A Dissertation

titled

Numerical Simulations of Microturbulence in Hot Stellar Atmospheres

by

Michelle Deady

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Doctor of Philosophy Degree in Physics

Dr. Lawrence Anderson-Huang, Committee Chair

Dr. Jon Bjorkman, Committee Member

Dr. Michael Cushing, Committee Member

Dr. Victor Karpov, Committee Member

Dr. Biao Ou, Committee Member

Dr. Amanda Bryant-Fredrich, Dean
College of Graduate Studies

The University of Toledo
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Most of what we know about stars comes from their stellar spectral features. Among other things, these features can tell us about the star’s temperature and chemical composition. The spectral features are not delta functions and have some width that can be explained by some well known and understood broadening mechanisms. In addition to the standard broadening mechanisms, an additional term called microturbulence must be added to models to match observed features. In stars similar to the sun or cooler, microturbulence is well understood to be due to sub-surface convection zones near the upper portion of the star’s atmosphere, but the cause of microturbulence in hot stars is not fully understood. This thesis will explore Doppler shifts in the stellar atmosphere as a possible cause of microturbulence to see if it matches empirical trends. These Doppler shifts occur within the stellar spectral features themselves and would cause changes in the opacity of these features, leading to a local acceleration and producing a small velocity field. I will explore this by modeling different stellar atmospheres of different temperatures and surface gravities.
Acknowledgments

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<td>H-R</td>
<td>Hertzsprung Russel</td>
</tr>
<tr>
<td>LMC</td>
<td>Large Magellanic Cloud</td>
</tr>
<tr>
<td>SMC</td>
<td>Small Magellanic Cloud</td>
</tr>
<tr>
<td>Si</td>
<td>Silicon</td>
</tr>
<tr>
<td>O</td>
<td>Oxygen</td>
</tr>
<tr>
<td>Fe</td>
<td>Iron</td>
</tr>
<tr>
<td>LAPACK</td>
<td>Linear Algebra Package</td>
</tr>
<tr>
<td>ScaLAPACK</td>
<td>Scalable Linear Algebra Package</td>
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<tr>
<td>1D</td>
<td>One Dimensional</td>
</tr>
<tr>
<td>3D</td>
<td>Three Dimensional</td>
</tr>
<tr>
<td>ZAMS</td>
<td>Zero Age Main Sequence</td>
</tr>
<tr>
<td>MPI</td>
<td>Messaging Processing Interface</td>
</tr>
<tr>
<td>BLAS</td>
<td>Basic Linear Algebra Subroutines</td>
</tr>
<tr>
<td>BLACS</td>
<td>Basic Linear Algebra Communication Subroutines</td>
</tr>
<tr>
<td>FWHM</td>
<td>Full width at half maximum</td>
</tr>
<tr>
<td>EW</td>
<td>Equivalent width</td>
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<tr>
<td>ESO</td>
<td>European Southern Observatory</td>
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<td>M-S</td>
<td>Main Sequence</td>
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List of Symbols

\( a(\nu) \) \ldots \ldots The absorption cross section of an atom in terms of frequency. Given in terms of \( \phi(\nu) \)

\( \phi(\nu) \) \ldots \ldots Line Profile

\( B_{lu} \) \ldots \ldots Einstein B coefficient

\( \Gamma \) \ldots \ldots Damping Constant in Lorentzian function

\( u_0 \) \ldots \ldots Thermal velocity. Given in terms of \( \text{cm s}^{-1} \)

\( T \) \ldots \ldots Temperature. Given in terms of \( \text{K} \)

\( k \) \ldots \ldots Boltzman constant. Given in terms of \( 1.380658 \times 10^{-16} \text{erg K}^{-1} \)

\( M_\odot \) \ldots \ldots Mass of the Sun

\( c \) \ldots \ldots Speed of light given in terms of \( 3 \times 10^{10} \text{ cm s}^{-1} \)

\( \Delta \nu \) \ldots \ldots Change in frequency. Given in terms of \( \text{Hz} \)

\( \xi \) \ldots \ldots Mictoturbulent velocity. Given in terms of \( \text{km s}^{-1} \)

\( \nu_0 \) \ldots \ldots Initial frequency. Given in terms of \( \text{Hz} \)

\( V_{max} \) \ldots \ldots Outflow velocity given in terms of \( \text{cm s}^{-1} \)

\( V_s \) \ldots \ldots Isothermal sound speed given in terms of \( \text{cm s}^{-1} \)

\( P \) \ldots \ldots Pressure given in terms of \( \text{g cm}^{-1} \text{ s}^{-2} \)

\( G \) \ldots \ldots Gravitational constant

\( \AA \) \ldots \ldots Angstrom which is \( 1 \times 10^{-10} \text{m} \)

\( L_\odot \) \ldots \ldots Solar Luminosity

\( L \) \ldots \ldots Luminosity

\( \log g \) \ldots \ldots Surface gravity of a star given in terms of \( \text{cm s}^{-2} \)

\( W \) \ldots \ldots Equivalent width

\( \lambda \) \ldots \ldots Wavelength given in terms of \( \text{cm} \)

\( \rho \) \ldots \ldots The mass density. Given in terms of \( \text{g cm}^{-3} \)

\( f \) \ldots \ldots External force given in terms of \( \text{erg} \) \( \text{s}^{-1} \text{ cm}^{-2} \)

\( T \) \ldots \ldots Stress tensor

\( a^2 \) \ldots \ldots Isothermal sound speed given in terms of \( \text{cm s}^{-1} \)

\( \alpha \) \ldots \ldots The acceleration due to radiation given in terms of \( \text{cm s}^{-2} \)

\( H_\nu(\mathbf{m}) \) \ldots \ldots The radiation flux per unit frequency of the atmosphere.

\( U \) \ldots \ldots Internal energy given in terms of \( \text{erg} \)

\( \zeta \) \ldots \ldots Fraction of total pressure to electron pressure, unitless

\( P_e \) \ldots \ldots Electron pressure given in terms of \( \text{g cm}^{-1} \text{ s}^{-2} \)
\( \mu \ldots \) Mean weight of atomic nuclei given in terms of amu

\( j_\nu \ldots \) Emissivity

\( k_\nu \ldots \) Absorption

\( J_\phi \ldots \) Profile weighted to mean intensity given in terms of erg s\(^{-1}\) sr\(^{-1}\) cm\(^{-2}\) Hz\(^{-1}\).

\( J_\nu \ldots \) Intensity given in terms of frequency given in terms of erg s\(^{-1}\) sr\(^{-1}\) cm\(^{-2}\) Hz\(^{-1}\).

\( C_{ul} \ldots \) Collisional coefficient given in terms of cm\(^3\) s\(^{-1}\) erg\(^{-1}\)

\( A_{ul} \ldots \) Collisional coefficient for transition from upper to lower states. Given in terms of s\(^{-1}\)

\( \delta \ldots \) Fractional destruction by collisional deexcitation

\( \sigma_T \ldots \) Thompson cross section

\( \overline{N}_w \ldots \) Transition mean extinction

\( m \ldots \) Mean mass of hydrogen given in terms of g

\( \kappa_c \ldots \) Kramer opacity given in terms of cm\(^2\) g\(^{-1}\)

\( f \ldots \) Oscillator strength of a given transition

\( n \ldots \) Number density given in terms of cm\(^{-3}\)

\( R(\nu', x'; \nu, x) \ldots \) Redistribution function

\( g(n, n') \ldots \) Phase function

\( \gamma \ldots \) Angle between \( \mathbf{n} \) and \( \mathbf{n}' \)

\( x \ldots \) Averaged difference in frequency in Hummer redistribution functions, unitless

\( \mu \ldots \) Directional angle, unitless

\( V \ldots \) Volume given in terms of cm\(^3\)

\( u(m) \ldots \) The bulk velocity of the fluid in the atmosphere in the given \( m \)th direction. Given in terms of km s\(^{-1}\)

\( B_\nu \ldots \) Blackbody radiation in terms of frequency. Given in terms of erg s\(^{-1}\) sr\(^{-1}\) cm\(^{-2}\) Hz\(^{-1}\)

\( \sigma \ldots \) Steffen Boltzmann constant

\( g \ldots \) Acceleration due to gravity given in terms of cm s\(^{-2}\)

\( F_{\text{rad}} \ldots \) Radiation force

\( S_\nu(m) \ldots \) The source function in the \( m \)th direction. Given in terms of erg s\(^{-1}\) sr\(^{-1}\) cm\(^{-2}\) Hz\(^{-1}\)

\( I_\nu(m) \ldots \) The source function in the \( m \)th direction. Given in terms of erg s\(^{-1}\) sr\(^{-1}\) cm\(^{-2}\) Hz\(^{-1}\)

\( P_\nu(m) \ldots \) Featurier P

\( R_\nu(m) \ldots \) Featurier R

\( \kappa \ldots \) Opacity given in terms of cm\(^2\) g\(^{-1}\).

\( T_{\text{eff}} \ldots \) The effective temperature in the photosphere, given in terms of K.

\( H \ldots \) Scale height

\( R \ldots \) Radius given in terms of cm
\begin{itemize}
  \item $\tau$ \hspace{1cm} Optical depth
  \item $\Delta \nu_D$ \hspace{1cm} Doppler frequency given in terms of Hz.
  \item $B_{lu}$ \hspace{1cm} Einstein B coefficient for atomic transitions. Given in terms of $\text{cm}^3 \text{s}^{-2} \text{erg}^{-1}$
  \item $N_e$ \hspace{1cm} Number of electrons given in terms of $\text{cm}^{-3}$
  \item $h$ \hspace{1cm} Planck constant given in terms of $6.6260755 \times 10^{-27} \text{erg s}^{-1}$
  \item $\hbar$ \hspace{1cm} The Planck constant divided by $2\pi$ given in terms of $1.05457266 \times 10^{-27} \text{erg s}^{-1}$
  \item $\nu$ \hspace{1cm} Frequency given in terms of Hz
  \item $\sigma_j$ \hspace{1cm} Upper state cross section
  \item $\sigma_i$ \hspace{1cm} Lower state cross section
  \item $n_e$ \hspace{1cm} Electron fraction, unit-less value.
  \item $N_a$ \hspace{1cm} Number density of atoms. Given in terms of $\text{cm}^{-3}$
  \item $N_e$ \hspace{1cm} Number density of electrons. Given in terms of $\text{cm}^{-3}$
  \item $F_{\text{rad}}$ \hspace{1cm} The radiation Force of the atmosphere.
\end{itemize}
A line profile in the spectrum of a star arises from an electronic transition between energy levels of an atom or molecule. These features indicate the elements present in a stellar atmosphere and are important in the understanding of stars. Observing the different spectral features in a star gives information on the temperature, pressure, and velocity structure within the atmosphere. Microturbulence is one of the key factors that determine the width of spectral features in stellar spectra. It is known to exist, but the exact cause of microturbulence has yet to be completely understood in hot stars such as spectral types O, B, and A. As seen in Figure 1-1, a model with added microturbulence matches the observed spectral feature better than the model without microturbulence. In current one dimensional (1D) models of hot stellar atmospheres, microturbulence is included as a single parameter applied throughout the atmosphere to match observed results. Other than some recent work on opacity-driven convective instability, there has not been much research on possible causes of microturbulence in hot stellar atmospheres.

1.1 The Line Profile

Absorption features arising from bound-bound transitions of electrons in the atomic constituents of stellar atmospheres are determined from the local absorption
cross section:

\[ a(\nu) = \frac{\hbar \nu}{4\pi} B_{lu} \phi(\nu) \quad (1.1) \]

where \( B_{lu} \) is the Einstein B coefficient for the transition from a lower state to an upper state, and \( \phi(\nu) \) is a profile function normalized over frequency \( \nu \) such that

\[ \int \phi(\nu)d\nu = 1. \quad (1.2) \]

This profile has a natural width, but can also be broadened by several different mechanisms.

1.1.1 Natural Line Profile

Natural line broadening follows directly from the Heisenberg Uncertainty Principle, which states that it is not possible to know exactly both the lifetime of an excited
state and its energy.
\[
\Delta t \Delta E \geq \frac{\hbar}{2} \quad (1.3)
\]

It follows that an excited state with a short lifetime will have a large energy uncertainty. This large energy uncertainty causes the line to be broadened in a Lorentzian distribution with the form of:

\[
\phi_\nu = \frac{\Gamma}{4\pi^2(\nu - \nu_0)^2 + \frac{\Gamma^2}{2}} \quad (1.4)
\]

where the damping width, \( \Gamma \), of the Lorentzian profile is almost always much narrower than the broadening due to thermal motions.

### 1.1.2 Thermal Broadening

Thermal broadening occurs naturally from thermal motions in the atmosphere. Not all particles in the atmosphere travel at the same velocity and, this spread in velocity broadens spectral features. This effect is purely dependent on the mass and temperature of the particles. The absorption profile resulting from a thermal Maxwellian distribution of atom velocities is a Gaussian profile in frequency in the form:

\[
\phi_v = \frac{1}{\sqrt{\pi} \Delta \nu_D} e^{\left(\frac{\Delta \nu}{2 \Delta \nu_D}\right)^2} \quad (1.5)
\]

where

\[
\Delta \nu = \nu - \nu_0 \quad (1.6)
\]

is the frequency offset from the line center at \( \nu_0 \),

\[
\Delta \nu_D = \frac{u_o}{c} \nu_0 \quad (1.7)
\]
is the fiducial Doppler broadening, and

\[ u_0 = \left( \frac{2kT}{M} \right)^{\frac{1}{2}} \]  

(1.8)

is the root mean square velocity for atoms of mass M at temperature T.

1.1.3 Pressure Broadening

Another mechanism that broadens spectral features is pressure. In a stellar atmosphere particles are close together and this proximity to each other causes particles to be more likely to collide. If the time between the collisions is shorter than the natural lifetime, from the Heisenberg Uncertainty Principle the energy is not as well defined.

Because this type of broadening is based on how often particles collide, factors that affect pressure broadening include the temperature of the atmosphere and the density. High temperature, very dense atmospheres will see more effects from pressure or collisional broadening compared to low temperature, or low density atmospheres. Due to the impact on lifetimes, the profile is Lorentzian.

1.1.4 Rotational Broadening

The final broadening mechanism is due to rotational effects. Rotational broadening is a more macroscopic effect compared to pressure and thermal broadening since it deals with the motion of the star itself. Stars rotate about their own axis of rotation. Rotational broadening Doppler shifts the contributions from different parts of the star, due to the shift of the line of sight velocity of the surface as the star rotates. This is different from the Doppler shifts from the thermal motions. The bulk motion does not influence the integrated absorption along the line of sight, so the local profile remains unchanged.
1.1.5 Convolution

Convolution is the combination of simultaneously acting broadening mechanisms. In most cases, there are multiple types of line broadening present that have to be taken into consideration, and since the different mechanisms can follow different probability distributions it is not as simple as just adding the two broadening mechanisms together. Some of the mechanisms show up predominately in the wings of the line versus line center and vice versa. What convolution does is to combine the different broadenings into a new feature. Convolution combines the different broadening features into a new feature by integration:

\[
\phi_V = \int_{-\infty}^{\infty} \frac{1}{\sqrt{\pi \Delta \nu_D}} e^{\left(\frac{-\Delta \nu}{\Delta \nu_D}\right)^2} \frac{\Gamma}{4\pi^2(\nu - \nu_0)^2 + \frac{\Gamma^2}{2}} d\nu
\]

(1.9)

It typically results in a Voigt profile rather than the original Gaussian, or Lorentzian profiles that are independently present.

