact of density inversions at a metallicity relevant to the progenitors of current gravitational wave observations (e.g., Stevenson et al. 2017). As we show here, the different methods used by 1D codes can have a non-negligible impact on the evolutionary properties of massive stars. These differences are important, as they can help us explain the formation of gravitational wave progenitors and other observations of stellar populations.

2 PHYSICS OF DENSITY INVERSIONS IN MASSIVE STARS

In this section, we describe the conditions for the formation of density and gas pressure inversions in stellar envelopes and their impact on modelling the evolution of massive stars.

For a spherically symmetric star containing mass $m(r)$ inside radius $r$ and with radiative opacity $\kappa(r)$ and density $\rho(r)$, the luminosity that can be carried by radiative transport of energy is given by

$$L_{\text{rad}}(r) = -\frac{4\pi r^2 c}{\rho(r) \kappa(r)} \frac{dP_{\text{rad}}}{dr},$$

where $P_{\text{rad}}$ denotes the radiation pressure and $c$ is the speed of light.

The Eddington luminosity gives the maximum value of luminosity that can be transported by radiation while maintaining hydrostatic equilibrium (Eddington 1926). The expression for the Eddington luminosity is given by

$$L_{\text{Edd}}(r) = \frac{4\pi c G m(r)}{\kappa(r)},$$

where $G$ represents the gravitational constant. The total pressure $P$ in the star is the sum of the radiation pressure, $P_{\text{rad}}$ and the gas pressure $P_{\text{gas}}$. Using equations 1 and 2 and the equation of hydrostatic equilibrium $dP/dr = -Gm(r)\kappa(r)/r^2$, the ratio of radiative luminosity to the Eddington luminosity can be defined as

$$\frac{L_{\text{rad}}}{L_{\text{Edd}}} = \frac{dP_{\text{rad}}}{dP} = \left[1 + \frac{dP_{\text{gas}}}{dP_{\text{rad}}}\right].$$

Normally, the luminosity transported by radiation ($L_{\text{rad}}$) is less than the Eddington-luminosity ($L_{\text{Edd}}$) inside a star, and the density and gas pressure of stellar material decrease with the stellar radius ($dp/dr < 0, dP_{\text{gas}}/dr < 0$). However, during the evolution of the star, changes in the elemental ionisation states can lead to an increase in the opacity $\kappa(r)$. In the low density ($\rho \ll 1$ g cm$^{-3}$) radiation pressure dominated ($P_{\text{rad}}/P \approx 1$) envelopes of massive stars, an increase in opacity can reduce the Eddington luminosity below the radiative luminosity ($L_{\text{rad}}/L_{\text{Edd}} < 1$). Since $dP_{\text{rad}}/dr$ is always less than 0, when $L_{\text{rad}}/L_{\text{Edd}} < 1$ Equation 3 implies $dP_{\text{gas}}/dr > 0$ i.e., a gas pressure inversion.

From the ideal gas equation of state, $P_{\text{rad}}$ can be expressed as a function of $\rho$ and $P_{\text{rad}}$. Using Equation 3, the condition for density inversion ($dp/dr > 0$) can therefore be written as

$$\frac{L_{\text{rad}}}{L_{\text{Edd}}} > \left[1 + \left(\frac{dP_{\text{gas}}}{dP_{\text{rad}}} \right) \rho\right]^{-1}$$

(Joss et al. 1973; Paxton et al. 2013).

The effect of density inversions on the evolution of massive stars is complex and remains an active field of research (Mihalas 1969; Éragna 1971; Langer 1997; Owocki et al. 2004; Cantiello et al. 2009; Sanyal et al. 2015). Gräfener et al. (2012) found that an increase
in the radiative luminosity near the opacity peak due to the iron-group elements (at \( \sim 2 \times 10^3 \) K) leads to the formation of an ‘inflated envelope’ containing density inversions (also see Ishii et al. 1999; Petrovic et al. 2006). In this state, the star has an extended radiative envelope with a relatively small convective core. As pointed out by Sanyal et al. (2015), these inflated stars are different to classical red supergiants, as envelope inflation does not require hydrogen shell burning and can even occur while the star is on the main sequence.

For hydrogen-rich stars, the formation of the inflated envelope reduces the opacity and therefore the radiative luminosity, driving down \( L_{\text{rad}} / L_{\text{Edd}} \). However, as the envelope expands, its outer layers become sufficiently cool to encounter opacity bumps due to helium ionization (at \( \sim 2 \times 10^4 \) K) and hydrogen recombination (at \( \sim 10^4 \) K) and further expansion no longer reduces \( L_{\text{rad}} / L_{\text{Edd}} \).

The presence of density inversions in the inflated envelopes makes it difficult to match solutions of stellar structure equations in the envelope (Maeder 1987, 1992). The combination of low gas pressure and the high entropy at the base of the inflated envelope leads to numerical difficulties if time-steps are large (Paxton et al. 2013). To avoid these difficulties, stellar evolution codes are forced to adopt exceedingly small time-steps and struggle to complete the evolution of these stars.

### 3 STELLAR MODELS: THE STANDARD SET

Module for Experiments in Stellar Astrophysics (MESA: Paxton et al. 2011, 2013, 2015, 2018, 2019) is an advanced one dimensional stellar structure and evolution code. MESA solves the coupled differential equations of stellar structure simultaneously with the energy transport equation (see Paxton et al. 2011, 2013, 2015, 2018, 2019). The set of models evolved using the physical inputs described above in our models to closely follow the evolution of massive stars. The network has been chosen to match globular cluster observations and has 72 elements, including Mg, Li and Fe. The reaction rates are determined using the Jina Reaclib database (Cyburt et al. 2010).

We use high spatial resolution with \( \text{mesh\_delta\_coeff} = 0.5 \) and the maximum relative cell size \( \text{max\_dq} = 5 \times 10^{-4} \). Model to model structure variation is kept modest with \( \text{var\_control} \) between \( 7 \times 10^{-4} \) and \( 10^{-3} \), and additional constraints are used to limit time steps where necessary.

