Modeling Chemically Homogeneous Evolution in COMPAS

Kaila Nathaniel
Department of Physics
Virginia Polytechnic Institute and State University

Advisor: Ilya Mandel
Mentors: Coenraad Neijssel, Alejandro Vigna-Gomez
School of Physics and Astronomy
University of Birmingham

July 2017

Contents

List of Figures

1 Introduction

According to Einstein's Theory of General Relativity, gravitational waves (GW), are ripples in the fabric of spacetime that move at the speed of light. GWs are created when massive objects move through spacetime, which changes the curvature of spacetime, thereby creating GWs. The detection of GWs has opened up a new field of GW astrophysics, focused on analyzing and modeling GW signals. GW data complements traditional electromagnetic data to gain a more complete understanding of a source's properties. While electromagnetic data allows us to see objects in space, GWs allow us to "hear" them as well.

Advanced LIGO has detected three confirmed GW signals since its launch in September 2015: GW150914, GW151226, and GW170104; and one lower-confidence signal, LVT151012. Modeling GW sources allows for better analysis, as detected data can be compared to models to determine source type and source properties.

Binary stars release energy in the form of gravitational waves as the bodies spiral inwards towards each other. The GW events observed so far appear to come from black hole binaries. Perfectly spherical single stars do not emit GWs, but even a neutron star with a small asymmetry would emit smaller GWs than two $30M_\odot$ compact objects orbiting each other at a close distance. The larger the amplitude, the easier to pick up a GW signal.

Massive binaries can undergo many physical processes as they evolve, and one of those processes is stellar rotation. If the objects rotate fast enough, the layers mix and prevent the build up of a chemical gradient between the core and the envelope. Chemically homogeneous stars are hotter, more luminous, and more compact, and are a potential source of GWs. Modeling stellar rotation is a new inclusion in theoretical modeling of massive star evolution (Mandel and De Mink 2016).

Normal binary systems go through a common-envelope phase as one of the stars expands. As the primary star expands, it is increasingly influenced by the gravitational field of the secondary star. When the primary star's envelope reaches the Lagrange point between the two stars, it is said to have overflowed its Roche lobe. More expansion means that material from the envelope of the primary accretes onto the secondary star. As the secondary star accretes mass, it expands to maintain thermal equilibrium, eventually expanding its Roche lobe as well. When the secondary has also filled its Roche lobe, the two stars share a common envelope (Izzard et al. 2011). This is important for binary evolution because common envelope can create compact object binaries that can become sources for gravitational waves.

COMPAS, or Compact Object Mergers: Population Astrophysics and Statistics, is one GW source modeling software package that is being developed by the Astrophysics and Space Research group at the University of Birmingham. COMPAS has a number of models for developing compact object mergers, but still requires a CHE model. COMPAS is designed to model populations of stars, rather than individual stars. In order to efficiently evolve millions of binaries to obtain population statistics, it simplifies parameters by choosing to use outputs from prescriptions, in order to evolve stars faster.

MESA, or Modules for Experiments in Stellar Astrophysics, is software primarily developed by Bill Paxton of University of California, Santa Barbara, with rotational CHE models mainly written by Pablo Marchant of Argelander-Institut fur Astronomie, Universitat Bonn. MESA can model individual stars in much greater detail than COMPAS. In order to develop a detailed CHE model for COMPAS, MESA must be used to create more comprehensive prescriptions. While MESA can be used to learn about individual stars in great detail, it is difficult to determine trends when looking at just a handful of stars at a time. Likewise, COMPAS can determine trends, but is not useful for learning about how individual stars behave in great detail. Together, MESA and COMPAS can be used to create detailed prescriptions from individual stars that can then be used to evolve millions of binaries to determine overall population trends.

This paper explains the process and methods behind creating prescriptions for chemically homogeneous stars using MESA and COMPAS. The rest of this paper is organized as follows: Section 2 will focus on CHE and its conditions, Section 3 will discuss modeling CHE, Section 4 will explain the methods used, Section 5 will analyze the results from the simulations, and Section 6 will talk about future possibilities with the work.