1.1.6 Dominant Mechanism

For this study the dominant form of broadening is due to thermal motions. If \(\Delta \nu_D \gg \Gamma\), natural broadening only adds to the far wings where turbulent Doppler shifts have less effect. Along with thermal motions, the other form of broadening that is included is natural broadening. The stars used in this thesis are fairly hot but not that dense, so pressure broadening is not needed. As this study is a numerical calculation of the local line formation and its influence on the local velocity fields, it also does not include rotational rotational broadening. Only the thermal broadening will be used to find the microturbulent velocities discussed in a later chapter.
1.2 Curve of Growth

A curve of growth is another way to analyze spectral features. While the line profile itself shows the wings and the central feature of the spectral line, the curve of growth shows the equivalent width of the line and the number of atoms of the spectral feature. The equivalent width is another way of looking at spectral features. Equivalent width is the small rectangular area that has the same value as the area of the entire spectral feature. This rectangle starts from the top of the continuum and goes down. Analyzing the curve of growth gives information about the abundance of the elements, temperature, microturbulence, and pressure.

The curve of growth can be broken into three different regimes of the spectral feature. In the first part of the curve of growth, the slope is equal to one. This is the regime where the spectral feature is optically thin so the equivalent width is proportional to the number of atoms. The second part of the curve of growth has a slope of the log of the number of particles. This is the part where the Gaussian profile is saturated and has a high optical depth. The third part of the curve of growth has a slope of close to one half. This is the upper portion of the curve of growth and the spectral feature is also very saturated at this point as well. Unlike the middle region where the Gaussian profile is dominate, the top portion of the graph is dependent on the Lorentzian profile due to collisional broadening. Figure 1-2 shows a full sample curve of growth.

In this particular case to see the impact of microturbulence on the curve of growth, the important region of the graph is the flat portion. If there is microturbulence or Doppler shifts involved in the line feature, then this portion of the curve of growth is raised compared to the same curve of growth without microturbulence. As seen in Figure 1-2, different values of microturbulence raise the flat portion of the curve of growth.
Figure 1-2: A sample curve of growth of a spectral feature. (Figure 16.5 Gray 2005) The y axis describes the equivalent width while the x axis is in terms of abundance of a specific element.

1.3 Microturbulence

Despite reasonably well-understood physics concerning the previous four broadening mechanisms, observed spectral features require additional broadening. This additional broadening appears in all spectral lines in about the same amount, and can be simulated by increasing the thermal width $\Delta v_D$ by a fixed value, usually expressed as an addition to the mean thermal velocity. The fact that one value fits all lines suggest the origin lies in bulk motions with a distribution similar to the thermal velocity distribution of individual atoms. This broadening is called microturbulence.

Microturbulence arises from turbulent motions that are close to one mean free path length of a photon in the star’s atmosphere. Typical derived values of microturbulence are anywhere between 2 km/s and 20 km/s or higher and are somewhat correlated with the effective temperature and surface gravity of the star, as seen in Figure 1-3. As the temperature of the atmosphere increases and/or the surface gravity decreases, the values of microturbulence increases. This dependence on temperature
and surface gravity suggests that the contribution of the radiation pressure working against gravity in the hydrostatic equilibrium of the atmosphere plays a significant role.

1.3.1 Microturbulence in Late Type Stars

Late type stars similar to the Sun are also impacted by microturbulence in spectral features, but the cause of the microturbulence is understood. These stars are cooler stars on the Hertzprung Russel (H-R) diagram. The energy transport mechanism in these stars differs from hotter stars and so the mechanism that causes microturbulence in low mass stars may not be the same as that in hot stars.

The structure of the interior of stars depends on the most effective way to transport energy throughout the atmosphere. Typically cooler layers become convective as they become too opaque to support radiative transport. Stars with temperatures around 8,000 K or cooler transport their energy from the core outwards through radiative zones to the convective outer layers of the stars’ envelope, this can form small sub-surface convection zones near the division between the radiative zones and the convective zones. These sub-surface convection zones are the source of microturbulence in stars whose masses are roughly equal to or less than that of the Sun. As a result, line profiles are well matched by radiative transfer in 3D models that include hydrodynamic convection.

1.3.2 Possible Causes of Microturbulence

Currently there are a few different theories on the cause of microturbulence in hot stars. One of the possible causes of microturbulence is instability in the upper radiative layers of the atmosphere due to buoyancy pressure. This instability arises because the upper layers are essentially floating on a sea of photons below. Figure
Figure 1-3: Graph of surface gravity (log g) vs Effective Temperature (K). The different values of microturbulence are listed in the table on the right with black being 0 km/s microturbulent velocity up to gray with a microturbulent velocity of 23.40 km/s. 1-4 from Cantiello et al. 2009 shows a schematic of where the microturbulence might be located. Notice in the figure that at the level where microturbulence is located there are also acoustic and gravity waves, which also contribute to the broadening.

One of the other strong possibilities for the cause of microturbulence is Doppler shifts of the photons in the atoms frame. Any bulk motion of the fluid will shift spectral features, exposing photons to higher or lower opacities in the line profile. These changes in opacity will contribute additional radiation pressure, which will in turn accelerate or decelerate the material, causing the opacity to shift even further. It is this mechanism that is explored in this thesis.

1.3.3 Historical Treatment of Microturbulence

Historically, microturbulence in hot stellar atmospheres has been treated by adding a term after the fact to help make synthetic spectra fit observed stellar line features.
The Doppler width becomes:

$$\Delta \nu_D = \frac{u_o + \xi}{c} \nu_o$$

(1.10)

where $\xi$ is expressed in km/s.

The value $\xi$ of the microturbulence is usually the same throughout the entire atmosphere independent of depth and atomic species. The argument for using a single value has been that generally all spectral features show roughly the same amount of extra broadening.

### 1.4 Stellar Winds as a Possible Cause of Microturbulence

Due to their high luminosities, early type stars usually have stellar winds and mass loss during their lifetimes. These winds have been suggested as one of the
possible causes of or a replacement for microturbulence. Stellar winds appear near the photosphere layer of the atmosphere and create their own velocity field. Depending on the strength of the wind, this could cause motions similar to that attributed to microturbulence. This method is discussed by Kudritzki (1992) in relation to weak metal lines.

1.4.1 Model

The model used by Kudritzki is a 1D plane parallel atmosphere code. This is justified because the scale height of portion of the atmosphere being modeled is much less than the radius of the star, so the problems with plane parallel atmospheres that are discussed in the next chapter are avoided (Kudritzki 1992). In order to model it, the atmosphere is broken into two portions, the part of the atmosphere that includes the stellar wind outflows and the portion not impacted by the stellar winds. The velocity field separating the two regimes is defined by the outflow velocity and the sound speed. When the outflow velocity reaches three times the isothermal sound speed that is the area that includes stellar winds (Kudrizki 1992):

\[
\frac{V_{\text{max}}}{V_s} = v_{\text{max}} = 3
\]  

(1.11)

where \(V_{\text{max}}\) is the outflow velocity, and \(V_s\) is the isothermal sound speed. By setting the stellar wind outflow velocity to three, the weaker lines were modeled with a lower stellar wind outflow. Having a larger stellar wind will cause other issues with the formation of the weaker lines in a stellar spectra and larger mass outflows of stars have to be modeled in a different fashion. So by setting the max value of the outflow velocity to three times the isothermal sound speed they did not have to worry about large mass outflows or stellar winds. This way they could model smaller winds and look at the weaker metal lines. The stars that were targeted by this work also did
not include stars with large stellar winds as they were focusing on B type stars on the main sequence.

In the portion of the atmosphere in which the stellar winds do not impact the radiative transfer, LTE conditions may be used. In the regime that the stellar winds are located, the temperature is not constant with mass outflow and the velocity fields, so local thermodynamic equilibrium (LTE) is not a valid assumption and it is necessary to use non local thermodynamic equilibrium (NLTE) calculations.

1.4.2 Results

Kudritzki finds that for small values of microturbulence it is possible to get the same results using only stellar winds in the upper portions of the atmosphere. The problem arises for larger values of microturbulence, as the stellar wind is only able to give small values (Kudriztki 1992). Therefore it can be concluded that stellar winds are not the entire cause of microturbulence in hot stars. Stellar winds can mimic the same effects as microturbulence for small values, but it fails for larger values, greater than 20 km/s, as seen in Figure 1-3. This provides evidence that microturbulence does exist and is not just an effect that can be masked by other portions of the star’s atmosphere.

The other problem with stellar winds being the sole cause of microturbulence in early type stars is the issue of the strength of the winds. The case discussed here has stellar winds with a maximum speed of three times the isothermal speed of sound and did include values for stars that have massive winds that would account for velocities higher than that. In the early star regime, the stars may have extremely large winds and mass outflows especially in O and B spectral type stars. When the stellar winds are large more mass is being lost, but these velocities are significantly higher than the isothermal sound speed.
1.5 Sub-Surface Convection Zones as a Possible Cause of Microturbulence

Other astronomers have touched on possible causes of microturbulence in hot stellar atmospheres. Cantiello et al (2009) is one of the most recent detailed papers that discuss causes of microturbulence. They suggest that a small sub-surface convection zone near the top of the atmosphere may create small-scale velocity fields that could be the cause of microturbulence. This form of microturbulence is found in stars later than type A, but this work is the first time that microturbulence in hot stars has been suggested to be a result of the same convection. In the past, sub-surface convection has been neglected in stellar atmosphere codes since it is assumed these would not affect the star’s spectra, but Cantiello suggests that convection driven by heavy element opacities, in particular iron, will be vigorous enough to reach the star’s photospheric, visible surface, layers (Cantiello et al 2009). They model these regions with a hydrodynamic stellar structure code and appropriate Ledoux criterion.

The model used by Cantiello is based on the observations done by the European Southern Observatory (ESO) FLAMES Survey of Massive Stars done in 2005 (Evans et al 2005). Cantiello modeled a variety of stellar masses and metallicities to determine whether the sub-surface convection zones would be an appropriate cause of microturbulence in hot stars. The metallicities used in this model are Z=0.02, Z=0.004, and Z=0.008 which simulate a star with near solar metallicity, and semi-metal poor star and a metal poor star respectively. The masses used in the model range from 5\(M_\odot\) to 100\(M_\odot\), a wide range of masses for early type stars and all significantly more massive than the Sun.
1.5.1 Sub-Surface Convection Zones

The Ledoux criterion determines whether perturbations are stable or unstable on the macroscopic level. In the specific case of stellar atmospheres, it determines whether otherwise radiative layers of the atmosphere would be stable against convection based on the inequality:

\[ \nabla_{\text{rad}} < \nabla_{\text{ad}} + \frac{\varphi}{\delta} \nabla_{\mu} \]  

(1.12)

The thermodynamic gradients are given by:

\[ \nabla_{\text{rad}} = \left( \frac{d \ln T}{d \ln P} \right)_{\text{rad}} = \frac{3}{16 \pi acG} \frac{\kappa l}{m T^4} \]  

(1.13)

the gradient required to carry the entire energy flux by radiation alone,

\[ \nabla_{\text{ad}} = \left( \frac{d \ln T}{d \ln P} \right)_{\text{ad}} \]  

(1.14)

the local adiabatic gradient, and

\[ \nabla_{\mu} = \left( \frac{d \ln T}{d \ln P} \right)_{\mu} \]  

(1.15)

the local gradient due to stratification of the chemical potential.

As discussed in the previous section, the sub-surface convection zones are a potential source of microturbulence in hot stellar atmospheres. It is the source of microturbulence in low mass stars and is well understood in that regime. These convection zones are close to the photosphere itself and form weak helium and iron convection zones. The iron convection zones follow the Ledoux criterion discussed above. There may also be helium sub-surface convection zones that exist in certain circumstances, but these are in general much weaker than the iron convection zones and are able to
Figure 1-5: Opacity versus temperature of a 60 $M_\odot$ Zero Age Main Sequence Star (ZAMS). Notice that the iron and helium bumps appear at roughly the position and temperature range no matter what the metallicity. The different colored lines corresponds to different stellar metallicities used going from a close to solar metallicity star to a metal poor star. Cantiello et al 2009

be neglected (Cantiello et al 2009). As seen in Figure 1-5, no matter the metallicity of the star there is a very strong iron peak at approximately the same temperature. This result shows that even in the metal poor stars that there exists a possibility of an iron sub-surface convection zone near the photosphere. The depth of these zones will be dependent on the metallicity, temperature, and luminosity of the star. Very metal poor stars are less likely to have iron convection zones simply because there is not enough iron in the star for convection so the energy transport in the iron regime would be predominately radiation (Cantiello et al 2009).

These sub-surface convection zones will have an impact on the microturbulent velocity of the atmosphere. As seen in Figure 1-6 for the Large Magellanic Cloud (LMC) the higher luminosity corresponds to a larger value for microturbulence.

The occurrence of these iron convection zones facilitate the gravity and acoustic waves in the atmosphere that can be the cause of microturbulence. Gravity waves are
caused in atmospheres by the change in pressure and density of the convection zones in the atmosphere itself as it reaches an equilibrium with buoyancy and gravity. These zones are usually considered to be subsonic which allows for gravity waves within the atmosphere to move freely compared to the sound waves. The propagation of these waves causes perturbations in the density of the photosphere. As the iron convection zones become larger, there is a greater chance of gravity waves forming at the surface, causing a change in density and microturbulence (Cantiello et al 2009).

### 1.5.2 ESO-FLAMES Survey

Cantiello’s work on sub-surface iron convection zones in the atmosphere uses values of microturbulence and other data for the LMC and SMC that comes from the ESO-FLAMES Massive Star Survey (2005). This survey looked at 61 B spectral type stars...
in four fields within the Milky Way for narrow line spectra (Trundle et al 2007). The stars used as part of the survey had to meet the following criteria: the stars could not be earlier than spectral type O9, could not be contaminated by a secondary object, and had to have silicon lines in order to calculate the effective temperature (Trundle et al 2007). After the observations are reduced the next step is to simulate these stars in a hydrodynamical code called TLUSTY to get information about metallicity of the stars, effective temperature, microturbulence, and surface gravity.

1.5.3 Calculations of the Microturbulence

The values for the microturbulence used for Cantiello’s work on the cause of microturbulence comes from Hunter’s (2007) work from the FLAMES survey. Similar to the method used in Steffen et. al. (2013), which will be discussed later, the values of microturbulence come from studying the equivalent width of specific spectral features. To find the equivalent width of the chosen spectral feature after data reduction the spectra of each star was normalized and fitted to find the width of the absorption features. These features are then fitted by a Gaussian profile and from that the equivalent widths are calculated.