We compute the evolution of stars in the mass range of 10–110 \( M_\odot \) at metallicity, \( Z = 0.00142 \) ([Fe/H] = -1). All stars start from the pre-main-sequence (PMS) with uniform composition and the goal is to evolve each model until the point of carbon depletion in the core (\( X_C < 10^{-2} \)). Following Choi et al. (2016), we adopt solar scaled abundances from Asplund et al. (2009), with Solar metallicity \( Z_\odot = Z_{\odot,\text{protosolar}} = 0.0142 \). The primordial helium abundance \( Y_p \) is taken to be 0.249 while the protosolar helium abundance \( Y_{\odot,\text{protosolar}} = 0.2703 \). Initial hydrogen (X) and helium abundances (Y) for PMS models are calculated using the following formula

\[
Y = Y_p + \left( \frac{Y_{\odot,\text{protosolar}} - Y_p}{Z_{\odot,\text{protosolar}}} \right) Z, \tag{5}
\]

\[
X = 1 - Y - Z. \tag{6}
\]

Models are evolved without mass loss from the PMS until the zero-age main sequence (ZAMS), defined as when the central hydrogen abundance reduces by 1 percent of the initial value. Evolution is then restarted (including mass loss) using the stellar model saved at ZAMS, and continues until either the termination condition is reached (\( X_C < 10^{-2} \)) or the end of 96 CPU-hrs (running parallel on 4 cores for 24 hrs).

#### 3.1 Results

The set of models evolved using the physical inputs described above fail to reach the end of carbon burning in the core within the allocated time (24 hrs) for stars more massive than 20 \( M_\odot \). Hereafter, we refer to this set as the ‘standard set’ and label it as ‘NoModifier’ in the figures, since the models were computed without any modifications to facilitate their evolution. The results for the standard set are unaffected by the increase in temporal and spatial resolution.

Figure 1 presents the stellar tracks in the Hertzsprung-Russell (HR) diagram for our standard set of models. In the left panel, the tracks are coloured by the maximum of \( L_{\text{rad}} / L_{\text{Edd}} \), while the right panel shows the minimum of \( P_{\text{gas}} / P_{\text{total}} \) for each stellar model. We see that in these models \( L_{\text{rad}} \) can become close to \( L_{\text{Edd}} \) and even exceed it by factors of a few during the evolution as the stars encounter opacity bumps in their envelopes. These opacity bumps are due to the partial ionisation states of iron and helium, as well as the recombination of hydrogen. However, for 10 and 20 \( M_\odot \) stars, \( P_{\text{gas}} / P_{\text{total}} \) remains high enough (>0.5) for their evolution to proceed uninterrupted (see Section 2).

Models with initial masses between 30 and 110 \( M_\odot \) fail during core helium burning at similar effective temperatures, \( \log T_{\text{eff}} / K \approx 3.7 \). In these models, the stellar envelope inflates in response to the iron-opacity peak, thereby preventing density inversion. However, as the star expands and cools, the minima in gas pressure fraction at the opacity peak decreases as highlighted in the right panel of Figure 1. The evolution of these models progresses smoothly until stars encounter the opacity peak due to hydrogen and helium in their subsurface layers at \( \log T_{\text{eff}} / K \approx 4.0 \). The envelope inflation there is
### Figure 1.
Hertzsprung-Russell (HR) diagram showing stellar models from the standard set coloured by the maximum of $L_{\text{rad}}/L_{\text{Edd}}$ (left panel) and the minimum of $P_{\text{gas}}/P_{\text{total}}$ (right panel). The blue cross marks the end of core hydrogen burning and the red cross marks the end of core helium burning (where applicable). The brown dashed line in the left panel denotes the position of the observational Humphreys & Davidson (1979) limit beyond which few stars are observed, while the grey dashed line signifies the luminosities of the brightest red supergiants as inferred by Davies et al. (2018). Density inversions in the envelopes of stars with initial masses $30 \, M_\\odot$ and above causes the evolution of these stars to become halted at $\log T_{\text{eff}}/K = 3.7$, and their models fail to finish core carbon burning.

### Figure 2.
Temperature profile of a $110 \, M_\\odot$ star at the ZAMS evolved using the standard set. Opacity peaks due to partial ionisation states of iron are present at $1.5 \times 10^3$ and $1.8 \times 10^3 \, K$. However, $L_{\text{rad}}$ is less than $L_{\text{Edd}}$ throughout the star and the evolution of the star proceeds smoothly. See Section 3.1 for details of each panel.

### Figure 3.
Temperature profile of a $110 \, M_\\odot$ star at the end of the simulation, evolved using the standard set. Vertical black dotted line marks the boundary of the helium core. The high luminosity of the star combined with the peak in opacity due to hydrogen and helium ionisation around $10^3 \, K$ causes $L_{\text{rad}}$ to exceed $L_{\text{Edd}}$. This causes density and gas pressure inversions at $3 \times 10^3 \, K$. However, the low-density of the environment renders convection inefficient and the star struggles to evolve despite reaching supersonic convective velocities.
not sufficient to prevent the radiative luminosity from exceeding the Eddington luminosity, which leads to the density inversions.

To elaborate on the conditions in the stellar interior, the temperature profiles for a 110 $M_\odot$ star at the ZAMS (at log$_{10}$Teff/$K = 4.77$), and at the end of the track (at log$_{10}$Teff/$K = 3.72$, corresponding to the final model reached after 24 hrs of computation), are shown in Figure 2 and Figure 3.

In panel (a) of Figure 2, $L_{\text{rad}}$ shows a small increase corresponding to the opacity peaks due to partial ionisation of iron at $1.5 \times 10^9$ and $1.8 \times 10^5$ K (panel b). In response to the increase in $L_{\text{rad}}$, gas pressure dips a little (visible as a minimum in $P_{\text{gas}}/P_{\text{total}}$ in panel c), although, density consistently decreases outwards (shown in panel e). The bottom panel (g) shows the variation of the actual temperature gradient and the adiabatic temperature gradient inside the star. Their difference, $\nabla_T - \nabla_{\text{ad}}$, is known as superadiabaticity (see Section 4.3 for details). At the location of the opacity peak, superadiabaticity is positive but small and the convective velocity ($v_{\text{conv}}$) is less than the sound velocity ($v_{\text{sound}}$) (panel f), signifying efficient convection. The specific entropy ($S/NABr$) in panel (d) at the base of the convective region is small and the evolution of the star proceeds smoothly.