2 Chemically homogeneous evolution

The evolution of massive stars, defined here as stars greater than $5M_\odot$, can be affected by multiple physical parameters, such as mass, metallicity and rotation. If a star rotates fast enough, it can trigger mixing between the various layers of chemicals. The mixing changes the chemical composition, or the metallicity, of the star, which affects mass loss from stellar winds and alters the star's evolution. As might be expected, chemically homogeneous stars evolve very differently from their normal counterparts.

The rotation of the star causes the loss of a chemical gradient between the core and the envelope. The entire star is the core, with no envelope. The mixing moves material from the hydrogen rich envelope into the central burning regions and vice versa, creating a star that is approximately chemically homogeneous. While normally evolving stars contract and expand in cycles over time, chemically homogeneous stars only slowly contract as they become more helium rich (Mandel and De Mink 2016). This is because chemically homogeneous stars have no envelope, unlike normal stars.

In most stars, the envelope expands as the core contracts, in order to remain in hydrostatic equilibrium. However, in very well mixed stars, there is no distinction between the core and the envelope, and the whole star contracts. This leads to a star that is smaller, hotter, and more luminous than normally evolved stars (Mandel and De Mink 2016). However, these stars are likely only found in metal-poor environments, because CHE is likely to only be possible with metallicity at solar or lower (Martins et al. 2013; Sźecsi et al. 2015). At $Z < Z_\odot = 0.02$, excessive mass loss due to stellar winds can be avoided. Otherwise, the star does not stay well mixed during core hydrogen exhaustion, and is not chemically homogeneous (Marchant et al. 2016).

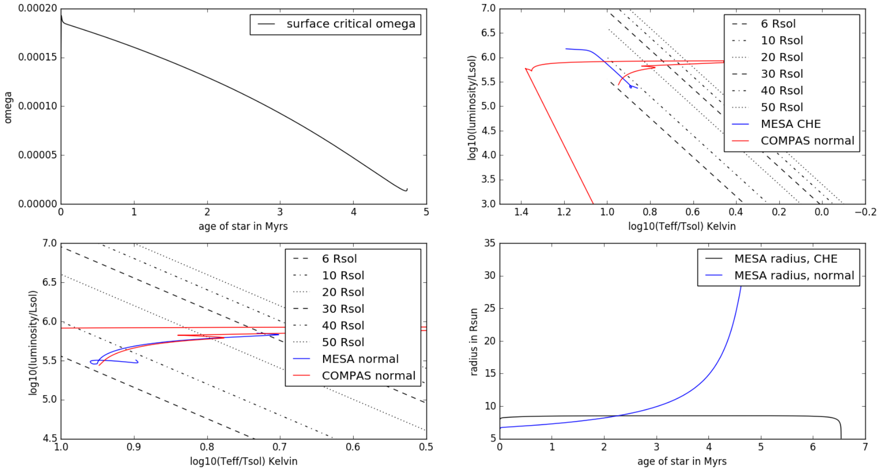

Figure 1: Comparison of normal star and a CHE star, with luminosity-temperature lines in the Hertzsprung-Russell diagrams.

Mandel and De Mink 2016 suggest that chemically homogeneous binary systems avoid mass transfer and common envelope phases, but Marchant et al. 2016 propose that binary systems can undergo an early mass transfer and common envelope phase and still go on to become chemically homogeneous. During early core hydrogen burning, the stars swap mass back and forth during contact stages, so that they end up with a mass ratio close to 1. The stars avoid merging, and still evolve chemically homogeneously during the main sequence and the post-core-hydrogen-burning phase (Marchant et al. 2016). Software such as COMPAS chooses to exclude stars undergoing mass transfer and common envelope phases as not chemically homogeneous, but future, more comprehensive modeling will likely take mass transfer and common envelope into account.

There are some observational clues that could be interpreted as evidence for chemically homogeneous stars, although there is no hard evidence at present. This is because rapidly rotating binaries are relatively rare, and it is difficult to observe in metal-poor environments. However, Martins et al. 2013 have found some Wolf-Rayet stars with Z between 0.5 and 1.0 in the SMC that cannot be created with standard evolutionary tracks, due to their position in the HR diagram and chemical composition. These stars appear to be evolving semi-chemically homogeneously, although more analysis is necessary.

Binary chemically homogeneous systems evolve into two massive helium stars, which may eventually collapse into two stellar-mass black holes. Chemically homogeneous systems are therefore a potential source of gravitational waves. GW observations and analysis may help determine the physics of such systems, including their merger rate.