In this case since the stars that are being considered here are B stars, silicon (Si) and oxygen (O) ions are good candidates to fit the curve of growth to find the equivalent width of the feature. Because there are many ions in close proximity of each other with oxygen’s triplet states, the spectral feature used to determine the microturbulence for the survey is the Si III triplet occurring between 4552-4574 Å (Hunter et al 2007). The argument for using this triplet compared to singlet lines of Si or other metals that have well defined features is that the Si III line appears in all of the stars in the survey whereas some of the other metals may not appear or have well defined equivalent width approximations. By using the triplet compared to the singlet, one can eliminate systematic errors that could appear in the oscillator
strength calculations since it will be averaged out over all the lines. Choosing the same spectral features for all stars in the survey brings consistency to the measurements of microturbulence. In general, microturbulence is not based on the specific ion or element in question as all spectral features will show the same amount of broadening, but due to measurements and calculations there can be some variance of microturbulence. Figure 1-7 shows the results of the microturbulent velocity calculations from the FLAMES survey.

Using information from the FLAMES survey Cantiello used an initial value of $\xi=10$ km/s in their model as a starting basis. This gives a starting point consistent with the observations of stars of this temperature but allows for the fluctuations of both gravity and temperature along with the effect of the different metallicities of the stars. They then modified this value to find the actual values of microturbulence by looking at the energy caused by microturbulence. Instead of looking directly at the microturbulent velocities Cantiello instead looked at the energy caused by microturbulent motions and compared it to the energy from gravity waves to find the values of their model’s microturbulence. For the sub-surface convection zones to cause microturbulent motions, the ratio of the gravity waves and microturbulence has to be greater than 1 (Cantiello et al 2009):

$$\frac{E_g}{E_{\xi}} \geq 1 \quad (1.16)$$

1.5.4 Results

As seen in Figure 1-6, the values of microturbulence found from Cantiello’s work on sub-surface convection zones fit with a similar pattern to other work on the subject but leaves the question concerning the lower limit of luminosity. At certain luminosity thresholds for the three different areas, $10^{3.2}L_\odot$ for the Milky Way, $10^{3.9}L_\odot$ for
Figure 1-7: Values of microturbulence versus surface gravity for 50 B stars from the FLAMES survey (Hunter et al 2008)

the LMC, and $10^{4.2}L_\odot$ for the SMC there are no helium or iron sub-surface convection zones (Cantiello 2009). This poses a problem as stars below these luminosity thresholds are still considered to be early type stars and show the signatures for microturbulence but do not have these convection zones attributed to them. This method works for stars that are above the threshold set, but is not applicable for stars below.

Sub-surface convection zones are a possible cause for microturbulence but as discussed above do not work for all early type stars and so cannot be said to be the sole reason of microturbulence in hot stellar atmospheres. If this was the case, then the cause of microturbulence for all stars would be the sub-surface convection zones no matter what the mass or luminosity of the star. Since not all early type stars have this sub-surface convection zone, another method needs to be used that can include the star set that does not form the convection zones. This could be the Doppler shift method discussed in this thesis. The Doppler shift method is not dependent on the metallicity or the luminosity of the star to the extent required for the sub-surface
convection zones to form, so this allows for the existence of microturbulence in these stars at low metallicity or lower luminosity.

1.6 Closing Remarks

The next chapter will go into a detailed discussion of the physical processes that are involved in the calculated model atmosphere. The equations will include all the equations and descriptions of terms within the equations to set up the physical picture of the atmosphere and all of the assumptions that will be included in further detail. This will include the equations for mass, momentum, and energy conservation, radiative transfer, the source function, and accurate frequency and direction redistribution for the radiation. The physical assumptions will be defended as usable with the model. The following chapter will discuss the numerical process. It will include a discussion on the grid itself and how the cell size is to be calculated. Included in this chapter is a discussion of the assumptions needed for the numerical simulation including a discussion on why the simulation of a single spectral feature in the atmosphere is a valid replacement for the standard treatment of simulating multiple spectral features within the atmosphere. In later chapters I will discuss computational algorithms, and results for a velocity dependent radiation field for three different stars along with future work.
Chapter 2

Assumptions and Equations

2.1 The Model

While Cantiello et al. looked at one possible source of microturbulence, they did not explore any other possible sources, such as turbulence due to changing radiation pressure. Our model is a 3D radiation hydrodynamic code used to study the atmospheric dynamics of hot stars with radiation pressure gradients comparable to gravity. In order to calculate a velocity field entirely consistent with the acceleration driven by the Doppler shifts of spectral features arising in that same velocity field, we make one great simplification; the entire radiation field is transported over a narrow range of frequencies surrounding one characteristic bound-bound transition.

2.2 Assumptions

Stellar atmosphere models require a good understanding of the underlying physics involved from magnetism to fluid dynamics. Because of this, these models can get complicated fairly quickly if all the physics is included. We can make some simplifying assumptions, however, without affecting qualitative behavior.
2.2.1 A Fully Three Dimensional Atmosphere

Using a plane parallel atmosphere is a common simplification that takes the atmosphere and breaks it up into horizontal layers that stack to create the atmosphere, where it is assumed that all variables remain constant on horizontal surfaces. This simplification means one only has to follow the radiation field as a function of height, direction (zenith angle), and frequency. All other state variables will depend only on height. As a corollary, line absorption profiles will also be essentially isotropic and horizontally self-similar. However if velocity fields are significantly turbulent, the Doppler shift of a narrow spectral line will not be horizontally self-similar, and photons may escape differently in different directions and from different horizontal locations. That inhomogeneity will then stir up the atmosphere, making temperatures and pressures also inhomogeneous. Our model uses a fully three dimensional atmosphere, allowing both atoms and photons to move freely in any direction. A fully three dimensional model requires knowing the values for the temperature, pressure, and radiation field at every location in the atmosphere as it is allowed to vary from cell to cell.

2.2.2 Non-Magnetic Fluid

The atmosphere is assumed to be non-magnetic so magnetohydrodynamics are not included in the model. In general, stars have a magnetic field that should be taken into consideration, but the interactions between the field and the particles may not be strong enough to impact the strength of the spectral features. If this is the case, then it is a valid to state that the fluid is non-magnetic without losing any of the physics involved with magnetism.

This holds true in the model discussed because the main source of line broadening is from the Doppler shifts. Doppler shifts do not depend on the alignment of the
electrons in the atom, which is one of the effects from magnetohydrodynamics if there is a weak magnetic field. The alignment changes the polarization, but not the speed of the fluid itself. Since both the bulk velocity of the fluid and the speed of sound is independent of the magnetic field of the star, the details of the magnetic field are irrelevant to the problem considered here.

2.2.3 Non-Relativistic Fluid

Relativity becomes a concern when the speed of the particles approaches the speed of light. At that point, particles start to behave differently and general relativity should be considered as the velocities get large. If the velocities of the fluid or object are not near the speed of light, then the classical equations are valid and will give the same results as special relativity. For Main Sequence (M-S) stars the atmosphere is non-relativistic. The magnitudes of the speed of sound and the bulk velocity do not approach relativistic speeds. Since this is the case there is no need to use the relativistic equivalent of the classical equations. The cases where relativity should be considered are stellar remnants such as white dwarfs, black holes, and neutron stars.

2.2.4 Local Thermodynamic Equilibrium

The model used here assumes that the stellar atmosphere is not in local thermodynamic equilibrium (LTE) and instead uses two level atom. Local thermodynamic equilibrium describes the balance between the radiation temperature and the velocity temperature in the atmosphere. If the two temperatures are equal to each other locally then the atmosphere can be assumed to be in LTE, and the radiative source function (emissivity/absorption) becomes isotropic and equal to the Planck function.

This model does not assume local thermodynamic equilibrium, and does not use Boltzmann statistics to find the number of electrons in the different states. Instead,
the information for the ratio of electrons in the different states comes from the opacity and the radiation field at each time step. This is a more realistic approach than the local thermodynamic equilibrium assumptions since the ratio of electrons in the different states of the atom becomes dependent on the radiation field and its scattering properties. Therefore a weaker radiation field would not have as many electrons in an upper state as an atmosphere with a stronger radiation field.

2.3 Equations for a Fluid

In the stellar atmosphere model mass, momentum, and energy are conserved.

2.3.1 Conservation of Mass

The equation of mass continuity in general form is:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$ (2.1)

where $\rho$ is the density within volume element $dV$ and $\mathbf{u}$ is the bulk velocity of the field. The natural logarithm of the density is used instead as it is nearly linear with height in an otherwise hydrostatic atmosphere. The continuity equation for the system can then be written in derivative format as:

$$\rho \frac{\partial \ln \rho}{\partial t} + \nabla \cdot (\ln \rho \mathbf{u}) = 0$$ (2.2)

or in integral form:

$$\frac{\partial \ln \rho}{\partial t} = \frac{-1}{\rho dV} \int \rho' \mathbf{u} \cdot dA.$$ (2.3)

where $dV$ is the differential volume element and $dA$ is a surface element normal to that volume.
2.3.2 Conservation of Momentum

For fluids the main equation to describe the motion is the Navier-Stokes Equation. This equation is the conservation of momentum and Newton’s second law for fluids, and in the generalized form is given by:

$$\rho \left( \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla P + \nabla \cdot \mathbf{T} + \mathbf{f}$$  \hfill (2.4)

where \(\mathbf{u}\) is velocity, \(\rho\) is density, \(P\) is pressure, \(\mathbf{T}\) is the stress tensor, and \(\mathbf{f}\) is the external force. The external force in this case is the force due to the gravity of the star and the force applied by the radiation field. The stress tensor contains terms relating to the viscosity of the fluid and the heat conduction terms. For this system, there are no viscosity and heat conduction terms so instead Euler’s equation is a valid approximation:

$$\rho \left( \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla P + \mathbf{f}$$  \hfill (2.5)

For a component in the \(m^{th}\) direction Euler’s equation becomes:

$$\frac{\partial u_m}{\partial t} + \mathbf{u} \cdot \nabla u_m = -\frac{1}{\rho} \frac{\partial P}{\partial s_m} + \frac{1}{\rho} f_m$$  \hfill (2.6)

Knowing that:

$$u_m = \mathbf{u} \cdot \mathbf{n}_m$$  \hfill (2.7)

with \(\mathbf{n}_m\) the unit vector pointing in the \(m^{th}\) direction, and where \(ds_m\) is a differential length element along \(\mathbf{m}\).

Focusing on the pressure term, we can rewrite the pressure in terms of \(\rho\) and the isothermal sound speed \(a\). The square of the isothermal sound speed is given by:

$$a^2 = \frac{P}{\rho}$$  \hfill (2.8)
then we can write the momentum equation as:

$$\frac{1}{\rho} \frac{\partial \rho}{\partial s_m} = \frac{1}{\rho} \frac{\partial (\rho a^2)}{\partial s_m} = \frac{1}{\rho} \left( \frac{\partial a^2}{\partial s_m} \right) = \frac{1}{\rho} \left( \frac{\partial a^2}{\partial s_m} + a^2 \frac{\partial \rho}{\partial s_m} \right)$$

(2.9)

which can be further simplified into:

$$\frac{1}{\rho} \frac{\partial \rho}{\partial s_m} = \frac{\rho a^2}{\rho} \left( \frac{1}{a^2} \frac{\partial a^2}{\partial s_m} + \frac{1}{\rho} \frac{\partial \rho}{\partial s_m} \right) = a^2 \left( \frac{\partial}{\partial s_m} \left( \ln a^2 + \ln \rho \right) \right)$$

(2.10)

The external force acting on the atmosphere is the combination of the force of gravity and radiation force so \( \mathbf{f} \) can be written in component form as:

$$f_m = \rho g_m + \rho \alpha_m$$

(2.11)

where radiation acceleration \( \alpha \) is given by:

$$\alpha_m = \frac{4\pi}{c} \int \kappa_{\nu,m} H_{\nu,m} d\nu$$

(2.12)

and \( H_{\nu,m} \) is the net radiative flux per unit frequency in direction \( \mathbf{m} \) and \( \kappa_{\nu,m} \) is the opacity in cm\(^2\) gram\(^{-1}\). Notice that the opacity is direction-dependent. This results from the directional dependence of the Doppler shifts. Then the total momentum conservation equation in component form becomes:

$$\frac{\partial u_m}{\partial t} + \mathbf{u} \cdot \nabla u_m = g_m + \alpha_m - a^2 \left( \frac{\partial}{\partial s_m} \left( \ln a^2 + \ln \rho \right) \right)$$

(2.13)
2.3.3 Conservation of Energy

One of the other major conservation equations is the conservation of energy. A general form of the energy conservation is given by:

\[
\frac{\partial}{\partial t} \left( \frac{1}{2} \rho u^2 + \rho U \right) + \nabla \left[ \left( \frac{1}{2} u^2 + U + \frac{P}{\rho} \right) \cdot \rho u \right] = \rho u \cdot f + \rho \frac{Dq}{Dt} \tag{2.14}
\]

Conservation of energy in a non-relativistic non-viscous radiating fluid may be expressed as:

\[
\frac{\partial}{\partial t} \left( \frac{1}{2} u^2 + U \right) = a^2 \frac{\partial \ln \rho}{\partial t} - u \cdot \nabla \left( \frac{u^2}{2} + U + a^2 \right) - \frac{1}{\rho} \nabla \cdot F_{\text{rad}} + u \cdot g \tag{2.15}
\]

where \( U \) is the internal energy per gram and \( F_{\text{rad}} \) is the radiative flux.

Characteristically, the dynamic terms on the right hand side are of order \( a^3 H \) where \( H \) is the density scale height and \( ag \), which for this work are both of order \( 10^{10} \text{ergs gram}^{-1} \text{s}^{-1} \). On the same scaling, \( \frac{F_{\text{rad}}}{\rho H} \), the radiation divergence is minimally of order 1000 times greater at the base of the models here and much greater at optical depths near unity. Thus, the material’s internal energy equilibrates with the radiation field considerably faster than either adiabatic expansion or advection. So one can instead find the local radiative equilibrium instead of using energy conservation.

Local radiative equilibrium may be written

\[
a^2 = \frac{\zeta k T}{(\zeta - 1) \mu} = \frac{\zeta k}{(\zeta - 1) \mu} \left( \frac{cB_{\text{rad}}}{4 \sigma} \right) \tag{2.16}
\]

Here \( \zeta = \frac{P_{\text{tot}}}{P_e} \), the ratio of total gas pressure to electron pressure, \( \mu \) is the mean weight of atomic nuclei, and \( B \) is a suitably chosen Planck energy density of radiation as determined from the equation of radiative equilibrium.
2.4 Radiative Transfer

2.4.1 Equation for Radiative Transfer

Radiative transfer describes the transport of radiation energy in the system in a specific direction. Radiation is described in terms of the specific intensity \( I_\nu \). We will assume that the radiation can be treated in an instantaneous manner with no time dependency. This assumption is related to the assumption of local radiative equilibrium, and is accurate as long as the photon diffusion time is much shorter than the dynamic relaxation time.