In panel (b) of Figure 3, in addition to the iron opacity peak, opacity peaks corresponding to partial ionisation of helium and hydrogen recombination can be seen at $3.5 \times 10^4$ and $10^4$ K. In contrast to Figure 2, the increase in opacity due to hydrogen and helium ionisation increases $L_{\text{rad}}$ such that it exceeds $L_{\text{Edd}}$ by more than a factor of two, causing density and gas pressure inversion that can be seen in the other panels. However, the high value of superadiabaticity ($\nabla_T - \nabla_{\text{ad}} \approx 10$) renders convection inefficient and prone to radiative losses. The convective velocity increases to increase the amount of flux convection can carry, becoming more than the local sound speed. However, the high value of specific entropy ($S/NABr \geq 300$) at the base of the convective envelope causes time-steps to be small, of the order of days.

The evolution of the star is essentially halted until it is able to get rid of the density inversion as mass loss slowly chips away the outer convective layers. However, evolving the star this way requires a lot of computational time (e.g., it takes $\approx 200$ CPU-hrs for a $40 M_\odot$ star) which might not be feasible.

4 STELLAR MODELS: THE MODEL VARIATIONS

In the absence of efficient convection, the radiation dominated envelopes of massive stars in 1D modelling are prone to numerical difficulties (Stothers & Chin 1979; Maeder 1987). Therefore, stellar evolution codes adopt various techniques to compute the evolution of massive stars beyond these numerically difficult points (Aloni et al. 1993; Ekström et al. 2012; Paxton et al. 2013). The exact technique differs from code to code, however, they can be summed up into the three main categories: using higher mixing length to increase the efficiency of the mixing process, using higher mass-loss rates to remove layers with numerical instabilities, or suppressing the numerical instability by limiting the temperature gradient and thereby suppressing density inversions. We explore each of them in details in the following subsections.

4.1 Enhancing internal mixing

In the convective transport of energy by MLT, the mixing length, $l$ travelled by a fluid element before dissolving in the surroundings is given in terms of the local pressure scale height $H_p$ and mixing length parameter $\alpha_{\text{MLT}}$ such that $l = H_p \times \alpha_{\text{MLT}}$. For a given $H_p$,
a higher value of $\alpha_{\text{MLT}}$ implies a higher $\ell$ and therefore better convective efficiency. $\alpha_{\text{MLT}}$ is a free parameter with a value that is often calibrated from the observations of the sun and eclipsing binaries. For example, in the standard set of models in this work the value of $\alpha_{\text{MLT}}$ has been calculated using solar data (see Choi et al. 2016, for details). There is increasing evidence that the value of $\alpha_{\text{MLT}}$ is not universal and varies with the evolutionary phase, mass and metallicity of the stars (Joyce & Chaboyer 2018; Johnston 2021).

While MLT gives fairly good results in the deep interiors of stars where density is high and convection is nearly adiabatic (with negligible radiative losses), its limitations start becoming apparent in low-density environments where the convection is highly superadiabatic and prone to radiative losses (Maeder 2009). In the presence of density inversions, convective velocity becomes supersonic and convection is time-dependent. In such situations both standard and non-adiabatic theories of MLT are out of their domain of applicability.

While testing the models with a different theory of convective energy transport is beyond the scope of this work, we do test the role of increased efficiency of convection on the convergence properties of the models from the standard set that fail to reach the end of carbon burning. Beginning with $\alpha_{\text{MLT}} = 1.82$ (used in the standard set), we compute a series of stellar models with $\alpha_{\text{MLT}} = 3.0, 3.64, 4.0, 5.0, 5.46, 7.28, 8.0$ for stars with initial mass 30 $M_\odot$ and above. We find that for $\alpha_{\text{MLT}} \geq 5.46$, which is three times the value used in the standard set, the models are able to evolve without any numerical instabilities until carbon depletion in the core.

The top panel of Figure 4 shows the evolutionary tracks evolved with $\alpha_{\text{MLT}} = 5.46$. From the figure we see that $L_{\text{rad}}$ still exceeds $L_{\text{Edd}}$ in the stellar envelope, however, this does not limit the time-steps of the computation of the stellar models. The reason for this can be understood from Figure 5, where we show the temperature profile of a 110 $M_\odot$ star at a similar location in the HR diagram where the computation for the 110 $M_\odot$ star from the standard set became stuck. Similar to Figure 3, the stellar profile contains opacity peaks due to ionisation of iron, helium and hydrogen (panel b), resulting in excess $L_{\text{rad}}$ (panel a) and the density and gas pressure inversions (panel c and e). However, higher convective velocities resulting from higher $\alpha_{\text{MLT}}$ imply that the convective fluid element travels faster and transports more energy before it leaks out due to radiative losses. The superadiabaticity in the outer layers is also smaller compared to the standard case ($\nabla_T - \nabla_{\text{ad}} \approx 2$), meaning radiative losses are also smaller. The overall convective flux is, therefore, higher than the standard case. The specific entropy remains small ($S/N_A k_B < 100$) and time-steps large enough to efficiently compute the evolution of the star until the end of carbon burning.

Increasing convective efficiency in this way helps compute the evolution of stars until core carbon burning. However, it also changes the effective temperature of these stars and makes them appear bluer in the HR diagram (Maeder 1987; Kippenhahn et al. 2012). Comparing the tracks with extra mixing (top panel of Figure 4), with the standard set (left panel of Figure 1), we find that stellar models with extra mixing are indeed limited to $\log T_{\text{eff}}/K \approx 3.73$ in the HR diagram which is greater than the minimum $\log T_{\text{eff}}/K \approx 3.63$ reached by models in the standard set. We discuss this further in Section 5.

### 4.2 Enhancing mass loss

Winds of hot massive main-sequence stars are optically thin line-driven winds. Due to their high luminosity, massive stars can generate a high number of photons which can be scattered via ions, transferring momentum with them which then accelerates material outwards that
can escape the gravitational potential of the star. As the star evolves to the cool red supergiant phase, these winds transition to being dust-driven where they are generated by the interaction of photons with dust grains instead of ions. Massive stars can lose a substantial amount of mass through stellar winds, even their entire hydrogen envelope to become naked helium stars. The mass loss in naked helium stars is again driven by radiation pressure and can be higher by a factor of ten or more than their hydrogen-rich counterparts (Smith & Tombleson 2015).