3 Modeling CHE

COMPAS was built upon Hurley, Pols, and Tout 2000; Hurley, Tout, and Pols 2002 models, which do not take rotation into account. COMPAS is rapid population synthesis software, which means that it does not calculate individual stars in detail. Rather than including prescriptions for every parameter, COMPAS uses the outputs from the prescriptions when evolving stars. This means that COMPAS can evolve large populations, but it requires models, since it cannot calculate all parameters. COMPAS requires a separate analytical prescription to determine which stars, given a mass and metallicity, should be flagged as chemically homogeneous. MESA was used to create that prescription. MESA is stellar evolution code that evolves one star at a time, and evolves them in great detail. While MESA does not evolve populations of stars, it can be used to calculate a prescription that can then be input into population synthesis software to create large populations. In order to create a prescription for chemically homogeneous stars in COMPAS, it is necessary to model grids of stars undergoing CHE in MESA, and then translate the data into a prescription that can be coded into COMPAS. This requires learning how to identify stars undergoing CHE, both manually and automatically; and then how to evolve stars so that they undergo CHE. Once the boundaries for CHE are understood, a fit can be made from the data, and a prescription can be put into COMPAS.

Mandel and De Mink 2016 approximated a basic model with a minimum ω_c for single stars to evolve quasi-chemically homogeneously using a Z = 0.004 grid.

$$\omega_c = \begin{cases} 0.2 + 2.7{\times}10^{-4}(\frac{m}{M_\odot} - 50)^2 & \text{for } m < 50M_\odot \\ 0.2 & \text{for } m \geq 50M_\odot \end{cases} \tag{1}$$

Using Kepler's Third Law, a threshold period can be found for binary stars undergoing CHE. Once a threshold period is found, it is easy to calculate the ω of a star to see if it is greater than the ω_c, and therefore undergoing CHE.

$$P = \frac{\pi r^{\frac{3}{2}}}{\sqrt{GM}} \tag{2}$$

$$\omega = \frac{2\pi r}{P v_k} \geq \omega_c \tag{3}$$

$$v_k = \sqrt{\frac{Gm}{r}} \tag{4}$$

Where v_k is the Keplerian velocity, M is the combined masses of the binary system, and m is the mass of a single star. r can be taken as the star radius, or can be approximated with the following formula at solar metallicity.

$$\mathrm{r} = \mathrm{R}_\odot\left(\frac{M}{M_\odot}\right)^{0.6} \quad \text{for } m > M_\odot \quad (5)$$

At low metallicities, this radius formula is no longer very accurate. Calculations at $Z = 0.004$ show that the radius is about 1.2 times larger than the true radius of the star. There is not currently a better fit for the radius, as only a rough approximation is necessary.

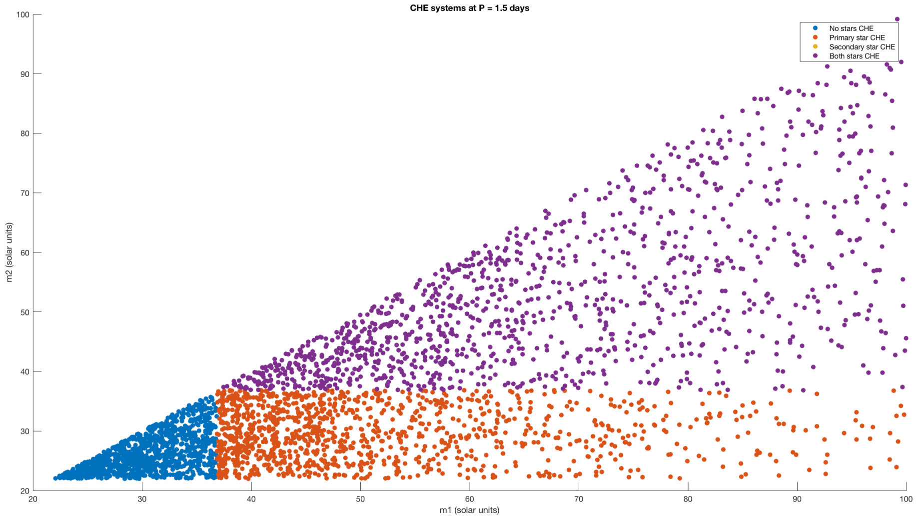

Figure 2: Window for CHE in binary stars, with a fixed period of 1.5 days.