The standard form of the time independent equation of transfer is given as:

\[
\frac{\partial I_\nu(s)}{\partial s} = \rho \kappa_\nu (S_\nu(s) - I_\nu(s)) \tag{2.17}
\]

where \( I_\nu(s) \) is the specific intensity in the \( s \)th direction, \( S_\nu \) is the source function, \( \rho \) is the density and \( \kappa \) is the opacity in terms of \( \frac{cm^2}{g} \). Considering a ray in the \( m \)th direction we can write the equation for radiative transfer as:

\[
\frac{\partial I_\nu(m)}{\partial s_m} = \rho \kappa_\nu (S_\nu(m) - I_\nu(m)) \tag{2.18}
\]

This holds true for static, non-relativistic fluids in the lab frame. In this frame both \( \kappa_\nu \) and \( S_\nu \) are direction dependent in the presence of bulk motions. If instead one transposes the Doppler shifts of the material into the co-moving frame, there is an additional term added to the equation of radiative transfer to account for the shift since the opacity is no longer the same for all photons. Since the Doppler shifts within the line profile moves the line center the opacity in the line feature changes. Along with this fact at times it is necessary to deal with radiative transfer in the co-moving frame. This is because when the photons get Doppler shifted they get exposed to
different opacities of the material, so the equation of radiative transfer becomes:

\[ \frac{\partial I_\nu(m)}{\partial s_m} = \rho \kappa_\nu(S_\nu(m) - I_\nu(m)) + \frac{\nu}{c} \frac{\partial u_m}{\partial s_m} \frac{\partial I_\nu(m)}{\partial \nu} \]  

(2.19)

in the co-moving frame, where we may assume that \( \kappa_\nu \) and \( S_\nu \) are isotropic.

### 2.4.2 Source Function

The source function \( S_\nu \) in the radiative transfer equation should account for all contributions from thermal emission and scattering into the beam from other directions and frequencies. \( S_\nu \) can be written in terms of the emissivity \( j_\nu \) and the total extinction \( \chi_\nu \), which includes both absorption and scattering terms:

\[ S_\nu = \frac{j_\nu}{\chi_\nu} \]  

(2.20)

It helps to break this function into components for the line and continuum:

\[ S_\nu = \frac{\chi_l j_l + \chi_c j_c}{\chi_l + \chi_c} \]  

(2.21)

This source function is easiest to formulate in the co-moving frame of the fluid, where \( \chi_\nu \) is isotropic. Also, in local radiative equilibrium total photon energy is conserved, so we can effectively write all contributions in terms of scattering redistribution functions in the co-moving frame.

### 2.4.3 Redistribution

The source function includes scattering redistribution in frequency and direction. A general form of redistribution in the co-moving frame is the following:

\[ R(\nu', n'; \nu, n) = f \left( \nu - \frac{\nu_0}{c} n \cdot u \right) P \left( \nu - \frac{\nu_0}{c} n \cdot u, \nu' - \frac{\nu_0}{c} n' \cdot u \right) \frac{g(n, n')}{4\pi} \]  

(2.22)
where \( f(\nu - \frac{\omega_0}{c} \mathbf{n} \cdot \mathbf{u}) \) describes the absorption probability in the scattering atom’s frame and \( P(\nu - \frac{\omega_0}{c} \mathbf{n} \cdot \mathbf{u}, \nu' - \frac{\omega_0'}{c} \mathbf{n}' \cdot \mathbf{u}) \) describes the probability of a photon being absorbed in the atom’s frame. The \( g(\mathbf{n}, \mathbf{n}') \) term gives the phase function for scattering.

Common phase functions used in scattering for isotropic scattering:

\[
g(\mathbf{n}, \mathbf{n}') = \frac{1}{4\pi} \tag{2.23}
\]

and dipole scattering:

\[
g(\mathbf{n}, \mathbf{n}') = \frac{3}{16\pi} (1 + \cos^2(\theta)) \tag{2.24}
\]

The redistribution function itself is always assumed to be normalized to one so that it looks like:

\[
\oint \oint \int_0^\infty \int_0^\infty R(\nu', \mathbf{n}'; \nu, \mathbf{n}) \frac{d\omega'}{4\pi} \frac{d\omega}{4\pi} = 1 \tag{2.25}
\]

We consider three different types of redistribution: complete redistribution, coherent redistribution, and partial redistribution.

### 2.4.3.1 Complete Redistribution in the Co-moving Frame

In complete redistribution, the scattered direction and frequency is uncorrelated with the incident direction and frequency during the event. This is a valid approximation in cases where the excited electron are randomly redistributed across the upper state. Situations that cause this form of redistribution are usually attributed to collisional and damping in the states involved. With complete redistribution, \( R \) is given by:

\[
r = \frac{1}{\sqrt{\pi}} \sqrt{\frac{T_{\text{eff}}}{T}} e^{-x^2} \tag{2.26}
\]
where $x$ is the averaged frequency between $\nu$ and $\nu'$, and the source function for any component in complete redistribution (comR) is:

$$S_{\nu,m,\text{comR}} = \frac{\chi_{\nu,\text{comR}}}{4\pi} \int \frac{\phi_{\nu,\text{comR}} P_{\nu,m} d\nu d\Omega}{\chi_{\nu,\text{total}}^4}$$  \hspace{1cm} (2.27)

### 2.4.3.2 Coherent Redistribution in the Co-moving Frame

In the case of coherent redistribution, the scattered frequency is identical to the incident frequency. The directional redistribution of the photon is still given by the phase function. This happens when the scattering atoms are at rest in the lab frame, or when dealing with scattering in the continuum. One case in particular involves coherence in the atom's frame. In this case, it can be assumed that that the photon's frequency stays constant in the atom's frame but the angle is allowed to change. By treating the photon's redistribution in the atom’s frame as coherent, the form of the redistribution becomes easier to work with. One Doppler shifts the photon into the atom’s frame before the collision happens, calculate the redistribution and then Doppler shifts the photon back into the observers frame afterwards. Coherent redistribution was used in some test cases, however, thermal Doppler redistribution always causes some redistribution in frequency, except in the forward direction.

### 2.4.3.3 Partial Redistribution

The last form of redistribution that can appear in the source function is partial redistribution. When appropriate, we use Hummer’s (1962) $R_I$ redistribution function.

$$R(x, n; x', n') = \frac{g(n, n')}{4\pi^2 \sin \gamma} \exp(-x^2 - (x - x' \cos \gamma)^2 \csc^2 \gamma)$$  \hspace{1cm} (2.28)
The component of the source function using $R_I$ (parR) is:

$$S_{\nu} = \gamma(n, n')\chi_{\nu} + (1 - \chi_{\nu})\phi \int R_I$$

This redistribution assumes coherent scattering in the atom’s rest frame, redistributed by thermal Doppler shifts in the co-moving frame. It is appropriate when the natural damping $\Gamma$ is much narrower than the thermal Doppler width $\Delta \nu_D$.

In this case the redistribution function is symmetric in opposite directions in the atom’s rest frame. However when shifted to the frame co-moving with the bulk velocity, opposite directions are shifted to the other side of the co-moving radiation field. This shift is shown diagrammatically in Figure 2-1.

![Figure 2-1: Diagram showing the symmetry of coherently scattered radiation in the atom’s rest frame where $\phi_{\nu} = \delta(\nu, \nu_0)$ as redistributed to the laboratory frame. The cyan grid is the rest frame of the observer while the magenta grid is the rest frame of the atom.](image)

Figure 2-1 shows the symmetry of the scattering process. The x and y axis are in terms of the frequency space where each square is one frequency bin. For directional purposes the y axis is parallel in frequency to the outgoing photon, while the x axis
is in the direction of the incoming photon. The black dot represents the location where the scattering event occurs in the two different frames. The incident radiation corresponds to the incoming photon’s original direction before the scattering event while the arrow pointing to the right corresponds to the outgoing photon. The grids represent incoming and outgoing frequencies in a scattering event. The cyan grid is the rest frame of a stationary observer. The magenta grid is the rest frame of the scattering atom. The offset of the two frames measures the Doppler shift induced by the components of the atom’s motion in each direction. The out-going arrows show the frequency shifts for the scattered photon in the four possible directions.

2.4.3.4 Redistribution Summary

In the previous sections we have presented the various options for frequency and direction redistribution in the frame co-moving with the bulk velocity of the fluid. This frame is the easiest for computing these redistributions. The model code calculates opacities and redistribution functions in this co-moving frame, and then applies Doppler shifts in the incident direction \( m \) and the scattered direction \( m’ \) according to the \( m \)-components of the velocity field. These Doppler shifts preserve normalization and remain fully conservative in photon number.

The next chapter details the description of the numerical set up to solve the equations and situations described in this chapter. Topics include a description of the how the grid is set up as well as the shape of the cell used in this model. As discussed later, the shape of the cell is different from the standard 3D model to allow for a more realistic atmosphere with more degrees of freedom. Also included will be the description of the equations used for the model with the explanation of how the equations go from a one directional approach to the numerical equivalent. After going through the equations numerically, the simplifications and numerical assumptions will be described including how the line formation region is treated and how to incorporate
a changing opacity into the source function.
Chapter 3

Numerical Set Up

3.1 The Grid

3.1.1 Description of the Cell Shape

In most 3D models of stellar atmospheres the grid cell shape is cubic, which allows for material to move along the three axes of the cube. The model in this research instead uses a rhombic dodecahedral shape. This arrangement has 6 axial directions with the same unit separation between adjacent cells, allowing for a more accurate resolution of the direction dependence of the radiation field within the stellar atmosphere. Allowing for axes every sixty degrees, the model doubles the number of degrees of freedom compared to a cube. This enables the particles to move along the diagonals and gives a better representation of an actual atmosphere. Figure 3-1 shows the comparison between a cubic and rhombic dodecahedron cell with the different directions shown. To track the largest number of photon paths, one needs to allow for the particles to move in as many possible directions as possible.
Figure 3-1: The left figure is the standard cubic shape commonly used in 3D models with the $x, y, z$ axes labeled and the forward directions for the different directions indicated. The right figure is the cell shape used in our model. Once again the $x, y, z$ axes are labeled and the 6 forward direction faces are also labeled. The faces are each $60^\circ$ from each other. On both figures the axes start from the center of the cell. Positive directions are all upward except for direction $m=6$ which is parallel to $y$.

3.1.2 Grid Arrangement

One reason most codes use the cubic grid cell shape is that the cells stack uniformly in the axial directions and may be oriented with gravity so as to reduce to hydrostatic conditions. The rhombic dodecahedral cells stack next to each other to form a 3D honeycomb. Figure 3-2 shows a horizontal slice of grid cells.

Yellow cells are displaced one-half unit above and below cyan cells. The center-to-center distance from one cell to any of its neighbors is constant. Layers in the model are added vertically in the $z$ direction. This honeycomb shape is chosen so that cells can be placed next to each other to set the horizontal repeating boundary conditions. The six directions from the center of any one cell have zenith cosines $\mu$ as follows: one direction (along the $z$-axis) with $\mu = +/-1$, four directions with $\mu = +/-0.5$, and one direction (along the $y$-axis) with $\mu = 0$.

In this case the cell grid size is set to include a total number of a 102 cells. This allows for a better resolution of what is happening in the atmosphere versus a cell grid of 10 which was the original model size because the scale height is independent of
Figure 3-2: Figure shows the stacking of cells with cell spacing labeled looking down on the grid. $\Delta s$ is the cell spacing in this figure. This spacing is the same for all cells in the grid. Each cell is offset in the up or down from the other cell so that there is no space between consecutive cells.

the grid cell itself. So while two atmospheres with the same temperature and surface gravity will have the same scale height, the larger grid gives a better resolution to see the changes in the atmosphere.

Figure 3-3 shows the top down view of the cell locations in the xy plane. The cells are placed such that the the particles are able to move freely in each direction continuously with the repeating boundary conditions. These cells are stacked on top of each other to create the 3D honeycomb at all depths in the atmosphere.

3.1.3 Mapping of the Cells

For a better resolution of the atmosphere, a larger grid cell is necessary. To do this, one has to map the 102 cell grid from the 10 cell grid. This allows for the same information one would get from the 10 cell model to be distributed properly across
Figure 3-3: Physical location on the xy grid for the 102 cell grid. The x-axis cells are all offset by factors of $\sqrt{2}$, while the cells are offset by a factor of $\frac{1}{2}$ in the y direction.

The larger grid for each depth. The cell grid needs to be designed so that boundary conditions are still applicable, and material flows in the proper direction. This means that making certain that the up cells in the 102 grid match with the corresponding up cell with the 10 cell grid and that the surface behaves in the expected manner.

One of the requirements for the cell grid is to make certain that it follows all of the appropriate boundary conditions. The material should be able to move freely from one cell to another in the larger grid size in the same way one would expect the material to move with several smaller grid columns sitting next to each other. This can be seen in the top figure of Figure 3-4. This is the larger column grid size.
Figure 3-4: Figure on the top shows the layout of the 102 cell grid broken into the smaller 10 cell grids lined up properly with repeating boundary conditions. The figure on the bottom is the same 102 cell grid with the different colors corresponding to the same number cell in the 10 cell grid.
overlaid with individual 10 column models of different colors. All of the different colors corresponds to an individual grid cell placed in the appropriate position so that the material can flow from one cell grouping to the next grouping freely.

Once the layout of the individual cell groupings is known, the next step is to figure out how the individual cells in the 102 cell grid correspond to individual cells from the 10 cell model. This is shown in the bottom figure in Figure 3-4 where each of the 10 different colors represents one of the 10 cell model cells. This is done by looking at the groupings of the 10 cell models on top of the 102 cell model and figuring out where each of the 10 cell grid begins. The first cell in each grouping would be cell number 1 and so on. This makes certain that the boundary conditions are still valid. Since one can treat the larger grid size as several smaller grids put together with the material from one grouping moving to the next with no breaks, the larger grid must follow the same behavior.

The individual cells not only need to be matched with the appropriate cell from the original 10 cell grid, they also have to make certain that they are in the proper place for the two different surfaces in the model. Since the rhombic dodecahedron are situated such that the cells are a half a scale height off from each other, all of the appropriate up and down cells need to be aligned. This is related to the individual mapping of the cells themselves. As seen in Figure 3-5, the light blue corresponds to all of the down cells while the light purple corresponds to the up cells. Each up cell and down cell are located along diagonals with other corresponding cells.

Once all of the individual cells have been mapped appropriately, the next step is to figure out how the different directions look in the 102 cell grid. As the cells allow for movement on all six sides, one has to know how the grid is arranged in all of these different directions. For the $m=1$ direction, it is the cell grid seen in Figure 3-5 or Figure 3-4, but for the other five directions those grids are slightly different. To do this part of the mapping, one puts ghost grids sitting next to the original grid so
that the material would be flowing into the next grid if needed. After that one looks at the directions coming from all of the other sides so $m=2,3,4,5,$ and $m=6$ in cell 1 along with the cell next to it in each of the directions. After that one looks at what the grid would look like from each of the different directions, this grid will be the one for each other directions.