The mass-loss rates for massive stars are highly uncertain (Renzo et al. 2017) and can be affected by instabilities and processes other than described above. For example, Gräfener & Hamann (2008) and Vink (2011) have shown the contribution of optically thick (clumped) winds in the presence of sub-surface opacity bumps in massive stars. Moreover, massive stars exceeding the classical Eddington limit can also experience episodes of much stronger mass-loss rates (up to $10^{-3} \text{M}_\odot \text{yr}^{-1}$), known as LBV eruptions or super-Eddington winds (Lamers & Fitzpatrick 1988; Humphreys & Davidson 1994; Smith et al. 2004). Despite being the stronger contributor to mass-loss rates for massive stars, the exact rates and the mechanism behind the LBV eruptions remains disputed (Puls et al. 2008; Smith 2014; Owocki 2015) and most stellar evolution models often exclude their contributions in the mass-loss rates.

Apart from the uncertainties in the mass-loss rates of massive stars, the differential equations of stellar structure and evolution do not include stellar mass loss. In stellar evolution codes, the mass change at each time step is computed from parameterized algorithms as time-averaged mass loss, before solving the equations of stellar structure. The stellar variables are then adjusted accordingly to account for the mass change. High mass-loss rates can therefore help remove outer layers in the stellar model containing the density inversion, helping the stellar model avoid numerical instabilities (Petrovic et al. 2006; Cantiello et al. 2009).

To determine the impact of enhanced wind mass-loss on the convergence properties of models that fail to evolve in the standard set, we recomputed these models with increased wind mass-loss rates for different evolutionary phases until the models are able to evolve without numerical difficulties. We find that setting the mass loss scaling factor to $\eta_{\text{Dutch}} \geq 8.0$, i.e., at least eight times the mass loss used in the standard set, whenever the stellar luminosity exceeds the Eddington luminosity, leads to smooth evolution of the stellar models with initial mass greater than or equal to 30$\text{M}_\odot$.

We also find that this mass-loss enhancement is only required for stars with a hydrogen-rich envelope ($X_{\text{surf}} \geq 0.4$). Although naked helium stars can also exceed the Eddington-limit and can develop density inversions in their envelopes, their evolution proceeds uninterrupted for our models without any numerical instabilities.

The models with extra mass loss as described above, with $\eta_{\text{Dutch}} = 8.0$, are shown in the middle panel of Figure 4. A 110$\text{M}_\odot$ star with extra mass loss is able to evolve to the end of carbon burning, while the maximum of $L_{\text{rad}}/L_{\text{Edd}}$ remains close to unity throughout the evolution. However, for models less massive than 70$\text{M}_\odot$, the maximum of $L_{\text{rad}}/L_{\text{Edd}}$ can be up to 8, similar to models in the standard set. These values of $L_{\text{rad}}/L_{\text{Edd}}$ do lead to the formation of density inversions, as shown in the temperature profile of the 70$\text{M}_\odot$ star in Figure 6, but enhanced mass-loss rates ($\sim 10^{-4} \text{M}_\odot \text{yr}^{-1}$ at this point) help remove the outer layers containing density inversions before specific entropy at the base of the envelope becomes large or time-steps become too small. Thus, all models are able to evolve smoothly to completion without any numerical instability.

Extra mass loss helps compute the evolution of massive stars all the way through to carbon depletion in their core. However, it also influences the structure and evolutionary properties of the stars as explained in Section 5.

### 4.3 Suppressing density inversions

According to the MLT, convection sets in when the temperature gradient of the surrounding material is greater than the gradient interior to the moving element: $\nabla_T > \nabla_{\text{ad}}$. For convection to transport the maximum possible energy, the element should move adiabatically, i.e. without dissipating energy in the surroundings or $\nabla_T \sim \nabla_{\text{ad}}$.

The difference between $\nabla_T$ and $\nabla_{\text{ad}}$ is termed as the superadiabaticity and is a measure of the efficiency of convection (Maeder 2009; Kippenhahn et al. 2012). For efficient convection, superadiabaticity is positive but close to 0. It means that the element loses hardly any energy as it traverses the mixing length. However, a higher value of superadiabaticity ($\sim 10^{-2}$) implies that the element suffers energy-losses as it travels, and by the time it reaches the end of the mixing length it is left with hardly any energy, thereby, rendering the convective transport of energy quite inefficient.

In the envelopes of massive stars superadiabaticity is the order of unity and the convective transport of energy given by MLT is inefficient, providing fertile ground for density inversions to form and be sustained. Some authors even consider density inversions to be non-physical, possibly an artifact of the MLT and 1D stellar evolution (Ekström et al. 2012) while others consider the possible presence of some unknown mixing mechanism that helps stars get rid of density inversions in nature (Paxton et al. 2013). Either way, since these density inversions are associated with numerical instabilities in the models of massive stars, many stellar evolution codes suppress...
them either by limiting $\nabla T$ or by reducing $\nabla T$ to make it closer to $\nabla ad$. This reduces the superadiabaticity, thereby making convection efficient and helping stellar models overcome numerical instabilities.

MESA uses the latter approach of reducing $\nabla T$ in the stellar envelope through a method known as MLT++. In this method, whenever the superadiabaticity exceeds a pre-defined threshold $\text{grad}_T \text{excess}_f_1$, MESA decreases $\nabla T$ to make it closer to $\nabla ad$. The amount of decrease is given by the combination of the parameter $\text{grad}_T \text{excess}_f_2$ which can be defined by the user, and the parameter $\text{grad}_T \text{excess}_\alpha$ which is calculated based on the the maximum of $L_{rad}/L_{Edd}$ and the minimum of $P_{\text{gas}}/P_{\text{total}}$ (see Appendix A for details). In general, a smaller $\text{grad}_T \text{excess}_f_2$ implies a larger reduction in the superadiabaticity and more efficient convective transport of energy.

We find that using the default values of the MLT++ parameters completely suppresses density inversions but it also gives unrealistic values of luminosity for the most massive stars in our set. Therefore, we test the models in the standard set with different combinations of parameters in MLT++, as described in Appendix A. Compared to the default values of the MLT++ parameters, we find that using a smaller value of $\text{grad}_T \text{excess}_f_2=10^{-1}$, therefore a smaller reduction in the superadiabaticity but occurring more frequently inside the star (with $\lambda_1 = 0.6$ and $\beta_1 = 0.05$) is sufficient for the smooth evolution of the models without any numerical instabilities or inaccuracies.