However, these formulae can only be used to create chemically homogeneous binaries, rather than single stars, and it is a definition of CHE that does not take chemical composition into account.

3.1 Identifying CHE

In order to create a prescription for chemically homogeneous stars in COMPAS, it is necessary to model individual stars undergoing CHE in MESA, and then translate the data into a prescription that can be coded into COMPAS. This requires learning how to identify stars undergoing CHE, both manually and automatically; and then how to evolve stars so that they undergo CHE.

While a regular star's HR diagram goes to the right after ZAMS, a star undergoing CHE has a HR that diverts to the left after ZAMS is completed. Additionally, a regular star has its radius expand as it evolves, while a star undergoing CHE has a radius that stays fairly constant until near the end of its life, where the radius will rapidly decrease as the star contracts. This is because a CHE star does not have a separate core and envelope, so there is no expansion and contraction over the lifetime of the star. These are indicators that can be seen visually in plots, but are difficult to detect automatically. A better way to detect stars that are undergoing CHE is by chemical composition in the core and surface of the star. A normal star will have a fairly large difference between the abundance of helium in the surface and the core, while a chemically homogeneous star will have a much smaller difference. As per Marchant et al. 2016, stars that reach a point where the difference between the surface and core helium abundance is greater than 0.2 are deemed to be evolving normally. Stars with a difference of less than or equal to 0.2 are chemically homogeneous and flagged as such.

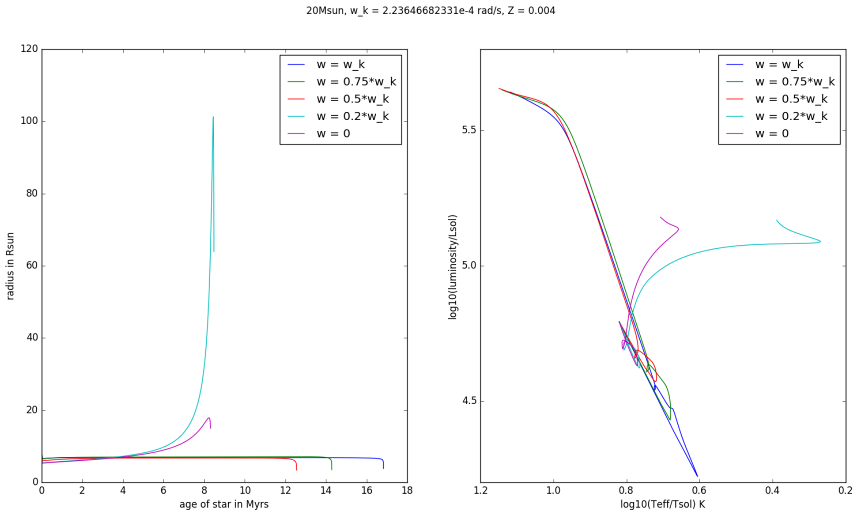

Figure 3: The purple and teal lines are non-chemically homogeneous stars evolving normally. The blue, green, and red lines are stars rotating fast enough that they are evolving chemically homogeneously.

4 Methods

4.1 Convergence Tests

When using simulation software, it is important to determine if the results converge when run under different conditions. MESA evolves stars using variable timesteps, and all stars should ideally evolve in the same way, regardless of the size of the timestep. In order to confirm this, stars were evolved at timesteps equaling half and twice the original timestep, and compared to the stars evolved at the original timestep to ensure that all stars still evolved in the same way.

If the stars do not evolve in the same way, then the results are noise from internal MESA processes and cannot be trusted. Fortunately, all stars evolved identically, regardless of timestep used.