### 3.2 Numerical Set Up

To simulate the atmosphere one has to set up the equations numerically. The equations defined in the previous chapter are physically correct but are not directly solvable. This section discusses how the equations are changed to be able to solve them numerically.

At each time step in the model the values for the temperature, velocity, density, radiation field, radiative acceleration, and pressure are calculated. The process is iterative, as these values are needed for the next time step. The number of time steps
needed can change and the simulation will be run until the atmosphere reaches a quasi-steady state or periodic behavior.

3.2.1 Numerical Equation for Continuity

Mass is a conserved quantity that is calculated at the cell center at each time step. As the material is allowed to move from one cell to the next adjacent cell, the material from a previous time step may move to an adjacent cell in the next time step. One starts with the integral version of the continuity equation discussed in the previous chapter:

$$\frac{\partial \ln \rho}{\partial t} = -\frac{1}{\rho dV} \int \rho' \mathbf{v} \cdot d\mathbf{A}$$ (3.1)

Consider cells labeled (i,l) where i is the vertical column index and l is the depth layer index varying from l = 1 at the top and l = L at the bottom of the atmosphere. All state variables ($\rho, T, P$) are defined at cell centers (i,l), and velocities are defined at cell faces with the same index if the face is in the positive direction in Figure 3-1. Then the numerical form of the continuity equation becomes:

$$\Delta \ln \rho_{i,l} = -\frac{\Delta t \Delta A}{2 \Delta V} \sum_{m=1}^{m} (\rho_{i,l} + \rho_+) u_{i,l,m} - (\rho_{i,l} + \rho_-) u_{i}$$ (3.2)

Where the (+) and (-) subscripts indicate cells forward and backward along the direction m.

When dealing with differential equations one needs to consider the boundary conditions at the modeled volume. At the lower boundary of the atmosphere we assume there is no material coming from below the cells so the entering velocities are zero. At the top of the atmosphere we assume that the cell above is in hydrostatic equilibrium and that the effective gravity at that layer includes the average radiative flux. Material may move freely through this boundary. At all cells within the atmosphere in the horizontal direction we assume periodic boundary conditions to allow for horizontal
movement of the material.

### 3.2.2 Numerical Equation for Momentum Conservation

The equation for momentum conservation calculates the value of the velocity in each of the given directions at each given time step. The general form of the momentum equation in component form from the previous chapter is:

\[
\frac{\partial u_m}{\partial t} + \mathbf{u} \cdot \nabla u_m = g_m + \alpha_m - a^2 \left( \frac{\partial}{\partial (\ln a^2 + \ln \rho)} \right) \tag{3.3}
\]

In the same manner that the equation for continuity is adapted for numerical calculations the momentum conservation equation for a given cell center in a particular \(m\)th direction is the following:

\[
\Delta u_{i,l,m} = \Delta t \left[ g_m + \alpha_{i,l,m} - \mathbf{v} \cdot \nabla u_m - \frac{1}{2} \left( a_+^2 + a_{i,l}^2 \right) \frac{1}{\Delta s} \left( \ln a_+^2 - \ln a_{i,l}^2 + \ln \rho_+ - \ln \rho_{i,l} \right) \right] \tag{3.4}
\]

One of the complicated terms to deal with here is the advection term, \(\mathbf{v} \cdot \nabla u_m\). This is caused by the directions are not along a straight Cartesian coordinate system one has to consider the fact that the velocity in the \(x, y, z\) directions will include multiple velocity components. At the same time if one uses the standard Cartesian coordinate system then some directions become even more complicated than others, so to take simplify the problem one sets a coordinate system based on the direction being computed. In this case define the \(z\) axis parallel to the \(m\)th direction computed, the \(y\) axis will be parallel to the \(n \perp m\) direction and the \(x\) axis perpendicular to the long dodecahedron axis. The decomposed dot product becomes:

\[
\mathbf{v} \cdot \nabla u = w \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + u \frac{\partial u}{\partial z} \tag{3.5}
\]

Where \(w\) and \(v\) are the velocity components in the \(x\) and \(y\) directions. To find

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the values for each of the components of the dot product one takes the averaged difference equations for the three terms, including all of the velocity components in that direction, to get:

\[ w \frac{\partial u_{i,l,m}}{\partial x} \approx \overline{w} \frac{1}{\sqrt{2}\Delta s} (u_{+x,m} - u_{-x,m}) \]  

(3.6) in the x direction

\[ v \frac{\partial u_{i,l,m}}{\partial y} \approx \frac{1}{4} (u_{i,l,6} + u_{+z,6} + u_{-y,6} + u_{-y,z,6}) \frac{1}{2\Delta s} (u_{x,y,m} - u_{-y,m}) \]  

(3.7) in the y direction and

\[ u \frac{\partial u_{i,l,m}}{\partial z} \approx u_{i,l,m} \frac{1}{2\Delta s} (u_{+z,m} - u_{-z,m}) \]  

(3.8) in the z direction. As the velocities in the x direction contain velocity from multiple m directions the velocity in the x direction becomes:

\[ u_{\pm x,m} = \frac{1}{4} (u_{\pm 2,m} + u_{\pm 3,m} + u_{\mp 4,m} + u_{\mp 5,m}) \]  

(3.9)

and

\[ \overline{w} = \frac{\sqrt{2}}{8} (u_{i,l,2} + u_{i,l,3} - u_{i,l,4} - u_{i,l,5} + u_{+4,2} + u_{+5,3} - u_{+2,4} - u_{+3,5}) \]  

(3.10)

The subscript \( \pm n \) indicates the value for an adjacent cell in the \( \pm n \) direction. From the discussion earlier on the shape of the cell, the directions 2 through 5 are the four \( 60^\circ \) away from m in the counter-clockwise direction with x between directions 2 and 3. The direction 6 is the y direction perpendicular to z.

As with the continuity equation, the equation for momentum conservation has repeating boundary conditions in the horizontal direction to allow for continuous
movement in that direction. For the bottom layer of the atmosphere the value for the velocity at the faces of the cells coming up from below is zero.

### 3.2.3 Numerical Equation for Energy Conservation

The equation of radiative equilibrium is given by:

\[
a^2 = \frac{\zeta k}{(\zeta - 1)\mu} \left( \frac{cB}{4\sigma} \right)
\]  
(3.11)

where all state and radiation values are defined at cell centers. The equation for radiative equilibrium gives the value for the speed of sound at the cell volume center.

### 3.2.4 Numerical Equation for Radiative Transfer

The form of the equation for radiative transfer in the frame of the atmosphere:

\[
\frac{\partial I_\nu(m)}{\rho k \partial s_m} = S_\nu - I_\nu(m)
\]

When looking at a particular cell within the grid, one has to account for both the radiation coming into the cell and the radiation going out of the cell itself. This movement of material through the cell will cause the radiation field to change compared to using one value for the radiation field in the cell. To counter the fact that the material is free to move to adjacent cells, I use two averaged forms of the radiation field, the forward moving material and the backward moving material into an added and subtracted average:

\[
P(m) = \frac{1}{2} (I_{+\nu}(+m)) + I_{-\nu}(-m))
\]

(3.13)
and

\[ R(m) = \frac{1}{2} (I_{+\nu}(+m) - I_{-\nu}(-m)) \]  

(3.14)

where \( I_{+\nu}(+m) \) is the value for the intensity coming in from the forward \( m \) direction while \( I_{-\nu}(-m) \) in the backwards \( m \) direction.

The additive and subtracted versions have the following form:

\[ \frac{\partial R_{\nu}(m)}{\rho \kappa \partial s_m} = S_{\nu} - P_{\nu}(m) \]  

(3.15)

and

\[ \frac{\partial P_{\nu}(m)}{\rho \kappa \partial s_m} = -R_{\nu}(m) \]  

(3.16)

If one substitutes the added average equation for radiative transfer into the subtracted equation for average radiative transfer one gets a second order differential equation in terms of just the added average equation which has the form of:

\[ \frac{\partial^2 P_{\nu}(m)}{\rho^2 \kappa^2 \partial s_m^2} = P_{\nu}(m) - S_{\nu} = P_{\nu}(m) - \frac{1}{4\pi} \int P_{\nu}(m) d\Omega \]  

(3.17)

When using an averaged form of the radiative transfer equation one needs to check the upper and lower limits and set the boundary conditions. At the bottom of the atmosphere we assume the diffusion limit with the appropriate flux entering from below, defined by the chosen effective temperature of the model in question. At this point the value for \( R_{\nu}(m) \) becomes:

\[ R_{\nu}(m) = \mu \frac{3}{4\pi} \sigma T_{eff}^4 \]  

(3.18)

where \( \mu \) is the cosine of the zenith angle in the particular \( m \)th direction.

At the upper boundary of the cell grid the main factor is the radiation entering from the source function integrating through the gas above the upper boundary. We
assume the source function along the ray \( m \) is constant above the upper boundary, and that the optical depth of the boundary is given by the extinction at the boundary times the local density scale height. Using those assumptions, the boundary condition for the upper portion of the atmosphere then becomes:

\[
\frac{\partial P_{\nu}(m)}{\rho \kappa \partial s_m} = I_{-\nu}(-m) - P_{\nu}(m) \tag{3.19}
\]

where in this case \( I_{-\nu}(-m) \) is given by:

\[
I_{-\nu}(-m) = S_0 (1 - e^{-\tau_0}) \tag{3.20}
\]

The second order differential equation becomes:

\[
\frac{1}{\chi_{+,n} \Delta s} (P_{+,m,n} - P_{+,l,m,n}) - \frac{1}{\chi_{-,n} \Delta s} (P_{-,l,m,n} - P_{-,m,n}) = \chi_{i,l,n} \Delta s \left( P_{i,l,m,n} - \frac{1}{6} \sum_{m'} P_{i,l,m',n} \right) \tag{3.21}
\]

where \( \chi = \rho \kappa \) is given by:

\[
\chi_{\pm,n} = \frac{1}{2} \left( \frac{1}{\chi_{+,n}} + \frac{1}{\chi_{-,n}} \right) \tag{3.22}
\]

Again, at the vertical boundaries we use repeating boundary conditions so that the radiation is free to move to adjacent cells. Using the two defined upper and lower boundaries we get the following equations:

\[
\frac{1}{\kappa_{+,2} \Delta s} (P_{+,l,m,n} - P_{-,m,n}) = (1 - e^{-\tau_{l,5}}) \frac{1}{6} \sum_{m'} P_{i,l,m',n} - \frac{1}{2} (P_{i,l,m,n} + P_{-,m,n}) \tag{3.23}
\]
and the upper boundary when \( m \neq 6 \) and:

\[
\left[ \frac{1}{\chi_{+,n} \Delta s} (P_{+,m,n} - P_{i,L,m,n}) + \frac{3\mu}{4\pi}\sigma T_{eff}^4 \right] = \chi_{i,l,n} \Delta s \left( P_{i,l,m,n} - \frac{1}{6} \sum_{m'} P_{i,l,m',n} \right)
\]  

(3.24)

at the lower boundary when \( m \neq 6 \).

Figure 3-6: Figure shows the vertical view of the stacked cells looking along the directions marked by the dashed line. For the points at the center of each cell is where the values for the intensity, density, and speed of sound are calculated. For the radiative transfer equation the two adjacent center cells are also included in the calculation.

3.2.5 The Horizontal Ray Problem

In a plane parallel atmosphere, the intensity in the horizontal direction is equal to the isotropic source function since the atmosphere in the horizontal direction is infinite in that direction. There is also no dependence on the opacity. This poses a problem near the surface as at some point the radiation needs to escape the stellar atmosphere. The result is an artificial limb brightening at zenith cosine \( \mu = 0 \) compared to what
one would expect in a real stellar atmosphere. To deal with this problem one can make the following assumption.

\[ \chi = \chi_0 e^{\frac{x^2}{2RH}} \]  

(3.25)

Where \( \chi_0 \) is the given opacity calculated at the cell center. This causes the optical depth along this direction to become:

\[ \tau = \chi_0 \int e^{-x^2/2RH} dx = \frac{1}{2} \chi_0 \sqrt{2\pi RH} \]  

(3.26)

Figure 3-7 shows a ray going in the horizontal \( x \) direction away from the computed cell center. At a distance \( x \) away the departure height is given by \( x^2/2R \). If the source function and opacity are constant along that horizontal ray, and using the given density scale height \( H \), the extinction along that ray is given by:

\[ \chi = \chi_0 e^{\frac{x^2}{2RH}} \]  

(3.25)

Where \( \chi_0 \) is the given opacity calculated at the cell center. This causes the optical depth along this direction to become:

\[ \tau = \chi_0 \int e^{-x^2/2RH} dx = \frac{1}{2} \chi_0 \sqrt{2\pi RH} \]  

(3.26)
which is no longer infinite. If we assume the source function is constant along the ray, we can integrate over this approximate horizontal optical depth to determine the Feautrier $P$. At depth, we recover the formal solution that $P = S$. This approximation gives back the boundary conditions defined at the upper and lower boundary conditions for the radiative transfer. Since at the upper boundary the radiation is related to the source function along a constant depth from the gas above, if one puts in the artificial darkening into the equation of radiative transfer, one gets the appropriate value for $P$ in this direction.

3.3 Line Simulation

Most 3D models simulate thousands of lines in a stellar atmosphere over a range of opacities. This is the standard method for stellar atmosphere models because stars contain multiple elements with different ionizations at different temperatures and photons coming out of the atmosphere at different energy levels. Instead, the model used here simulates one single spectral line repeatedly over a thousand times rather than computing a thousand single spectral lines. The idea is that repeating the same line that many times is as effective as simulating a thousand lines.

This is because we are only interested in determining the microturbulent velocity. In general this value is not dependent on the atom or ionization level of the specific atom as all spectral features show the same amount of broadening. Therefore it is just as valid to look at an emergent profile independent of any particular atom to find the value for the microturbulence as it is to look at at several different spectral features of different ionization levels. Both methods would show the same value for microturbulence as the only dependence on the microturbulence velocity in general is the temperature and surface gravity of the star.
3.4 Opacity

Due to the different transitions that occur in the atmosphere, opacity is always changing. In a given line feature the opacity will be different at the line center compared to the wings of the spectral feature. This change of opacity inside of one spectral feature causes acceleration which causes microturbulence, so this change in opacity has to be considered.

3.4.1 Sources of Opacity

Opacity is an important component of stellar atmospheres. There are a multitude of causes of opacity that have to be accounted for, mostly dealing with different types of transitions that occur. The transitions involved are bound-bound transitions, bound-free transitions, free-free transitions, and electron scattering. Bound-bound transitions involve a photon exciting an electron into a different bound state within the atom or molecule. Electron scattering involves scattering a photon by a free electron or molecule in the atmosphere. In this case it is Thompson scattering that is more significant due to the fact that the temperature would be too high for many molecules to form. Bound-free transitions occur when a photon excites an electron from a bound state to the continuum which is also called photoionization. The last source of opacity comes from free-free transitions involving ions and photons.