The stellar models evolved using MLT++ are shown in the bottom panel of Figure 4. The evolutionary paths of models computed with MLT++ are quite similar to models evolved with extra mixing. Although, unlike the models with extra mixing, models with MLT++ are not limited to log$L_{\text{eff}}/K \approx 3.73$ and evolve to lower effective temperatures. The temperature profile of a 110$M_\odot$ star evolved with MLT++ (Figure 7) again shows a similar behaviour compared to the temperature profile of the 110$M_\odot$ star evolved with extra mixing (Figure 5), at similar log$L$ and log$L_{\text{eff}}$. However, MLT++ artificially reduces $\nabla T$, such that the superadiabaticity and the specific entropy at the base of the convective envelope remain small despite having smaller convective velocity compared to the 110$M_\odot$ model with extra mixing.

5 IMPLICATIONS

Each of the three methods described in Section 4 help compute the evolution of massive stellar models in the standard set until the end of carbon burning. However, in the process they also modify the evolutionary pathway of the stars and impact their evolutionary outcome. In this section, we compare the set of stellar models obtained with the minimum numerical enhancement from each method and determine the impact of these methods on the structure and evolution of the massive stellar models.

5.1 Structure of the star

Figure 8 shows the Kippenhahn plot of a 110$M_\odot$ star—depicting regions within the star by mass as a function of time in the period leading up to the end of the run—for each of the models computed with the numerical fixes described in Section 4. The evolution of the 110$M_\odot$ model evolved using MLT++ is similar to the model with extra mixing but quite different to the evolution of the model computed with extra mass loss.

All three models start with a 90$M_\odot$ convective core, (shown by the green hatching) accompanied by a 3$M_\odot$ overshoot region outside the core, (shown by the purple hatching). The convective core decreases in size as the star evolves through the main-sequence.

In models computed with extra mixing and MLT++, thin strips of convection, two close to the surface and the third at about 90$M_\odot$, are formed as the star encounters the hydrogen, helium and iron opacity bumps in the final 10^6 years of its evolution. The envelope inflation due to the iron opacity bump causes the star to become a red supergiant before core hydrogen burning can finish. The star suffers higher mass-loss rates as a red supergiant that can be – seen as a rapid decline in the total mass of the star (black solid line) – until a 60$M_\odot$ helium core is formed – depicted by a blue dotted line in the figure. The star continues to lose mass, as the core helium burning and the hydrogen shell burning ensues, although at a comparatively lower rate. It ultimately loses its envelope to form a naked helium star in the final 10^5 years of its evolution, before finally forming a roughly 50$M_\odot$ carbon core in the end.

In the model computed with enhanced mass loss, mass-loss rates are quite high ($> 10^{-3} M_\odot$ yr^{-1}) during the main-sequence evolution. The convective core shrinks rapidly in response to high mass-loss rates. The star loses its outer layers before any sub-surface convection region can form, becoming a naked helium star shortly after a 50$M_\odot$ helium core is formed. The final product is a 40$M_\odot$ naked helium star with a 35$M_\odot$ carbon core.

The similarities in the evolution of the models using MLT++ and enhanced mixing can be understood as follows. In models with enhanced mixing, convection is already efficient in the core, owing to its high density and increasing $\alpha_{\text{MLT}}$ (and therefore the mixing length) hardly makes any difference. However, the density in the sub-surface of layers of the star can be $\approx 10^{10}$ g cm^{-3} and convection is highly inefficient, therefore increasing $\alpha_{\text{MLT}}$ leads to more efficient convective transport of energy in the stellar envelope.

For models using MLT++ to suppress density inversions, the story is similar. Reducing the temperature gradient (superadiabaticity) prevents radiative losses from the convective cells, making them more efficient at transporting energy. However, near the centre convection is nearly adiabatic and the value of superadiabaticity is small ($<10^{-4}$), therefore MLT++ is not applicable there. Thus models with high $\alpha_{\text{MLT}}$ and MLT++ produce similar core structure.

For models with extra mass-loss the evolution is quite different from the first two cases as the star loses quite a lot of mass even on the main sequence. This same trend continues for the post-main sequence evolution. Therefore, it has the least of both the helium and carbon core masses. Similar to the other two methods, the 110$M_\odot$ model again loses all its envelope and ends up as a naked helium star during the core helium burning phase.

Interestingly, the maximum mass-loss rate encountered by the 110$M_\odot$ star with extra mass loss is lower than the models with enhanced mixing and with MLT++, as shown in Figure 9. However, models with extra mass loss by construction have higher mass-loss rates during most of the main sequence, therefore they become a naked helium star without ever undergoing the red supergiant phase where the peak in mass-loss rates usually occurs (due to the large radius of the star). Models with enhanced mixing and MLT++ lose their envelope later in the evolution as they encounter high mass-loss rates as a red-supergiant and therefore end up with higher total mass compared to the model with extra mass loss.

5.2 Final mass and remnant properties

Massive stars are expected to end their lives in supernovae, leaving behind compact remnants (neutron stars and black holes) in a core-collapse or a pulsational-pair instability supernova or undergoing
Figure 8. Kippenhahn plots showing the structure of a $110M_\odot$ star evolved with enhanced mixing (left), with MLT++ (middle) and with enhanced mass loss (right). The Y-axis represents the mass co-ordinate inside the star while the X-axis represents the time remaining in the life of the star before end of the run is reached. Green, purple and red hatching mark the regions with convection, overshooting and semiconvective mixing, respectively. In all three panels, the helium core boundary is the outermost location where the hydrogen mass fraction is less than 0.01, while the helium mass fraction is $\geq 0.01$, and is represented by the blue dashed line. Similarly, the carbon core boundary is defined as the outermost location where the hydrogen and helium mass fraction are less than 0.01 while the carbon mass fraction is $\geq 0.01$. It is represented as the red dashed line.

