

# Simulation go Burrr....

A Thesis Proposal

Submitted to the Faculty  
in partial fulfillment of the requirements for the  
degree of

Doctor of Philosophy

in

Physics and Astronomy

by

Thomas M. Boudreaux

DARTMOUTH COLLEGE

Hanover, NH

May 10, 2022

The Examining Committee:

---

Dr. Brian Chaboyer

---

Dr. Elisabeth E. Newton

---

Dr. Aaron Dotter

The equations of stellar structure have proven astonishingly predictive when describing stars interior structures. In their most basic form they constitute 4 ordinary, first-order, differential equations. However, they are not on their own well enough constrained to solve. In addition to the four ODEs, an equation of state, thermal conductivities, nuclear reaction rates, and opacities are all required when modeling a star. Some of these additional constraints can be computed on the fly; however, as yet there is no effective way to compute opacities at run time. Rather, stellar structure programs use pre-tabulated opacities over a range of temperatures, densities, and chemical compositions. The Dartmouth Stellar Evolution Program (DSEP) has used OPAL opacities for the last decade and a half; however, there are now more up to date elemental opacity tables from OPLIB. Moreover, OPAL opacities can no longer be reliably generated for different chemical compositions. Here we present an overview of how we update DSEP to use opacities from OPLIB in addition to preliminary results from two studies making use of these updated opacities.

## 1. INTRODUCTION

Over the last half of the 19th and first decade of the 20th centuries Lane, Ritter, and Emden codified the earliest mathematical model of stellar structure, the polytrope (Equation ??), in *Gaskugeln* (Gas Balls) (?).

$$\frac{d}{d\xi} \left( \xi^2 \frac{d\theta}{d\xi} \right) = -\xi^2 \theta^n \quad (1)$$

Where  $\xi$  and  $\theta$  are dimensionless parameterizations of radius and temperature respectively, and  $n$  is known as the polytropic index. Despite this early work, it wasn't until the late 1930s and early 1940s that the full set of equations needed to describe the structure of a steady state, radially-symmetric, star (known as the equations of stellar structure) began to take shape as proton-proton chains and

the Carbon-Nitrogen-Oxygen cycle were, for the first time, seriously considered as energy generation mechanisms (?). Since then, and especially with the proliferation of computers in astronomy, the equations of stellar structure have proven themselves an incredibly predictive set of models.

Low mass stars form an important component of the stellar population, with stars less than [MASS HERE] making up more than 70% of stars in the galaxy.

There are currently many stellar structure codes (e.g. ???) which integrate the equations of stellar structure — in addition to equations of state and lattices of nuclear reaction rates — over time to track the evolution of an individual star. The Dartmouth Stellar Evolution Program (DSEP) (???) is one such, well tested, stellar evolution program.

DSEP solves the equations of stellar structure using the Henyey method (?). This is a relaxation technique making use of a Newton–Raphson root finder and therefore requires some initial guess to relax towards a solution. This guess will be either some initial, polytropic, model or the solution from the previous timestep. In order to evolve a model through time DSEP alternates between solving for reaction rates and the structure equations. At some temperature and pressure from the solution to the structure equations DSEP finds the energy generation rate due to proton-proton chains, the CNO cycle, and the tripe-alpha process from known nuclear cross sections. These reaction rates yield both photon and neutrino luminosities as well as chemical changes over some small time step. Thermodynamic variables are calculated using an equation of state routine which is dependent on the initial model mass. All the updated physical quantities (pressure, luminosity, mean molecular mass, temperature) are then used to solve the structure equations again. This process of using a solution to the structure equations to calculate reaction rates which then inform the next structure solution continues until DSEP can no longer find a solution. This can happen as the stellar structure equations are extremely stiff. In addition, for finite radial mesh sizes, discontinuities can occur.