In our models we assume, bound-bound transitions, and Thompson scattering are the significant source of opacity. In hot stars, the temperature is too high for the molecules that are stable at lower temperatures to exist. We also add a generic Kramers-like opacity to account for bound-free transitions, but it only there to set the overall flux-weighted mean optical depth to occur at the appropriate column density of material.
3.4.2 Terms of Opacity

Opacity shows up predominately in the equation of radiative transfer and in the source function. As discussed earlier this change of opacity causes an acceleration which causes microturbulence. At the microscopic level, the opacity can change within the line profile itself due to the Doppler shifts. As photons may be shifted from an area of higher opacity to an area of lower opacity within the single line feature itself this may mean that a single value of microturbulence may not be accurate to match spectral features.

\[ S_\nu = \frac{\kappa_\nu}{\kappa_\nu + \sigma_\nu} B_\nu + \frac{\sigma_T}{\kappa_\nu + \sigma_\nu} \int \oint I_\nu(n) R_\nu(n', \nu'; n, \nu) \frac{d\Omega}{4\pi} d\nu' \]  

(3.27)

where the first term is the condition for LTE conditions and the second term describes the scattering portion of the source function. The \( \kappa_\nu \) term, which is the opacity, will change based on the Doppler shift of the material. To find the opacity at a given part of the atmosphere, one has to know the optical depth at that portion of the atmosphere:

\[ \tau_\nu = \int_0^l \sigma_\nu n(z) dl' = \sigma_\nu nl = \kappa_\nu \rho l \]  

(3.28)

Therefore

\[ \kappa_\nu = \frac{\sigma_\nu n}{\rho} \]  

(3.29)

if the absorption cross section and number density are independent of path length in the atmosphere.

Optical depth refers to how far in the atmosphere one can see and is used to define where the start of the photosphere when \( \tau_\nu = \frac{2}{3} \). The number density can be considered constant as the part of the atmosphere modeled is a smaller portion where density and number density can be considered to be isotropic. Though the number density can be considered constant, the actual density and temperature increases with
depth in the atmosphere.

\[ a(\nu) = \frac{h\nu B_{lu}}{4\pi} \phi(\nu) \] (3.30)

The profile used is the thermal Gaussian profile with the Doppler shifts which is dependent on the velocity field. A velocity dependent opacity:

\[ \kappa_\nu = \frac{h\nu B_{lu}N_e e^{-\frac{(\Delta\nu)^2}{4\Delta\nu_D^2}}}{4\pi^{\frac{3}{2}}N\Delta\nu_D \rho} \] (3.31)

and discussed in the next section \( \Delta\nu_D \) has the form of:

\[ \Delta\nu_D = \frac{-u_m \nu_0}{c} \] (3.32)

which is related back to the bulk motions of the fluid.

As one can see from the prior equations, if the velocity changes in the different directions, the opacity will not have the same value throughout the atmosphere. This becomes important when finding the radiation in all directions as the value of the radiation field will change as well in the different directions to compensate for the different values of the opacity.

### 3.5 Doppler Shifts

Doppler shifts have a significant role in the model used here as it could be the cause of microturbulence in hot stars. Since the material is moving the atoms can be exposed to different portions of the same spectral feature as they Doppler shift out of an absorption line. This increases the opacity in the laboratory frame leading to an increase in radiation pressure thereby accelerating the gas, ultimately, causing the microturbulence. Because of this, it is important to understand where the Doppler shifts are occurring in the spectral feature and incorporate that into the model. The
Doppler velocity is given by:

$$u_D = \frac{-u_m}{u_{D\text{thermal}}}$$  \hspace{1cm} (3.33)

where $u_D$ is the Doppler velocity and $u_{D\text{thermal}}$ is the thermal Doppler velocity and the Doppler width is given by:

$$\Delta \nu_D = \frac{\nu u_D}{c}$$  \hspace{1cm} (3.34)

Once the Doppler width is known, one can easily shift into the co-moving frame of the atom and from there see how the photon gets redistributed. This has to be done for each of the six directions as the velocity and direction is allowed to change causing the photons to be exposed to different portions of the line profile. After following the photon through redistribution in the co-moving frame one switches back to the lab frame, though the photon does not necessarily come out in the same direction as before as described by redistribution.

### 3.6 Input Parameters

The boundary conditions, grid scales, and various internal quantities require the specification of several fixed parameters for a given model. As for any model atmosphere, the support and overall state of the material requires specifying the parameters for gravity and radiative flux, e.g. log $g$ and $T_{\text{eff}}$, the effective temperature. While less important in our spectrally simplified model, the abundance fractions of hydrogen (X), helium (Y), and metals (Z) do affect the ionization balance and electron number, as well as the background opacity. Setting the grid scale $\Delta s$ requires an estimate of the opacity resisting the radiative flux in the formula for the effective gravity. This estimate is only used in the grid scaling to keep $\Delta s$ 0.25 times the density scale height in the atmosphere. Setting upper boundary boundary conditions requires an initial value for the column mass density of the material above the boundary; this value is
revised every time step according to the instantaneous values of the density and the
density scale height at the upper boundary. Finally, the horizontal photon escape
probability requires an estimate of the stellar radius as discussed in the horizontal
ray problem.

Parameters for the spectral line feature include the ratio of the frequency-integrated
line opacity to the assumed background continuum, and the molecular weight of the
atom responsible. The latter is required for the frequency grid spacing $\Delta \nu_D$ and the
ratio of this spacing relative to the bulk velocity induced Doppler shifts.

## 3.7 Numerical Process

The code calculates the values for the speed of sound, density, specific intensity,
and face-normal velocities at each time step in the atmosphere. Since the current
step is dependent on the prior steps, these values are not independent of each other.
At each time step the values from the previous time step are used to find the cur-
rent values for the same input parameters in the following order. Given the material
velocities, the cell densities are updated one time step $\Delta t$ via the continuity equa-
tion. With the new densities and gravity and old radiation forces, update the new
face-normal velocities via the momentum equation. Then solve the instantaneous
radiative transfer equation for $P(i, l, n, m)$. It is this solution for $P$ that is the most
time consuming, because all cells are directly coupled to all other cells. Fortunately,
our transfer equation is linear so we may compute the solution via matrix inversion
techniques.

The next chapter discusses the different computational algorithms that could be
used to make the model more time efficient. To create the most realistic atmosphere
one has to have the best resolution available, but this can come at a computational
cost. Increasing columns, layers, and frequencies allows for a better resolution but
can become too costly in time. There are several different libraries that can solve this problem efficiently to allow for the increase in frequency and layers to the atmosphere.
Chapter 4

Computational Algorithms

The equations discussed in the prior chapter are solved for a total of $N \times l \times L \times M$ radiation elements, $i \times L$ densities, and $l \times L \times L$ velocities. Our model uses $N=11$ frequencies, $l=102$ columns, $L=45$ layers, and $M=6$ directions. Adding frequencies and layers gives a higher resolution in the atmosphere which allows for a clearer understanding of the physics happening. At the same time, this greater resolution requires more computational power and time. To help to eliminate some of the computational time, one looks at parallel processing.

4.1 Basics

4.1.1 How Parallel Processing Works

Parallel computing breaks up a large problem into smaller subsets that are then passed onto different computers or processors in a cluster environment. Doing this speeds up the computing time dramatically compared to solving the same problem using a serial code. With the ability to take a larger problem and solve it more quickly than the serial version of the problem, one can increase the grid size to give a more thorough description of the atmosphere. This allows for larger atmosphere that includes more frequencies to provide a more detailed description of redistribution and
the Doppler shifts. Including these details and solving the problem serially for the same code would take too long and may even be too large to compute at all.

4.1.2 Connecting to the Processors

The key difference between serial and parallel computing is the distribution of the code over different processors to spread the problem out into smaller portions. This difference is why using parallel processing is time efficient for certain problems. The program that distributes the code over the different processors is the message passaging system. The message passaging system takes the program, and with a given number of available processors or computers in a cluster, breaks the problem up over the different processors. The processors then each work on their own to solve the required program and send the results back to the main program. By sending smaller portions of the code to each of the processors instead of using one processor to run through the entire process, the computers together do the same amount of work in a shorter span of time instead of using a single processor. This is generally done

![Diagram](image)

Figure 4-1: Left figure shows the general form of computing for serial computers where given the code after compiling it goes to one single processor. Right figure shows the general form of parallel computing where given the code after compiling it gets distributed over 3 processors instead on one.

by using a message processing interface (MPI). There are two common open source MPI’s: MPI and OpenMPI. Both of these MPI systems work with all programming languages and can be used interchangeably, depending on the need of the user. This
removes the user from having to set up the communication between the different processors and computers being used.

### 4.1.3 Running the Program

Once the processors are connected and communicating the actual program can be run. This includes setting up a process grid, a grid for the matrix to be used and split over the different processors. Depending on the program or software package, multiple different methods can be used to do this part of the process. For example the method used and described in the next section for ScaLAPACK uses a block-cyclic method of distribution. After the matrix is distributed over the defined process grid, the program can do its computation and return the solution to the inverse back to the user. Once the solution is given there is no more need to use parallel processing so the grid gets shut down using MPI to go back to serial computing. This method is described in particular for ScaLAPACK in the next section.

### 4.2 ScaLAPACK and LAPACK

#### 4.2.1 Description of LAPACK and ScaLAPACK

Linear Algebra PACKage (LAPACK) is a library of numerical routines to solve various linear algebra problems commonly found in the sciences. Some of the routines include finding eigenvalues and eigenvectors, solving linear equations, factoring matrices, and finding least square values. These routines are optimized to use the least amount of computational power needed to solve these problems. LAPACK only does serial computing routines and does not include parallel processing. There is another set of routines based on LAPACK that does include parallel processing routines called SCAlable Linear Algebra PACKage (ScaLAPACK).
ScaLAPACK includes the same routines in LAPACK, except that it is able to use parallel processing. ScaLAPACK comes with routines and drivers that do the actual parallel processing and configuring of the computer cluster or processors to do the code. These drivers allow the LAPACK routines to run on a computer cluster rather than calling just the LAPACK routine to run on a serial computer.

Along with ScaLAPACK and LAPACK, there are other libraries that are required to use the routines and to do parallel processing. These libraries include Basic Linear Algebra Subroutines (BLAS), Basic Linear Algebra Communication Subroutines (BLACS), and a form of a message passage system to communicate the information across the different processors such as openMPI. Both BLAS and BLACS are common libraries that include routines called from LAPACK and ScaLAPACK. BLACS is required for ScaLAPACK routines, but not by LAPACK, as it helps with the process grid. Message passage systems are required for ScaLAPACK for parallel processing. Without openMPI or another message passage system, there is no form of communication between the different processors.

ScaLAPACK uses a specific grid system to spread the matrix over the different processors involved in the system, this grid is called the process grid. The process grid is used to distribute the matrix given in the problem over the different processors. The division of the matrix over the grid is dependent on the number of processors and the size of the matrix involved. ScaLAPACK uses a block-cyclic distribution over the different processors to create blocks of the matrix in a column array. The drivers break the matrix into a series of columns that are then put into blocks in each processor.

Figure 4-2 shows an example 9 x 9 matrix over a 2 x 3 process grid by ScaLAPACK. The left side of the matrix is the input matrix shown in 2 x 2 blocks before the block-cyclic distribution has been done. The right side is the same 9 x 9 sample matrix after it has been distributed over the 2 x 3. The columns and rows have been interchanged.
Figure 4-2: Figure on the left is a sample 9x9 matrix in blocks of 2x2 before being distributed over ScaLAPACK’s process grid. The figure on the right shows the same 9x9 matrix distributed over a 2x3 process grid by ScaLAPACK. Adapted from the ScaLAPACK user manual.

due to this. In the shown example, columns 2, 3, 4, and 5 have been interchanged into columns 3, 5, 2, and 4, respectively. The rows get shifted as well, as seen from looking from the left figure to the right figure. Rows 2, 3, 4, and 5 are exchanged with rows 4, 2, 5, and 3. The actual algorithm is more complicated than just switching the rows and columns; there is a specific way that this happens.

4.2.1.1 Reasoning for Using ScaLAPACK

ScaLAPACK is used in the model discussed previously is to find the inverse of a matrix. To find $P_\nu(n, i, l, m)$, one needs to find the value for the matrix equation.

$$A \ast X = I \quad (4.1)$$

where $X$ is the inverse.

One way is to use a Gaussian-elimination scheme to find the inverse. A Gaussian-elimination method is a linear algebra method of solving matrices by doing row reduction to find a determinant or inverse of a matrix. It does this by using the standard row operations till the matrix is put into row echelon format. This format requires that the left most value in each row be equal to one and all values following that
column is zero.

The reasoning behind using the ScaLAPACK version of the routine rather than LAPACK is the number of frequencies and the size of the grid that is capable of being used here. To do a standard Gaussian-Elimination routine with a sample atmosphere with 9 frequency values and 40 layers of the atmosphere takes approximately 8 seconds to complete whereas by doing the inversion routine supplied by ScaLAPACK takes less than a second to do the same thing and get the same result.

### 4.2.2 Routines Used from ScaLAPACK

There are a specific set of routines and drivers required to initialize and release ScaLAPACK’s grid and spread the given matrix over the grid, independent of the routine used.

#### 4.2.2.1 Initialize the Process Grid

Before any of the other routines can be called one first has to initialize the process grid. In this step, one defines the shape of the process grid and calls the subroutines sl_init, and blacs_gridinfo. The shape of the process grid can change the efficiency of the routine and cause longer times since it determines how the matrix will get distributed. The first routine, sl_init, initializes the process grid itself and requires the rows and columns of the grid to be used called here. The shape of the process grid can be any size as long as it does not surpass the total number of available processors or computers to be used in the arrangement. If the size of the grid is larger than the maximum available to the user, the computational time can get slowed and is no longer as efficient. The second routine, blacs_gridinfo, calls the BLACS library into the routine to help distribute the matrix over the grid itself, one of the outputs from the sl_init is required to call the BLACS library. After these routines are done the next set to do the actual computation is to distribute the matrix over the process
grid, as described in the previous section.

4.2.2.2 Distribute Matrix over ScaLAPACK’s Process Grid

The next set in process required to run ScaLAPACK’s routines is to distribute the matrix over the process grid. This routine is called descinit. Descinit does the block-cyclic distribution discussed in section 4.3.1 to the matrix involved. To call the routine, the following variables must be defined: the rows and columns of the matrix itself, the maximum column and rows allowed, the process row that the distribution is started on, the process column that the the distribution is started, and the location of the first element of the matrix in the array. After this routine is finished, the matrix will be ready to be manipulated in any of ScaLAPACK’s library of routines. If the matrix is not distributed over the grid properly in this step, the computational routines will have memory issues and will not run. Once the matrix has been distributed properly, the next set is to compute the inverse.

4.2.2.3 Call the Routines

After the matrix is distributed across the process grid, the actual computations can begin. The routine used here is the subroutine psgetri. Psgetri is a routine that is parallel real general factoring of the matrix and does an inverse. This routine takes the LU factorization from psgetrf and finds the inverse of the matrix. The only information needed for psgetri is the matrix itself, the size of the matrix, and the pointers for the memory.