Figure 9. Variation in mass-loss rates with time for a $110M_\odot$ star evolved with extra mixing (blue line), extra mass loss (pink line) and with MLT++ (orange line). While the maximum mass-loss rate encountered by the $110M_\odot$ model with extra mass loss is less than the maximum mass-loss rate encountered by the models evolved with the other two methods, it still ends up being the least massive of all in the end. See Section 5.1 for an explanation.

complete disruption in a pair-instability supernova. Their demise as a supernova explosion is also important for modifying the chemical and energy makeup of their surroundings, paving way for the formation of new generations of stars. Furthermore, stellar remnants are important for studies across a wide spectrum. They are the progenitors of X-ray binaries, gamma rays bursts, and compact binary mergers that lead to gravitational waves. Hence, it is important to quantify the differences between the properties of the remnants formed by the massive star models.

There are many prescriptions available in the literature that relate the final properties of the star with the end of supernova explosion (e.g., Eldridge & Tout 2004; O’Connor & Ott 2011; Fryer et al. 2012; Ertl et al. 2016). Here we use the Belczynski et al. (2008) prescription, which is the same as the StarTrack prescription in Fryer et al. (2012), to calculate the mass of the stellar remnants for each set of models. The method uses the total mass and the core mass of the star at the end of carbon burning to calculate the mass of the remnant (we refer the interested reader to Section 6.1 of Agrawal et al. 2020, for further details of the method).

Following Belczynski et al. (2010), we plot the remnant mass of the stars as a function of their initial mass as given by the three sets with numerical enhancements in Figure 10. The top panel of the figure shows the remnant mass of the stars while the bottom panel shows the final total mass of the star and mass of the carbon-oxygen core.

For all the sets of models, the Belczynski et al. (2008) prescription predicts the formation of black holes with masses in the range of $13–50M_\odot$. The difference in the mass of black holes as predicted by each set is less than $2M_\odot$ for stars with initial masses up to $60M_\odot$, with the exception of the $30M_\odot$ star where the model with extra mixing predicts a significantly higher remnant mass ($22M_\odot$ black hole) compared to other two sets ($13M_\odot$ black hole). For stars more massive than $60M_\odot$ the curve diverges rapidly, and the difference between the remnant masses can be up to $14M_\odot$. A similar trend can be seen in the total mass and core masses for each set. For the $30M_\odot$ star, the model with extra mixing predicts a higher final total mass but lower carbon-oxygen core mass compared to the other two sets. This is because a larger mixing length in the model leads to a more compact star with lesser mass loss. Thus, the $30M_\odot$ model is able to retain most of its envelope and ends up with the final total mass of $26M_\odot$. Similarly, the origin of differences in the black hole mass predictions can be traced back to the mass-loss rates experienced by each model which themselves are dependent on the surface properties of the star.

5.3 The maximum radial expansion

Figure 11 shows the maximum radial expansion achieved by the stars during their evolution, computed with the three different numerical fixes. The maximum difference in the maximum radial expansion is $\sim2000R_\odot$ which occurs between models with extra mass loss and models with MLT++, for the most massive $110M_\odot$ star in the set. For models with extra mixing and MLT++ which appear to undergo similar evolutionary paths and final fates, the difference in maximum radial expansion can still be up to $1000R_\odot$, especially for stars in the mass range $30–80M_\odot$. Even for the $110M_\odot$ star, where the
difference between models with extra mixing and MLT++ appears to be the least, the maximum radius can differ by 500 $R_\odot$. This has important implications for the binary evolution of the star, as radial proximity determines the episodes of mass transfer in close binary systems.

These differences in the stellar radii are again the result of the numerical enhancements used in each set. For models with initial masses greater than 60 $M_\odot$ and computed with extra mass loss, high mass-loss rates strip the envelope of the stars before they can become a red supergiant. Thus these stars evolve directly towards the naked helium star phase and show the least radial expansion. For stars with extra mixing, a higher mixing length means the fluid element is more efficient at transporting energy through convection. This decreases the size of the convective cells in the envelope and the model remains more compact and at higher effective temperatures than the models from the other two sets.

An interesting case is presented by models with MLT++ where reducing the temperature gradient can have the same effect as excess envelope mixing (Sabhahit et al. 2021). For stars up to 50 $M_\odot$, models using MLT++ closely mimic the behaviour of models with extra mass loss, although beyond 50 $M_\odot$, the excess envelope mixing in models with MLT++ makes them resemble more closely the models with enhanced mixing.

6 CLUES FROM OBSERVATIONS: THE HUMPHREYS-DAVIDSON LIMIT

It is well established that the evolution of massive stars is highly uncertain. It is riddled with many physical and numerical problems. Therefore the need for numerical fixes arises. To make matters worse, it is difficult to say which method is closer to reality as there is an apparent scarcity of massive stars in the region of the HR diagram where numerical issues with density inversions occur.

First characterised by Humphreys & Davidson (1979), the Humphreys-Davidson (HD) limit defines the region in the HR diagram above log$L/L_\odot = 5.8$ where very few massive stars in the Galaxy have been observed to date. Using recent observations of red supergiants in the Large Magellanic Cloud (LMC) and the Small Magellanic Cloud (SMC), Davies et al. (2018) found the limiting luminosity of the brightest red supergiants to be log$L/L_\odot = 5.5$ in both galaxies, slightly lower than previous studies. The LMC and SMC are lower metallicity environments than the Milky Way, closer to the metallicity used in this work. The findings of Davies et al. (2018) also suggest that the maximum red supergiant luminosity does not vary strongly with metallicity.

While the absence of massive stars as red-supergiants beyond the HD limit may not help trace the exact evolutionary path of massive stars, it does provide an important clue that stars more massive than about 40 $M_\odot$ do not spend much time in the HD region. In recent years, several studies (e.g., Castro et al. 2018; Kaiser et al. 2020; Vink et al. 2021) have tried to constrain the different mixing mechanisms (such as semiconvection, overshooting), mass-loss rates and binary properties of massive stars by using stellar models evolved with different physical inputs to reproduce the HD limit. However, they also employ numerical fixes for instabilities due to density in-
versions to compute the complete evolution of the stellar track. Using these numerical fixes interferes with other physical inputs and adds an implicit bias in the computation of models. As these numerical fixes can be different across different stellar evolution codes, results obtained with them might not reflect the true value of the physical parameter being constrained for the massive stars.