While other stellar evolution programs, such as the widely used Modules for Experimentation in Stellar Astrophysics (MESA) (?), consider a more complex handling of nuclear reaction rate calculations, and are consequently more applicable to a wider range of spectral classes than DSEP, DSEP has certain advantages over these other programs that make it well suited for certain tasks,

such as low-mass modeling. For one, DSEP generally can evolve models much more rapidly than MESA and has a smaller memory footprint while doing it. This execution time difference is largely due to the fact that DSEP makes some simplifying assumptions due to its focus only on models with initial masses between 0.1 and 5  $M_{\odot}$  compared to MESA’s more general approach. Moreover, MESA elects to take a very careful handling of numeric uncertainty, going so far as to guarantee byte-to-byte similarity of the same model run on different architectures (?). DSEP on the other hand makes no such guarantee. Rather, models evolved using DSEP will be accurate down to some arbitrary, user controllable, tolerance but beyond that point may vary from one computer to another. Despite this trade off in generality and precision, the current grid of isochrones generated by DSEP (?), has been heavily cited since its initial release in 2008, proving that there is a place for a code as specific as DSEP.

As DSEP pushes a star along its evolutionary track the radiative opacity must be known for a wide range of temperatures, pressures, and compositions. Specifically, opacity is a key parameter in the equation of energy transport. With current computational tools it’s infeasible to compute opacities on the fly; rather, Rossland Mean opacity ( $\kappa_R$ ) for individual elements must be pre-tabulated over a wide range of temperatures and densities. These opacities can then be somewhat arbitrarily mixed together and interpolated to form opacity lookup-tables. Multiple groups have preformed these calculations and subsequently made tables available to the wider community, these include the Opacity Project (OP ?), Lawrence Livermore National Labs OPAL opacity tables (?), and Los Alamos National Labs OPLIB opacity tables (?).

The OPAL opacity tables in particular are very widely used by current generation stellar evolution programs (in addition to current generation stellar model and isochrone grids). However, they are no longer the most up date elemental opacities. Moreover, the generation mechanism for these tables, a webform, is no longer reliably online. Consequently, it makes sense to transition to more modern opacity tables with a more stable generation mechanism.

Here we will present work transitioning DSEP from OPAL opacities to opacities based on measurements from Los Alamos national Labs T-1 group (OPLIB ?). Moreover, we will present two

projects which are in large part reliant on these updated opacities. For the first project we investigate the affects of chemically self consistent modeling of multiple populations within the globular cluster NGC 2808, and for the second project we present the effects of the OPLIB opacities on the location of the recently discovered Gaia M-dwarf gap.

This paper is organized as follows. In Section ?? we outline some basic information about OPLIB opacities, how we query them, and how we modify them to work with DSEP. In Section ?? we discuss scientific background of the first project along with the current work done towards its goal. Finally, in Section ?? we present our findings on the effects of OPLIB opacities on the location of the Gaia M-dwarf gap.

## 2. THESIS

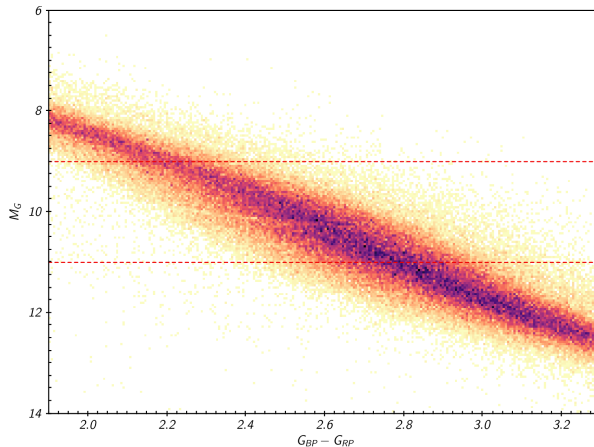
The thesis here proposed will be split into 5 chapters. Each chapter will consist of work focusing on models low mass stars.

### 2.1. *Jao Gap & Updated High Temperature Opacities*

Due to initial mass requirements of the molecular clouds which collapse to form stars, star formation is strongly biased towards lower mass, later spectral class, stars when compared to higher mass stars. Partly as a result of this bias and partly as a result of their extremely long main-sequence lifetimes, M-dwarfs make up approximately 70 percent of all stars in the galaxy. Moreover, some planet search campaigns have focused on M-dwarfs due to the relative ease of detecting small planets in their habitable zones (e.g. ?). M-dwarfs then represent both a key component of the galactic stellar population as well as the possible set of stars which may host habitable exo-planets. Given this key location M-dwarfs occupy in modern astronomy it is important to have a thorough understanding of their structure and evolution.