To compute the inverse, the matrix has to be a square matrix, $n \times n$, where the rows and columns have to match in rank. In this case, it does not matter whether the matrix is considered to be either dense or sparse, though the matrix used here is a sparse matrix. Dense and sparse describe how full the matrix is with nonzero values, so a sparse matrix is comprised of mostly zero values. At the same time, there is no
special formatting required for the matrix to use it in the ScaLAPACK routines.

The algorithm used in psgetri and psgetrf first does a partial pivot LU factorization of the given matrix. This will triangulate the matrix. LU factorization takes the given matrix $A$ and turns out three matrices:

$$A = PLU$$ \hspace{1cm} (4.2)

Where $P$ is the permutation matrix, $L$ is the lower triangle matrix, and $U$ is the upper triangle matrix. The $L$ and $U$ matrices combined create the triangular matrix of $\overline{A}$. Partial pivoting LU factorization only does row permutations instead of both row and column permutations. The permutation matrix, $P$, gives the description of the row changes of the original matrix $\overline{A}$. In general, the pivot point is the starting point for the row exchanges for different algorithms. In a Gaussian-elimination scheme, the pivot point is a zero entry, while for LU decomposition the pivot point is a nonzero entry.

Once the matrix is factorized from psgetrf, psgetri is then called to do the actual inverse computation. By this point the matrix has been factored and due to the convenience of the LU factorizing, the matrix equation to solve for the inverse is:

$$\overline{A}X = LU = B$$ \hspace{1cm} (4.3)

Where $LU$ is the factored format of $\overline{A}$, and $B$ is the identity matrix in this case. Given that $LU$ and $B$ are known the equation can rearranged to find $X$:

$$X = BLU$$ \hspace{1cm} (4.4)

And since the matrix has been turned into a triangular matrix via the LU factorization the inverse is easily read off and found.
4.2.2.4 Shut Down the Grid

After the routines are called to do the inverse of the matrix, the process grid is no longer needed for computations and is uninitialized to free up computational power. As with initializing the grid, the routines that leave the grid have similar features. The routines called in this case are blacs_gridexit, which exits the grid itself, and blacs_exit, which leaves the parallel processing portion of the code. These are both similar to sl_init and the blacs_gridinfo, from the grid initialization sequence explained previously. Blacs_gridexit is called first to inform the processor to leave and dismantle the process grid itself, blacs_exit is called which tells the processors to go back to serial computations.

4.3 ARPACK

4.3.1 Description of ARPACK

The ARnoldi PACKage (ARPACK) is a Fortran77 library of routines to solve eigenvalue problems for large scale matrices. ARPACK solves these systems of equations for all forms of matrices, whether they are sparse or filled matrices, that do not have to be symmetric. ARPACK may be used in serial computations or in parallel computations, but due to its innate ability to handle large matrices, the serial version is more than satisfactory for the size of the input matrix used for this model.

ARPACK requires no specific format for the input matrix, as it uses a reverse communication interface to retrieve the matrix (Lehoucq 1997). This allows the user to choose the type of matrix used and the format of the input matrix unlike SuperLU, which has a required input matrix format. ARPACK uses a reverse communication interface for inputting the matrix in terms of a matrix-vector product instead of a matrix alone. The matrix-vector product itself allows for any original input matrix
format, as the resultant will be a vector product for solving the eigenvector problem. This is required to use an Arnoldi iteration, the computational algorithm that is predominately used in ARPACK.

### 4.3.2 Algorithms used

ARPACK’s main algorithm used to compute the eigenvectors of the problem is the Arnoldi iteration process. The Arnoldi iteration is a linear algebra algorithm of finding the eigenvectors for the solution to:

$$\overline{A}x = \lambda x$$

(4.5)

Where $\lambda$ is the eigenvalues corresponding the the eigenvectors $x$, that when multiplied together return $\overline{A}$.

For large systems, finding every eigenvector is computationally intensive and unnecessary, as small eigenvalues can be considered negligible in the overall scheme of the needed quantities. The Arnoldi iteration uses this assumption to locate the nth largest eigenvectors for a given matrix. The Arnoldi iteration uses this assumption to compare a large matrix space and converge on the value of the needed eigenvalues after a few iterations (Lehoucq 1997). This is related to a power iteration of a Kyrov matrix space. This method takes the power multiple of the a given space and finds the largest polynomial eigenvector required for the matrix to converge (Lehoucq 1997). The Arnoldi iteration applies this method to systems of large matrices that have zero vectors which the power iteration diverges to find the inverse of a matrix with the fewest eigenvectors needed.

The other algorithm used in ARPACK is the input matrix vector itself with the reverse communication interface. This does the opposite of what is generally done when calling input matrices into programs. Reverse communication interface avoids having
a specifically called input matrix by using the matrix vector product. ARPACK, unlike ScaLAPACK and SuperLU, does not input a matrix directly into the routine called, it first gets passed through the user created matrix vector product and is then called.

\section*{4.3.3 Description of the Routines Used}

ARPACK has several routines that are called to find the inverse of the matrix-vector product. These routines create the matrix-vector product, retrieve the matrix-vector product, and compute the inverse itself. As the version of ARPACK that is discussed here is the serial version, it is not necessary to set up a process grid and distribute the matrix-vector product over multiple processors.

The first step to invert a matrix using ARPACK is to set up the matrix-vector product. In general, when solving for the eigenvectors the input is in a form of an input matrix with an output matrix or vector. This input matrix needs to be turned into a vector product to find the eigenvalues. This is done by a user created matrix-vector created program to turn the input matrix into a matrix-vector by using:

\[ \mathbf{A} \mathbf{x} = \mathbf{b} \Rightarrow \mathbf{w} = \mathbf{A}\mathbf{b} \quad (4.6) \]

Where \( \mathbf{b} \) is the identity vector which is given.

After the matrix-vector product is created from the input matrix, the routine dsaupd is called to input the matrix-vector product into the program. Dsaupd is the reverse interface routine required for the Arnoldi iteration to find the inverse of the matrix.
4.3.4 Reasoning for Using ARPACK

ARPACK’s routines are built to handle large sparse matrices and to compute the solution to these matrices in a time efficient manner without using parallel processing. This is done by only finding the larger eigenvectors of the input matrix instead of all the eigenvectors to the solution, including those that may be negligible in size, which can take up computational time. Rather than finding each of the small eigenvectors for large scale matrices, the program can find the solution to a few large vectors that are comparable to the entire solution.

ARPACK is built to handle large matrices without having to resort to parallel processing, unlike to LAPACK and SuperLU, although at a certain point it is more efficient to run the program over multiple processors. By not having to send the program over multiple processors it saves time by not having to call the processors or to distribute the matrix over a process grid of any shape. ARPACK takes the input matrix vector and finds the vectors immediately.

4.4 SuperLU

4.4.1 Description of SuperLU

The Super Lower Upper (SuperLU) is a set of routines written in C with a conversion to Fortran77 that solves the equation $\overline{A}X = \overline{B}$ where $\overline{A}$ is a sparse n x n matrix, $\overline{X}$ and $\overline{B}$ are n x n matrices. With SuperLU there is no constraint on the type of matrix that $X$ can be. It is allowed to be sparse, non-symmetric, or Hermitian. Since the LU factorization is used to solve for the matrix B, the input type does not matter. This can be used to find the inverse of a matrix as

$$\overline{A}^{-1}\overline{A} = \mathcal{I}$$

(4.7)
where $I$ is the identity matrix. As the goal for the problem at hand is to find the matrix $A^{-1}$, the requirement for this program is that $A$ should have an inverse.

SuperLU has the option of either serial computing or parallel computing, depending on the need. The parallel computing version of SuperLU can be split into two different categories, determined by whether the memory is a shared or a distributed version of parallel processing (Li 2005). The version used here is the serial version of the program.

Unlike ScaLAPACK and ARPACK, SuperLU requires the input matrices to be in a particular format called Harwell-Boeing. Harwell-Boeing matrix format is one of the compressed matrix input formats. This format requires a list of column and row indices and the assigned nonzero value at that location. This does not include any zero values in the actual format itself, as any value that is not listed is assumed to be zero. Figure 4-3 is an example of a sample 5 x 5 matrix in normal matrix format and the compressed matrix market format.

```
0 1 2 0 0
0 0 0 3 0
4 0 0 5 0
0 0 6 7 0
0 0 0 0 8
```

<table>
<thead>
<tr>
<th>row</th>
<th>column</th>
<th>value</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>5</td>
<td>8</td>
</tr>
<tr>
<td>1</td>
<td>2</td>
<td>1</td>
</tr>
<tr>
<td>1</td>
<td>3</td>
<td>2</td>
</tr>
<tr>
<td>2</td>
<td>4</td>
<td>3</td>
</tr>
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<td>3</td>
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<td>4</td>
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<td>4</td>
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<td>6</td>
</tr>
<tr>
<td>4</td>
<td>4</td>
<td>7</td>
</tr>
<tr>
<td>5</td>
<td>5</td>
<td>8</td>
</tr>
</tbody>
</table>

Figure 4-3: Figure on the left is a sparse 5 x 5 matrix, figure on the right is the same matrix in the given matrix market format required for SuperLU
4.4.2 Algorithms for SuperLU

Both the serial and parallel versions of SuperLU use variations of a Gaussian elimination scheme for solving the matrix problems. The general strategy for finding the solution to the matrix is to first triangulate the matrix (Demmel 1997):

\[ \mathbf{P}_r \mathbf{D}_r \mathbf{A} \mathbf{D}_c \mathbf{P}_c = \mathbf{LU} \]  \hspace{1cm} (4.8)

Where \( \mathbf{LU} \) is the upper and lower triangle forms of the input matrix \( \mathbf{A} \), and \( \mathbf{P}_r, \mathbf{D}_r, \mathbf{P}_c, \) and \( \mathbf{D}_c \) are the permutation and diagonal matrices to create the upper and lower triangle matrices. The two \( \mathbf{P} \) matrices do the row and column exchanges needed for Gaussian elimination, while the \( \mathbf{D} \) matrices diagonalize the row and column elements respectively for the given input matrix.

The permutation and diagonal matrices use the Choleskey factorization method for Gaussian elimination (Demmel 1997). For cases of sparse matrices, the input matrix is not symmetric or diagonal, so the the factoring into the upper and lower triangle matrices may not be transposes of each other, which occurs when doing LU factoring. In cases where it doesn’t, Choleskey factoring allows for decomposing the matrices into the respective upper and lower triangle matrices.

Choleskey factorization takes a positive Hermitian matrix and factors it into two matrices, the lower triangle matrix and its transpose. For symmetric matrices, the transpose of the lower triangle matrix would be the upper triangle matrix, but in cases where the matrix is not symmetric that is not always true.

After the input matrix has been turned into the two upper and lower triangle matrices the routine solves for the unknown matrix, \( \mathbf{X} \) with the result matrix. The equation for the inverse:

\[ \mathbf{A} \mathbf{X} = \mathbf{I} \]  \hspace{1cm} (4.9)
Becomes

\[ X = A^{-1}I \] (4.10)

Using the different permutation and diagonal matrices to turn \( A \) into a diagonal matrix, the equation becomes:

\[ X = (P_r D_r A D_c P_c)^{-1}I \] (4.11)

Which in the case described here would be the matrix that is needed.

4.4.3 Description of the routines used in SuperLU

There are two routines required to do the inverse of a matrix in SuperLU, dgsrtf.c and dgstrs.c. Both of which have Fortran wrappers that can be used to go from C to Fortran. The first routine called is dgsrtf.c, which factorizes the given input matrix. Dgsrtf factors the input matrix into the upper and lower matrices, as described in the previous section. Once this routine is called, the permutation matrices can be reused for future factorizations if SameRowPerm is called. After the matrix is factorized, dgstrs finds the inverse of the matrix by doing a triangular solve of the matrix after it has been factored by dgsrtf. Dgstrs has to be called after the factorization since the routine takes an already factored matrix to find the solution to the matrix equation; it cannot solve an unfactored matrix.

For solving matrices with similar matrices, another routine that can be used is dgsrfs.c. This routine does a refined version of the solution found by using dgstrs.c with the factored input matrix. By using the refined solution of the matrix, it takes into account that the same permutation matrices are used for similar layers in the atmosphere, allowing for computational efficiency.

The parallel version of SuperLU uses a similar pattern to the serial version, although it also includes setting up a process grid and then calling up the routines in
question. The computational routines themselves are the same as the serial version of SuperLU, so first the matrix has to be factorized then it can be inverted. The factorization routine, dgsrtrf.c, is done in parallel processing while the solving of the matrix itself is done in serial computing. The matrix that is to be factored is distributed over SuperLU’s process grid uses the block-cyclic method that is described previously in ScaLAPACK. Similarly to ScaLAPACK, the routine superlu_gridinit initializes the process grid and distributes the matrix over the given size of the grid itself.

4.4.4 Reasoning for Using SuperLU

SuperLU benefits from the fact that it has repetition built into its algorithm for solving the inverse. This allows for efficiency in layers, as the basic computational routine for the multiple layers of the atmosphere use the same process (Demmel 1997). By using a Choleskey factorization instead of an LU factorization, the column and row permutation matrices would not change when factoring the matrix. By not having to recalculate those two matrices, the code is able to compute the inverse more quickly than it would if the calculation were done from scratch.

SuperLU is not used in the code or the time tests because of the problems with the Fortran77 conversion with the C code itself are not complete. As the rest of the model is written in Fortran77, for the efficiency of large matrices of sparse values having portions of the code itself in another language removed the time efficiency provided by the reusable permutation matrices.

4.5 Time Results for the Different Programs

When dealing with multiple different packages with different algorithms, it comes down to which routines give the correct solution in the least amount of time. In theory ARPACK, LAPACK, and ScaLAPACK will give the same result for the inversion
of the same matrix, along with a serial Gaussian elimination routine but the time efficiency of the different methods varies. To select the most time efficient routine, one must run sample matrices through the different routines with various sizes. Nine sample sparse matrices of sizes 20x20, 50x50, 100x100, 200x200, 250x250, 300x300, 400x400, 500x500, and 660x660 were selected to invert with 40 iterations. The sample matrices were then run with ARPACK and seven different arrangements of process grids, using a maximum of four processors for the ScaLAPACK routine. The table below shows the results of the time tests.