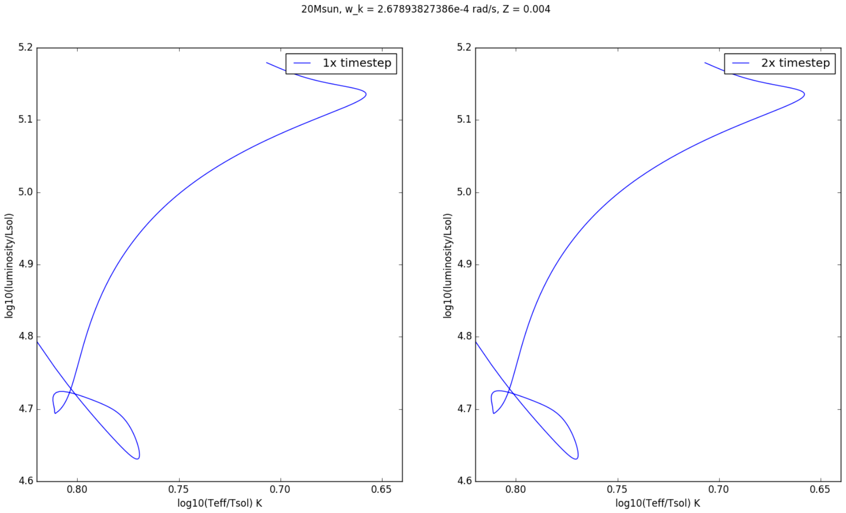
20Msun, w_k = 2.67893827386e-4 rad/s, Z = 0.004

Figure 4: An HR diagram of a 20Msun star, run at the default timestep and 2x the default timestep. The evolution is identical.

4.2 MESA Grids

Grids are runs of many stars, used to find trends that cannot be spotted with single stars. The grids run had three main parameters: mass, angular velocity (ω), and metallicity. The mass grid was calculated from $5M_\odot$ to $100M_\odot$, with 25 points; angular velocity and metallicity were calculated according to formulae to get correct boundaries as grid resolution was increased, with 10 points each for full grids. For the first set of grids, Z was set to $Z_\odot = 0.02$.

Initially, stars were evolved with a wide range of ω and $Z = 0.004$ and plotted against the Equation 1 line. Chemically homogeneous stars were found to be within ± 0.25 of the Equation 1 line, although in general chemically homogeneous stars had a higher threshold than the Equation 1 line suggests. For the second grid, ω was calculated according to Equation 1. The lower bound for ω was the star's $\omega_c - 0.25$, and the upper bound was $\omega_c + 0.25$, with 10 points evenly spaced between.

After the first two grids, the ω boundaries were set according to the thresholds found in the previous grid. 10 points were evenly spaced between the largest ω found in a normally evolving star and the smallest ω found in a chemically homogeneous star. This process was repeated for greater resolution and more

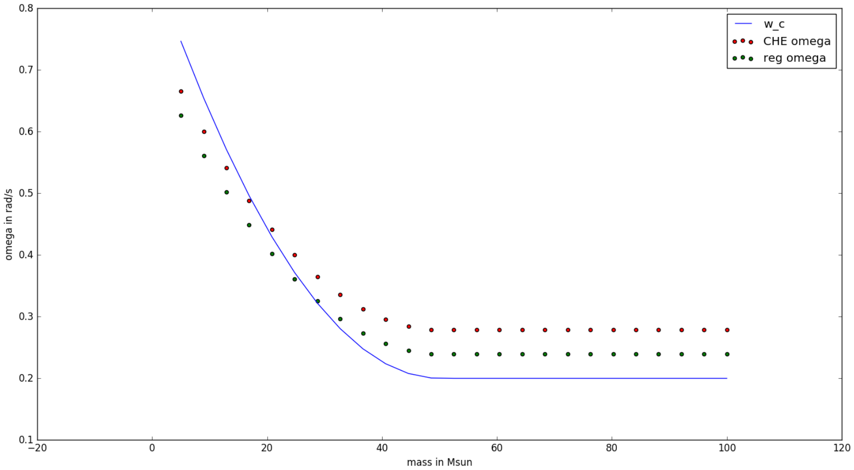

Figure 5: ω of normal and chemically homogeneous stars, plotted against the Equation 1 line.

defined fit, until ω was defined to the nearest hundredth-thousandth, in order to have as accurate a prescription as possible.