#### 2.1.1. *Observations and Instability*

Gaia Data Release 2 (DR2) revealed a previously unknown structure in in the  $G_{BP} - G_{RP}$ ,  $M_G$  color-magnitude diagram (Figure ??) corresponding to stars with a mass near that where a star



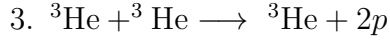
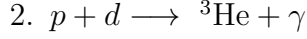
**Figure 1.** Figure 1 from ? showing the so called “Jao Gap” at  $M_G \approx 10$

transitions from fully convective to having both convective and radiative regions within (the fully convective transition mass) (?). The so called Gaia M-dwarf gap, or Jao gap, represents a decrease in luminosity and commensurately a decrease in stellar density — by approximately 17% — over this mass range. ?? suggest that this density deficiency is due to stars between a mass of 0.3 to 0.35  $M_\odot$  transitioning into full convectivity.

A theoretical explanation for such a density deficiency comes from ?, who propose that directly above the transition mass between a star with a radiative core and convective envelope and a fully convective star, due to asymmetric production and destruction of  $\text{He}^3$  during the proton-proton I chain (ppI), periodic luminosity variations can be induced. This process is known as convective-kissing instability. Take for example a star with a mass right on the fully convective transition. Such a star will descent the pre-MS with a radiative core; however, as the star reaches the zero age main sequence (ZAMS) and as the core temperature exceeds  $7 \times 10^6$  K, enough energy will be produced by the ppI chain that the core becomes convective. At this point the star exists with both a convective core and envelope, in addition to a thin, radiative, layer separating the two. At this Point asymmetries in ppI affect the evolution of the stars convective core.

The proton-proton I chain constitutes three reactions

1.  $p + p \longrightarrow d + e^+ + \nu_e$



Because reaction 3 of ppI consumes  ${}^3\text{He}$  at a slower rate than it is produced by reaction 2,  ${}^3\text{He}$  abundance increases in the core increasing energy generation. The core convective zone will therefore expand as more of the star becomes unstable to convection. This expansion will continue until the core connects with the convective envelope. At this point convective mixing can transport material throughout the entire radius of the star and the high concentration of  ${}^3\text{He}$  will rapidly diffuse outward, away from the core, again decreasing energy generation as reaction 3 slows Down. Ultimately, this leads to the convective region around the core pulling back away from the convective envelope, leaving in place the radiative transition zone, at which point  ${}^3\text{He}$  concentrations build up in the until it once again expands to meet the envelope. This process repeats until chemical equilibrium is reached throughout the star and the core can sustain high enough nuclear reaction rates to maintain contact with the envelope, resulting in a fully convective star.

### 2.1.2. *Modeling the Gap*

Since the identification of the Gaia M-dwarf gap, stellar modeling has been conducted to better constrain its location, effects, and exact cause (e.g. ??). When modeling the gap manifests as a discontinuity in the mass-luminosity relation. However, all modeling of the gap has been done using GS98 OPAL high-temperature opacities. This presents similar issues to the use of these tables when modeling multiple populations in GCs; namely, OPAL tables are no longer the most up to date in their component opacities .

? and ? identify that the gap's mass location is correlated with model metallicity — the mass-luminosity discontinuity in lower metallicity models being at a commensurately lower mass. ? suggests this dependence is due to the steep relation of the radiative temperature gradient,  $\nabla_{rad}$ , on temperature and in turn, on stellar mass.

$$\nabla_{rad} \propto \frac{L\kappa}{T^4} \quad (2)$$

As metallicity decreases so does opacity, which, by Equation ??, dramatically lowers the temperature where radiation will dominate energy transport (?). Since main sequence stars are virialized the core temperature is proportional to the core density and total mass (Equation ??). Therefore, if the core temperature where convective-kissing instability is expected decreases with metallicity, so to will the mass of stars which experience such instabilities.

$$T_c \propto \rho_c M^2 \quad (3)$$

### 2.1.3. *Consistently Modeling the Gap*

In order to address the two main issues with using OPAL opacity tables we use our OPLIB opacity table web scraper to generate a set of tables that consistently model lower metallicities. Specifically, we generate tables for  $Z_{\odot} = 0.017$ ,  $Z = 0.01$ ,  $Z = 0.001$ , and  $Z = 0.0001$ . Compositions are derived from the GS98 solar composition, with the mass fractions between metals remaining constant, and only the total metal mass fraction is allowed to vary. Moreover, Helium mass fraction is held constant as extra mass from the reduced metallicity is put into additional Hydrogen.