Studies that do not employ any numerical fixes (e.g., Klencki et al. 2018) are usually limited to stars less massive than 30 $M_\odot$ or to the evolutionary phases before numerical instabilities arise in more massive stars. While this helps avoid bias due to numerical methods, it also inhibits exploring the late stage evolution of massive stars, such as the end of core helium burning and beyond. Thereby, affecting the potential studies involving stellar remnants and transients.

Some studies also show that the HD limit can also be reproduced by stellar models by just using these numerical fixes. For example, using just MLT++ as the source of excess envelope mixing in massive stars up to 50 $M_\odot$, Sabhahit et al. (2021) were able to reproduce the lack of massive stellar models beyond the HD limit and the Davies limit at Galactic ($Z = 0.017$), LMC ($Z = 0.008$) and SMC ($Z = 0.004$) metallicity.

Recently, Gilkis et al. (2021) showed that using significantly enhanced mixing parameters in stellar models can reduce the time spent by stars beyond the HD limit. Following Gilkis et al. (2021), in Figure 12 we show the amount of time stars spend beyond the HD limit as a function of initial mass for each of our sets of models. We see that the models computed with extra mass loss spend the least time (except for a 40 $M_\odot$ stellar model) while most of the massive stars computed with enhanced mixing and MLT++ can spend between $2 \times 10^5$ and $4 \times 10^5$ years in the HD region. Therefore, models with extra mass loss may appear to be closest to observations (or lack of observations) of massive stars. This, however, has serious implications for gravitational wave observations, as the maximum black hole mass predicted by this set of the model is just 35 $M_\odot$ (see Figure 10).

To unravel this problem, we plot the evolutionary tracks, colored according to the mass-loss rates, from the set computed with the extra mass loss in Figure 13. Despite the enhancement near the Eddington-limit, the maximum mass-loss rates for models with enhanced mass loss seem to be consistent with the typical mass-loss rates for massive stars (Smith 2014). The maximum mass-loss rate of $1.8 \times 10^{-3} M_\odot$ yr$^{-1}$ is experienced by stars in the 40–60 $M_\odot$ mass range during the red supergiant phase of their evolution. However, these rates only last for a maximum of $7 \times 10^3$ yrs. For stars more massive than 60 $M_\odot$, the maximum mass-loss rates are an order of magnitude lower, about $3 \times 10^{-4} M_\odot$ yr$^{-1}$, and last between $3 \times 10^2$–$2 \times 10^4$ yrs. The lower mass-loss rates encountered by more massive stars are a consequence of the enhanced mass loss during their main-sequence evolution. These stars experience mass-loss rates of about $10^{-5} M_\odot$ yr$^{-1}$ for more than $3 \times 10^5$ years. Therefore, they lose a significant portion of their envelope while on the main-sequence and do not undergo the red-supergiant phase of evolution.

Whether massive stars can retain these high mass-loss rates for prolonged periods of time is currently questionable. Moreover, several authors have recently argued that mass-loss rates for massive stars should be lower, rather than higher, than what is commonly used in computing massive single star models (e.g., Beasor et al. 2020; Vink & Sander 2021). Interaction with a companion in a binary system can lead to higher mass-loss rates, but again the smaller radii predicted by these models (Figure 11) makes binary interactions less likely. Therefore, the validity of mass-loss rates in models computed with extra mass-loss, or in general any of numerical fixes used by the codes cannot be ascertained at present.

Mixing process such as rotation, semiconvection and overshooting have also been shown to have large impact on the red supergiant phase of evolution for massive stars and on the reproducibility of the HD limit (Schootemeijer et al. 2019; Higgins & Vink 2020; Gilkis et al. 2021; Sabhahit et al. 2021). Further, many studies suggest that magnetic fields can have a significant effect on the sub-surface convection regions of the stars and hence on the density inversions. For example, Jiang et al. (2018) have shown that the turbulent velocity fields around the iron opacity peak can be escalated in the presence of magnetic fields. We have not explored the role of semiconvection, rotation, magnetic fields and binarity in this work, each of which we acknowledge can have a significant impact on the evolution of massive stars. Evolving massive stellar models with these properties is important and will be a part of future work.
7 CONCLUSION

In this work, we performed a systematic study of the impact of the Eddington limit and the subsequent density inversions on computing the evolution of massive stars with the 1D stellar evolution code MESA. Using commonly used input parameters for massive stellar models, we compute the non-rotating evolutionary tracks of 10–110 M\(_\odot\) stars for \(Z = 0.00142\). Models with initial masses between 30 and 110 M\(_\odot\) in this standard set fail to reach the end of core carbon depletion (\(X_c \leq 10^{-2}\)) as the time-steps become too small (of the order of days) as models encounter density inversions in the sub-surface layers. We find that this is due to large specific entropy \((S/N_A k_B \geq 300)\) at the base of the convective envelope.

We recompute the models for 30–110 M\(_\odot\) stars using three numerical fixes: enhancing the mixing length parameter, enhancing mass-loss rates and suppressing density inversions through adopting MLT++. These three are a general form of the methods used by different stellar evolution codes to resolve numerical instabilities associated with density inversions in models of massive stars. With each method, we are able to compute the evolution of massive stars up to carbon depletion in the core.

To determine the least impact each method can have on the evolution of the star, we pick the sets with the minimum enhancement for each method. With these, we find that density inversion regions can still form in these models, but the specific entropy stays small and the evolution of models proceeds smoothly, i.e., without time-steps becoming too short.

We compare the stellar models evolved using each method. Even with sets of models with minimum numerical enhancement from each method, the remnant mass of the stars can vary by up to 14 M\(_\odot\) while the maximum radial expansion achieved by stars can vary by up to 2000 R\(_\odot\) between the sets. These differences are important for comparing stellar models with observations and the possible feedback on the evolution of massive stars. For example, the above differences can have huge implications for studies involving binary interactions of stars and stellar remnants.

We also find that the differences in the various evolutionary properties predicted by the set of models computed with extra mixing and those using MLT++ are quite small. However, these models show a difference of 1000 K in the minimum effective temperatures achieved by the star as a red supergiant (cf. Section 4.3). The effective temperature is critical for determining the spectral properties and surface abundances of the stars (Davies et al. 2013). Thus, this discrepancy in the effective temperature can be significant for studies involving abundance properties of massive stars, such as galactic chemical composition studies.