Once a 2D fit was established for stars at $Z = 0.02$, grids were run with an array of metallicities. The metallicity bounds were between $Z = 0.0002$ and $Z = 0.02$, in logspace. The same process as for the previous grids was repeated to determine the boundary conditions for chemically homogeneous stars, and a plane of data was generated. For a $50M_\odot$ star, ω must reach at or above $4.44741268179 \times 10^{-5}$ rad/s to be chemically homogeneous, but after that, the metallicity matters much more than the ω. Once a star has reached the minimum ω necessary for CHE, Z must be taken into account. Z boundaries for chemically homogeneous stars were calculated to the nearest hundredth for a grid of stars at $10M_\odot$, $50M_\odot$, and $100M_\odot$.

5 Results

Fitting the data from the 2D grids revealed a change in ω necessary for CHE around $50M_\odot$. Until that threshold, there is an exponentially decaying curve, but afterwards it changes to a shallow linear slope. This is because the necessary ingredients for convective mixing in a star are radiation pressure and a thermal gradient between the equator and poles to drive mixing through meridional circulation. At low masses, radiation pressure plays only a small role, so it is more important to have a large thermal gradient, supplied by the rapid rotation, to drive mixing. As the mass increases, the required thermal gradient drops, and the radiation pressure increases. Around $50M_\odot$, radiation pressure becomes dominant, so further mass increases do not change the thermal gradient. This makes the curve flatten out to a threshold rotation rate required to create enough of a temperature gradient. This equation can be used to create a prescription, so that COMPAS-created stars can be flagged as chemically homogeneous.

$$\omega(m) = (3.8145 \times 10^{-4}) \times e^{(-8.213285 \times 10^{-2}) \times m} + 4.0442 \times 10^{-5} \tag{6}$$

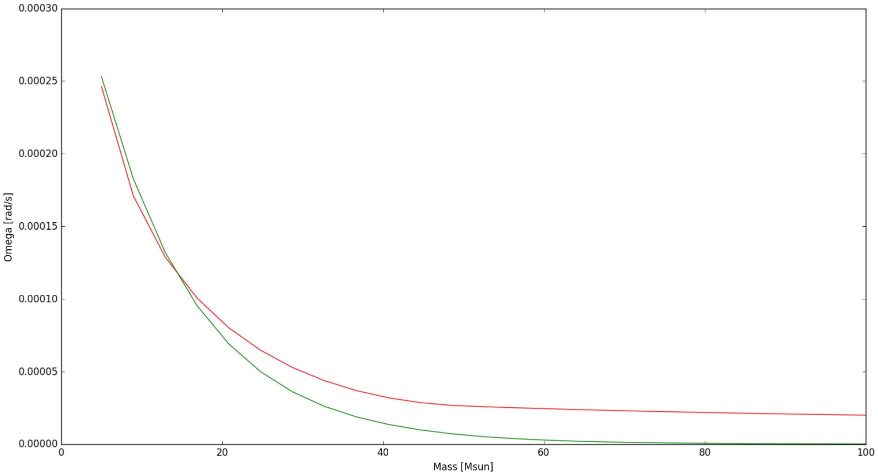

Figure 6: Comparison of the Equation 1 fit in red and the Equation 6 fit in green.

This fit is approximate, and requires more grids at a higher resolution to be complete, but it is a useful estimation of the ω required for stars of $Z = 0.02$. The threshold for CHE is lower than the threshold estimated in Mandel and De Mink 2016, but the Equation 6 was run at $Z = 0.02$, while the Equation 1 was run at $Z = 0.004$. More grids and greater analysis will lead to a better fit that can be used to determine the ω necessary for chemically homogeneous stars of varying masses.

As Table 5 shows, CHE depends very heavily upon metallicity. The greater the mass of the star, the lower Z had to be for the star to be chemically homogeneous. This holds true with understandings about wind mass loss. Greater metallicity in a star means strong winds, which will reduce the mass of the star, leading to the ω being too small for CHE. The table data shows that with stars of the same ω and mass, the Z of the chemically homogeneous star must be roughly double the Z of the star evolving normally. A star of $20M_\odot$ with a Z of 7.188×10^{-3} must have an ω roughly four times larger than a star of $100M_\odot$