For each metallicity 101, uniformly spaced, models from 0.3 to 0.5  $M_{\odot}$  (spacing of 0.001  $M_{\odot}$ ) are evolve with both the GS98 OPAL opacity table and OPLIB tables, hereafter these are the “coarse” models. For each set of coarse models the discontinuity in the mass-luminosity relation is identified at an age of 7 Gyr (Figures ?? & ?? shows a characteristic example).

Immediately, the difference in mass where the discontinuity manifests is clear. For each metallicity the discontinuity in the OPLIB models is approximately one one-hundredth of a solar mass lower than the discontinuity in the OPAL models. We can validate that this discontinuity is indeed correlated with the convective transition mass; Figure ?? shows an example of the model forming radiative zones at approximately the same masses where the discontinuity in the mass-luminosity function exists.



$Z =$	$Z_{\odot}$	0.01	0.001	0.0001
OPAL	0.3803 - 0.384	0.3583 - 0.3631	0.34 - 0.3448	0.362 - 0.3663
OPLIB	0.374 - 0.3767	0.3526 - 0.3567	0.3358 - 0.3406	0.3577 - 0.3621

**Table 1.** Mass ranges for the discontinuity in OPAL and OPLIB models. Masses are given in solar masses.

At this resolution only a few models exist within the mass range of the discontinuity. In order to better constrain its location we run a series of “fine” models, with a mass step of  $0.0001 M_{\odot}$  and ranging from where the mass derivative first exceeds two sigma away from the mean derivative value up to the mass where it last exceeds two sigma away from the mean. A characteristic fine mass-luminosity relation is shown in Figure ??.

Using the fine models we identify the location of the discontinuity in the same manner as before, results of this are presented in Table ?. Of note with the mass ranges we measure for the discontinuity is that are generally not in agreement with those measured in ?. However, the luminosity difference from over the gap ( $\approx 0.1mag$ ) is similar to both the observational difference and that reported in ?. Currently, it is not clear why our mass range is not in agreement with the ? mass range and further investigation is therefore needed.

## 2.2. Jao Gap Ageing - 1

Following the integration of updated high temperature opacities detiled in §?? we will investigate using the Jao-Gap color to age the local solar neighborhood.

Models predict that the location of the Jap Gap will shift with population age [CITATION]; in fact, we see this behavior, gap colors reddening as populations age, in populations evolved with DSEP [FIGURE] which span the mass range of the gap.

[DETAILS ON KINEMATIC AGEING]

We propose to model a population of stars of various ages and mettalicities sampled from the local stellar neighborhood. Each of these stars will be assigned kinematics — again sampled from empirical distributions. We will then extract kinematically derived ages from this population and

use these to segregate stars into rough age bins. Finally, we will measure if difference in Jao gap locations are statistically distinguishable between these rough age bins.

### 2.3. *Jao Gap Ageing - 2*

### 2.4. *NGC 2808*

Globular clusters (GC, ?) are among the oldest groupings of stars in the Universe, with typical ages greater than 10 Gyr. They are characterized by their compact size — typical half-light radius  $< 10$  pc but up to 10s of pc — and high surface brightness —  $M_V \sim -7$ . Traditionally, GCs were believed to contain a single stellar population, much like open clusters. However, chemical inhomogeneities in GCs have been known about since the early 1970s (e.g. ?) and by the late 1980s multiple clusters were known which exhibited features in their CMDs consistent with either bimodal or multimodal stellar populations (e.g. ?).

Whereas, people have have often tried to categorized objects as GCs by making cuts along half-light radius, density, and surface brightness profile, in fact many objects which are generally thought of as GCs don't cleanly fit into these cuts. Consequently, ? proposed a definition of GC based on observed chemical inhomogeneities in their stellar populations. The modern understanding of GCs then is not simply one of a dense cluster of stars which may have chemical inhomogeneities and multiple populations; rather, it is one where those chemical inhomogeneities and multiple populations themselves are the defining element of a GC.