In commonly used 1D stellar evolution models, a combination of these methods is used and not necessarily limited to their minimum value. Thus, the differences in the evolutionary properties of massive stars can be higher than what we get here, as shown in Paper I.

Here we considered an intermediate value of metallicity (\(Z = 1.42 \times 10^{-3}\)), as this is the metallicity where progenitors of current gravitational wave observations are more likely to form. Due to the dependence of opacity on chemical composition and the diminishing effect of opacity peaks at lower metallicities (Sanyal et al. 2017), numerical issues related to the proximity to the Eddington limit become less prominent at lower metallicities. For example, using the same set of input parameters as the standard set (Section 3), we find that stellar models fail to evolve for initial masses beyond 20 M\(_\odot\) at higher (solar) metallicity (\(Z = 1.42 \times 10^{-2}\)) but evolve smoothly for initial masses up to 100 M\(_\odot\) at lower metallicity (\(Z = 1.42 \times 10^{-4}\)).

Multi-dimensional stellar models suggest that convection can be more turbulent and non-localised than assumed by MLT (Kupka 2009). 3D modelling of the density inversion regions in massive stars by Jiang et al. (2015, 2018) showed a complex interplay of convective and radiative transport dependent on the ratio of the photon diffusion time to the dynamical time and a smaller convective flux compared to 1D codes. There are ongoing efforts to improve the treatment of mixing 1D codes using results from 3D simulations (Arnett et al. 2019; Schultz et al. 2020).

As observations of massive stars become more accessible, and our ability to compute 3D models of massive stars improves, the problem of density inversions might be resolved in future. Meanwhile, it is important to be aware of and acknowledge the impact different numerical methods can have on the evolutionary model sequences of massive stars.

DATA AVAILABILITY

The link to the MESA input files will be added in the final version of the paper.

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APPENDIX A: DETAILS OF MLT++

In MLT++, MESA makes convection efficient by reducing superadiabaticity in the stellar envelope. In the regions where superadiabaticity is greater than threshold $\gamma < \text{grad} T_{\text{excess}}$, it decreases $\gamma$ to make...
it closer to $\nabla_{ad}$. The fraction of decrease is determined by the parameter $gradT_{\text{excess, alpha}}$ or $\alpha$ and is calculated based on the value of (cf. equation 38 of Paxton et al. 2013):

$$\lambda_{\text{max}} \equiv \max \left( \frac{L_{\text{rad}}}{L_{\text{Edd}}} \right) \quad \text{and} \quad \beta_{\text{min}} \equiv \min \left( \frac{P_{\text{gas}}}{P} \right), \quad (A1)$$

For each stellar model, MESA computes $\alpha$ by comparing $\lambda_{\text{max}}$ with the thresholds $\lambda_1$ and $\lambda_2$ and $\beta_{\text{min}}$ with $\beta_1$ and $\beta_2$ using the following conditions.

If $\lambda_{\text{max}} \geq \lambda_1$ then,

$$\alpha = \begin{cases} 
1 & \beta_{\text{min}} \leq \beta_1 \\
\frac{1}{\beta_1 + d\beta - \beta_{\text{min}}} & \beta_1 < \beta_{\text{min}} < \beta_1 + d\beta \\
0 & \text{otherwise}
\end{cases} \quad (A2)$$

If $\lambda_{\text{max}} \geq \lambda_2$ then,

$$\alpha = \begin{cases} 
1 & \beta_{\text{min}} \leq \beta_{\text{limit}} \\
\frac{\beta_{\text{limit}} + d\beta - \beta_{\text{min}}}{d\beta} & \beta_{\text{limit}} < \beta_{\text{min}} < \beta_{\text{limit}} + d\beta \\
0 & \beta_{\text{min}} \geq \beta_{\text{limit}} + d\beta
\end{cases} \quad (A3)$$

If $\lambda_{\text{max}} > \lambda_2 - d\lambda$ then,

$$\alpha = \begin{cases} 
1 & \lambda_{\text{max}} + d\lambda - \lambda_2 \\
\frac{\lambda_{\text{max}} + d\lambda - \lambda_2}{d\lambda} & \lambda_{\text{max}} + d\lambda - \lambda_2 > \lambda_2 \\
0 & \text{otherwise}
\end{cases} \quad (A4)$$

The net fraction of decrease is determined by a combination of alpha and user defined $gradT_{\text{excess, f2}}$ or $f_2$ using the following equation,

$$\alpha_{\text{net}} = f_2 + (1 - f_2)(1 - \alpha). \quad (A5)$$

The excess fraction is then subtracted from $\nabla_T$, to give reduced $\nabla_{T,\text{new}}$ as,

$$\nabla_{T,\text{new}} = \alpha_{\text{net}} \times \nabla_T + (1 - \alpha_{\text{net}}) \times \nabla_{ad}. \quad (A6)$$

The default values for the different thresholds in the Equations A2–A4 are: $\lambda_1 = 1.0$ and $\lambda_2 = 0.5$, $\beta_1 = 0.35$ and $\beta_2 = 0.25$, $d\lambda = 0.1$ and $d\beta = 0.1$. $gradT_{\text{excess, f1}}$ defaults to $10^{-4}$ while the default value of $gradT_{\text{excess, f2}}$ or $f_2$ is $10^{-3}$. These values can be redefined by the user.

Equations A2–A4 yield a value of $\alpha$ between 0 and 1. The maximum fraction of $\nabla_T$ used in calculating $\nabla_{T,\text{new}}$ is limited to $f_2$ (when $\alpha = 1$), with smaller $f_2$ implying larger contribution of $\nabla_{ad}$ in the equation A6 and therefore larger reduction in superadiabaticity.

We tested our models with for different values of $f_2$, $\lambda_1$ and $\beta_1$. The HR diagram for 110 M$_\odot$ stellar model, calculated with the four different combinations of parameters in MLT++ is shown in Figure A1. We find that using a small reduction in superadiabaticity with $f_2 = 10^{-1}$ and setting $\lambda_1 = 0.6$ and $\beta_1 = 0.05$ helps the stellar models reach completion timely and without any numerical inaccuracies or difficulty.

This paper has been typeset from a \TeX/\LaTeX\ file prepared by the author.