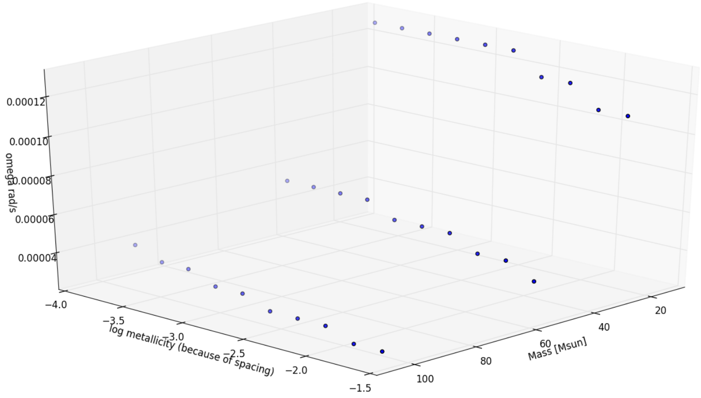

Figure 7: Plane of data generated for stars with varying mass, ω, and metallicity.

Mass ($M_\odot$)	CHE	ω ($\times 10^{-5} rad/s$)	Z ($\times 10^{-3}$)
20.0	False	12.0689209891	7.18762732761
20.0	True	12.0689209891	11.9896850064
20.0	False	13.1207704739	2.58309933003
20.0	True	13.1207704739	4.30886938006
50.0	False	4.44741268179	11.9896850064
50.0	True	4.44741268179	20.
50.0	False	5.17649672799	4.30886938006
50.0	True	5.17649672799	7.18762732761
50.0	False	5.90558077418	0.928317766723
50.0	True	5.90558077418	1.54852736536
100.0	False	2.81796615635	7.18762732761
100.0	True	2.81796615635	11.9896850064
100.0	False	3.37050853995	1.54852736536
100.0	True	3.37050853995	2.58309933003
100.0	False	3.92305092355	0.556511880441
100.0	True	3.92305092355	0.928317766723
100.0	False	4.47559330715	0.2
100.0	True	4.47559330715	0.33362010744

Table 1: Data from stars varying in mass, ω, and metallicity.

with the same Z. There is not currently a fit equation for Table 5, but the analysis is in process.

6 Future Work

The overall goal of this project was to create an equation that would determine the ω necessary to create chemically homogeneous stars of varying masses and metallicities that can then be input into a model for CHE in COMPAS. An equation has been found for stars of varying masses, and the next step is to create a COMPAS model. To do this, a new stellar evolution type must be created in COMPAS. While Marchant et al. 2016 determined that stars can undergo early mass transfer and still go on to be chemically homogeneous, for now the COMPAS model will assume that stars undergoing mass transfer are not eligible to become chemically homogeneous. Normal wind prescriptions will still apply, and the star will basically turn into a zero-age Wolf-Rayet star, evolving as a Hurley HeMS once it reaches HeMS. It will be assumed that the whole star becomes a helium core, with existing COMPAS prescriptions taking over once the star reaches HeMS.

Another future goal is to create an equation that can be used to determine chemically homogeneous stars of varying masses and metallicities. Currently existing equations are for stars at $Z = 0.004$ and $Z = 0.02$, and it would be helpful to have a prescription that can be used at an arbitrary metallicity. This requires more grids with greater resolution, and more analysis of results. This work is currently ongoing.

References

Hurley, Jarrod R., O. R. Pols, and Christopher A. Tout (2000). “Comprehensive analytic formulae for stellar evolution as a function of mass and metallicity”. In: *Royal Astronomical Society* 315, pp. 543–569.

Hurley, Jarrod R., Christopher A. Tout, and O. R. Pols (2002). “Evolution of binary stars and the effect of tides on binary populations”. In: *Royal Astronomical Society* 329.4, pp. 897–928.

Izzard, Robert G. et al. (2011). “Common envelope evolution”. In: *IAU Symposium.*

Mandel, I. and S. E. De Mink (2016). “Merging Binary Black Holes Formed Through Chemically Homogeneous Evolution in Short-Period Stellar Binaries”. In: *MSRAS.*

Marchant, Pablo et al. (2016). “A new route towards merging massive black holes”. In: *Astronomy and Astrophysics.*

Martins, F. et al. (2013). “Evidence for quasi-chemically homogeneous evolution of massive stars up to solar metallicity”. In: *Astronomy and Astrophysics.*

Sźecsi, Dorottya et al. (2015). “Low-metallicity massive single stars with rotation”. In: *Astronomy and Astrophysics.*