Variations in observed abundances were initially attributed to evolutionary mixing (?). However, enhanced abundances are still observed in scarcely evolved main sequence stars, ruling out evolutionary mixing as the primary mechanism (??). Moreover, mixing of a degree high enough to explain the observed anomaly in cyanogen abundances would result in extended lifetimes and a broadened main sequence turn off region in the CMD of ancient GCs, which is not observationally supported. More recently, precision Hubble photometry revealed that almost every cluster in orbit of the milky way comprises multiple main sequences (???) (MMP) as opposed to a single stellar population (SP).

Single stellar populations had been assumed due to spectroscopically uniform iron abundances (?) and very narrow principal sequences (?), both of which are indicative of a single stellar population. The first conclusive evidence for MMPs came with Hubble Space Telescope (HST) high precision crowded field photometry in which three distinct main sequences in NGC 2808 were identified (?). Since this discovery, split main sequences have been found in nearly all Milky Way globular clusters studied by HST (??). Split stellar populations are believed to be due to enhanced helium abundances in the stellar populations formed after the primordial population of stars (??). When compared to primordial helium mass fractions ( $Y$ ) of  $Y \sim 0.25$  (?) or solar helium abundances  $Y \sim 0.27$  (?) these populations have mass fractions as high as  $Y \sim 0.4$ . Helium enhancement is strongly suspected to be the result of an earlier, more massive population dying off, enriching the interstellar medium (???). The primary open question then is not why some populations are enhanced in helium; rather, it is to what extent they are enhanced.

Due to the relatively high and tight temperature range of partial ionization for helium it cannot be observed in globular clusters; consequently, the evidence for these enhanced helium abundances originates from comparison of theoretical stellar isochrones to the observed color magnitude diagrams of globular clusters. None of the isochrones used to date in these comparison have been generated from models with self consistent chemistries.

## 2.5. *Population Opacities*

Given the relative historic difficulty in generating new opacity tables, stellar models have tended to use opacity tables whos range of compositions is derived from simple rescaling of the some solar composition. Here we use our OPLIB web scraper to generate opacity tables with compositions specific to each population in NGC 2808.

These population have been studied in depth by Feiden and their chemical compositions were determined in ? (see Table 2 in that paper). While we cannot currently make fully self-consistent models due to still ongoing atmospheric modeling, we can make a first pass investigation of the affect of OPLIB opacities (Figure ??). Note how the models generated using OPLIB opacity tables



**Figure 2.** 10 Gyr &  $Y=0.33$  isochrones for models generated with OPAL and OPLIB opacities tables (top). Residuals between isochrones (bottom).

have a systematically lower luminosity. Recall, that this is consistent with the overall lower opacities of the OPLIB tables.

### 2.6. *Additional Consistency*

The lack of self consistency presents problems at other stages of stellar evolution codes. Perhaps most importantly, where the interior of a stellar model meets the atmosphere. Atmospheric models such as a grey (?), Krishna Swamy (?), or Phoenix (?) model atmosphere provide one pressure boundary conditions to solve the two-point boundary value problem that is the equations of stellar structure. Once again however, models tend to use atmospheres with non consistent chemistries. Therefore, one key element of NGC 2808 modeling is the incorporation of new atmospheric models, generated from the MARCS grid of model atmospheres (?), which match interior elemental abundances. Members of our collaboration are currently working on such atmospheric modeling.

Finally, The isochrones used to infer the degree of helium enhancements assume that convection operates in the same manner in metal-poor stars as it does in the Sun. However, observations from *Kepler* of metal-poor red giants (??), in concert with interferometric radius determination of the

metal-poor sub-giant HD 140283 (?), have shown that the efficiency of convection changes with iron content. We will additionally modify DSEP to capture this variation in convective efficiency. While we wait for atmospheric modeling to be completed it makes sense to investigate other locations where opacity differences on the order of 5% may affect results.”s

### 2.7. *47 Tuc & NGC 6752*

In addition to NGC 2808, Feiden has generated MARCS atmospheric models for the clusters NGC 6752 and 47 Tuc. We will conduct the same, self-consistent, modeling for these clusters as we do for NGC 2808.

This research has made use of NASA’s astrophysical data system (ADS). We acknowledge the support of an NASA grant (No. 80NSSC18K0634). Additionally, we would like to thank James Colgan for his assistance with the OPLIB opacity tables. We would like to thank Aaron Dotter, and Elisabeth Newton for their assistance. Finally, we thank our colleagues and peers in for their continuing and appreciated support.