Table 4.1: Time results for various computational routines with different size matrices

<table>
<thead>
<tr>
<th>Size</th>
<th>ARPACK</th>
<th>S 4x1</th>
<th>S 1x4</th>
<th>S 1x1</th>
<th>S 2x1</th>
<th>S 1x2</th>
<th>S 2x2</th>
<th>S 1x3</th>
<th>S 3x1</th>
</tr>
</thead>
<tbody>
<tr>
<td>20x20</td>
<td>0.010</td>
<td>1.618</td>
<td>1.651</td>
<td>0.651</td>
<td>1.181</td>
<td>1.540</td>
<td>1.161</td>
<td>1.406</td>
<td></td>
</tr>
<tr>
<td>50x50</td>
<td>1.477</td>
<td>1.675</td>
<td>1.294</td>
<td>0.552</td>
<td>1.287</td>
<td>0.949</td>
<td>1.808</td>
<td>1.420</td>
<td>1.327</td>
</tr>
<tr>
<td>100x100</td>
<td>0.289</td>
<td>1.577</td>
<td>1.587</td>
<td>0.522</td>
<td>1.066</td>
<td>1.019</td>
<td>1.615</td>
<td>1.098</td>
<td>1.364</td>
</tr>
<tr>
<td>200x200</td>
<td>1.817</td>
<td>1.515</td>
<td>1.546</td>
<td>0.546</td>
<td>1.167</td>
<td>0.978</td>
<td>1.428</td>
<td>0.988</td>
<td>1.429</td>
</tr>
<tr>
<td>250x250</td>
<td>4.954</td>
<td>1.917</td>
<td>1.332</td>
<td>0.589</td>
<td>1.288</td>
<td>0.933</td>
<td>1.591</td>
<td>1.031</td>
<td>1.519</td>
</tr>
<tr>
<td>300x300</td>
<td>5.811</td>
<td>1.721</td>
<td>1.294</td>
<td>0.515</td>
<td>1.457</td>
<td>1.172</td>
<td>1.961</td>
<td>1.372</td>
<td>1.372</td>
</tr>
<tr>
<td>400x400</td>
<td>13.338</td>
<td>1.489</td>
<td>1.309</td>
<td>0.561</td>
<td>1.083</td>
<td>0.921</td>
<td>1.577</td>
<td>1.187</td>
<td>1.278</td>
</tr>
<tr>
<td>500x500</td>
<td>25.605</td>
<td>1.786</td>
<td>1.380</td>
<td>0.599</td>
<td>1.175</td>
<td>0.945</td>
<td>1.624</td>
<td>1.267</td>
<td>1.288</td>
</tr>
<tr>
<td>660x660</td>
<td>38.497</td>
<td>5.540</td>
<td>2.433</td>
<td>2.733</td>
<td>2.613</td>
<td>2.533</td>
<td>2.568</td>
<td>2.744</td>
<td>2.576</td>
</tr>
</tbody>
</table>

The smaller size matrices have issues with computational time since most of the time required to calculate the inverse is from machine time rather than program time, so the smaller sizes results can be neglected.

Table 4.1 shows the data with all of the different computer algorithms. For all the small sparse matrices up to the 200x200 size, the time scales are all approximately equivalent to each other. This is because at that point in time the dominating part of the time to compute the matrix is the overhead needed by the computer and processors. After the 200x200 matrix, the computer algorithm itself takes most of the computational time and that when it is becomes clear that ScaLAPACK and LAPACK are efficient for the computations needed in this calculation rather than
ARPACK. ARPACK has an exponential increase in computational time to do the same inversion after the sample 200x200 matrix. So in this case ARPACK is not the most efficient computer algorithm to do the inversion.

Figure 4-4: Computational times for 9 different square sparse matrices using ARPACK, LAPACK, and multiple size process grids using ScaLAPACK

Figure 4-5 is the same nine sample matrix sizes with just the ScaLAPACK process grid sizes. This allows a close up view for comparison of the different configurations and size process grid efficiencies with the same sparse matrix. The main differences in the time for the different grids comes from the distribution of the matrix over the process grid. This can be seen when comparing the 1x1 process grid compared to all the other configurations of up to 4 processors.

The 1x1 process grid is characterized by the green circles and is noticeably below all of the other curves of the different process grids. This is because the input matrix is not actually distributed over multiple process grids and is similar to doing the same
routine using LAPACK. The configuration with the largest time for computation is the 4x1 and the 2x2 process grids. This is once again due to the distribution of the matrix over the grid shape itself using the block-cyclic distribution described earlier. In general, the faster time process grid configurations are the 1x3, 1x2, and 1x4 due to the shape itself. As these grid shape sizes are vertical rectangular process grids compared horizontal rectangular process grid shapes it is more efficient generally to distribute the matrix in that type of configuration.

![Figure 4-5: Computational time for the same 9 square matrices just showing the ScaLAPACK grids, notice that all the times are relatively close to each other for most of the process grid configurations](image)

After doing time runs on all of the different computer algorithms and different shape process grids used for ScaLAPACK, the most time efficient routine was ScaLAPACK. This allowed for an increase in frequencies over the line width itself, which in turn allowed for a better resolution of the spectral feature. This also allowed a
larger sample size of the atmosphere in the vertical direction as well, which gives a better defined atmosphere at multiple depths. By both increasing the resolution of the spectral feature and using a larger model atmosphere used the model is able to have a better resolution when looking at the cause of microturbulence with finer detail.

The next chapter deals with the model atmospheres and the results for the different test cases to see whether or not the we can reproduce appropriate microturbulence values that match known values or empirical trends. These models use the assumptions and equations discussed in chapter 2 along with the numerical processes discussed in chapter 3. There is detailed discussion about how the turbulence caused by the Doppler shifts evolve over different time scales along with how the emergent line profiles evolve with time. Atmospheres with two different temperatures and surface gravities are compared.
Chapter 5

The Model Atmospheres

A group of three test models were run using two different methods to compare the impact of the Doppler shifts in stellar atmospheres. First these models were run with the standard added microturbulence term and no Doppler shift. Then these same models were run with the Doppler shifts for at least 100 time steps. The models without the Doppler shifts had fixed microturbulence values added to them to match the model results in order to compare two atmospheres with the same value of microturbulence.

The models run are listed in the following table. The temperatures and surface gravities were chosen so that there could be a direct comparison with observed stellar spectra. Among the three models listed, parameters were changed one at a time. Before the models were run at the larger scale of 102 columns, the temperature and surface gravity combinations were run with a ten-column model to see how the model

<table>
<thead>
<tr>
<th>Model</th>
<th>Temperature (K)</th>
<th>Surface Gravity log g(cm/s²)</th>
<th>Eddington Flux</th>
</tr>
</thead>
<tbody>
<tr>
<td>3535</td>
<td>35,000</td>
<td>3.5</td>
<td>1.000 ± 0.12</td>
</tr>
<tr>
<td>3538</td>
<td>35,000</td>
<td>3.8</td>
<td>1.000 ± 0.1</td>
</tr>
<tr>
<td>4038</td>
<td>40,000</td>
<td>3.8</td>
<td>1.00 ± 0.09</td>
</tr>
</tbody>
</table>

Table 5.1: List of temperatures and surface gravities used for the test atmospheres. Also included is the Eddington flux for the ratio between gravity and the radiation field
behaved and let it reach equilibrium with any change in input parameters.

5.1 Equilibrium

The addition of the Doppler shifts into the model causes the atmosphere to become turbulent initially due to the inclusions of the perturbation. To measure the microturbulence, the atmosphere should first come to a new equilibrium state under the pressure from the radiation field and gravity. To determine whether the atmosphere has reached a new equilibrium position, one looks at the velocity in the upward direction. A steady negative velocity indicates that the atmosphere is contracting due to gravity, while a steady positive velocity indicates that the atmosphere is expanding due to the radiation field.

To see the overall motions of the atmosphere after the initial insertion of the Doppler shifts, one may check the average of the squared velocities over the course of the first 1000 time steps. Using the root mean square velocity (rms) instead of the individual velocity average allows the modeler to track the scale of velocities over time as the model comes to an equilibrium with the parameters. When the rms velocities approach zero or become periodic in the ten-column model one can then run the model with the larger grid size.

As seen in both Figures 5-1 and 5-2, it takes more than one quasi-oscillation period for the atmosphere to settle down from the initial conditions. In the case of 3535, it takes close to 13 hours for the velocity to consistently approach zero compared to approximately 6 hours for 4038. 4038 settles to a point of equilibrium more quickly due to the higher surface gravity of the star itself. In both cases, though the velocity approaches zero during the first period, the occasional spikes in velocity shows that star still has not settled into a new equilibrium. As discussed in a later section, these spikes will also correspond to larger spikes in mass loss at those points. Since different
Figure 5-1: Average of the squares velocity graph for 3535. The figure on the left is the velocity squared while the figure on the right is root mean squared velocity.

Figure 5-2: Average of the squares velocity graph for 4038. The figure on the left is the velocity squared while the figure on the right is the root mean squared velocity.
depths will have different velocity patterns we must choose a specific reference depth for comparison. The depth chosen for these velocity traces is $l=11$. This value is chosen to be in the upper portion of the atmosphere where the velocities would be larger but deep enough in the atmosphere to minimize the possibility that the velocities are affected by the upper boundary condition or any stellar wind.

All three models do hit a quasi-equilibrium by consistently having a squared average velocity close to zero with no further spikes, at which point the larger grid size will be used to study the further evolution of the atmosphere. If after the model reaches a new point of equilibrium there still is microturbulence found naturally in the spectral features, then the microturbulence should be found in the stellar features at anytime. This same idea holds true whether or not it might generate a stellar wind to appear. With the initial perturbation, there would most likely be a wind that appears just from the atmosphere expanding or contracting, causing mass loss or gain in the model. If after the star is no longer expanding and/or contracting, there is still mass being blown off with positive values, those events would be a consequence of Doppler shifts in the spectral features.

Figure 5-3: Average of the squares velocity graph for 3538. The figure on the left is the velocity squared while the figure on the right is the root mean squared velocity.
5.2 Model End Results

After the models run a desired number of time steps information on the end state of the atmosphere is useful. This information describes how several of the key parameters change as one goes deeper into the given atmosphere. Some input data for the given models can change the output parameters along with other parts of the atmosphere. Because of these effects, certain properties were kept the same so that changes in metallicity, or line opacity in the atmosphere would impact the comparison. The following is a list of the properties in the atmosphere that were not changed during any of model atmosphere runs (see section 3.6).

<table>
<thead>
<tr>
<th>Name</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>X</td>
<td>.899</td>
</tr>
<tr>
<td>Y</td>
<td>.100</td>
</tr>
<tr>
<td>Z</td>
<td>.001</td>
</tr>
<tr>
<td>Column Mass Densityx1000</td>
<td>0.3000</td>
</tr>
<tr>
<td>Star Radius</td>
<td>5.20 $R_\odot$</td>
</tr>
<tr>
<td>Opacity of Line</td>
<td>100.00 g/cm</td>
</tr>
<tr>
<td>Atomic Weight of Line Atom</td>
<td>56 amu</td>
</tr>
</tbody>
</table>

Table 5.2: List of unchanged data parameters

The atom used for the spectral line feature is iron with a mass of 56 amu, because iron spectral features are common in the ultraviolet of B stars. The radius of the star used is $R=5.20R_\odot$. This radius is approximate for stars of our surface gravities and effective temperatures. The other two values listed in the table are arbitrarily chosen. The opacity ratio of the line to the continuum is set to represent typical values that would have an impact from Doppler shifts.

While all of the above information was held constant for the different temperature and surface gravity combinations, information regarding the temperature, pressure, and density of the atmosphere are dependent on these choices. All of the models go down to forty-five depths but the scaling differs between all of the different models.
This scaling is related back to the density scale height in the atmosphere.

As discussed in a later section, the atmosphere moves more-or-less in horizontal plane waves instead of part of a horizontal surface moving up while another part moves down. Because of this, the temperature, pressure, and density also behave in a similar fashion. At any specific depth, the temperature remains relatively constant but does increase with depth as expected. As seen in Figure 5-4 all three of the models follow a similar pattern that the temperature is flat across the horizontal surfaces instead of having hot and cool pockets at each level. At the same time at any single depth both the pressure and density are relatively constant across horizontal surfaces similar to the temperature. Since the atmosphere is fairly flat across the horizontal surface there is no turbulent motion caused by the inclusion of the Doppler shifts.

5.3 Determining Whether or not There is Micro-turbulence in the Atmosphere

To tell whether or not there is microturbulence in the atmosphere without adding additional terms one can look at the emergent spectrum along with the equivalent width of the feature. To see whether or not the Doppler shifts created a microturbulent velocity, one can run the same temperature and surface gravity combination with no Doppler shifts added to it for comparison. If the equivalent width is larger than what it would be without the Doppler shifts, then this means that there is microturbulence showing up in the spectral feature with no added factor.

In fact, we see increases in equivalent widths for all models. This means that there is a natural form of microturbulence occurring with the addition of the Doppler shifts without needing to add an additional term. As seen in Table 5.3, the values are higher for the atmospheres with the Doppler shifts compared to the same values with no Doppler shifts. This increase is seen at all time steps. This can also be
Figure 5-4: Temperature versus column for 4 different depths in all three models. For all three models the temperature across horizontal surfaces is nearly constant. In clockwise order the top left figure is 3535, top right is 3538, and the bottom figure is 4038.
Table 5.3: Equivalent widths for the three models for both the Doppler shifts and an atmosphere with no Doppler shifts added.

<table>
<thead>
<tr>
<th>Star</th>
<th>Equivalent Width (Hz)</th>
<th>Equivalent Width no Doppler shift (Hz)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3535</td>
<td>3.300 ± 0.001</td>
<td>3.241 ± 0.004</td>
</tr>
<tr>
<td>3538</td>
<td>3.028 ± 0.011</td>
<td>3.010 ± 0.008</td>
</tr>
<tr>
<td>4038</td>
<td>3.231 ± 0.011</td>
<td>3.005 ± 0.001</td>
</tr>
</tbody>
</table>

Figure 5-5: Emergent profiles for 3535 and 4038 with both the model profile along with several different added microturbulent velocities to the non Doppler shifted model atmosphere. Notice that for both of the two models that the overall profile is broader compared to the profile from a microturbulent velocity of 0 km/s.

seen the emergent profiles themselves. If there is a microturbulent velocity the profile is broader than what it would be with zero microturbulence artificially added with no Doppler shifts. As seen in the following figure for the different models, all of the different curves for simulated emergent profiles with added microturbulence are centered about the standard line center for the model. For the model curve averaged overall time steps, they are generally shifted to one side and are not completely symmetric about the line center.
5.4 Calculation of the Microturbulent Velocities

We use the full width half maximum (FWHM) of the spectral feature to find the microturbulent velocities. The FWHM is full width of the spectral absorption line as measure at one half of its depth. Depending on the shape of the spectral feature, the FWHM is related to the standard deviation of the spectral feature. Since the dominant broadening type of broadening used in this atmosphere is due to thermal motions and has a Gaussian profile, the equation for the FWHM is:

\[ f_G = 2.35482\sigma \]

(5.1)

where \( \sigma \) is the standard deviation.

To find the actual value of the FWHM for the profile, one has to fit the emission profile to a Gaussian curve. Generally, the core of the spectral feature closely matches the Gaussian while the wings or outer portion of the spectral feature fits closer to the Lorentzian shape. The models were fit at each time step to both profiles to determine how the profiles changed over the course of the time steps.

Even though the Doppler shifts change the overall shape of the profile compared to a model without the Doppler shifts, one can still use a traditional Gaussian curve to match it. This was double checked with LMfit, a python library used to fit different functions to data sets. This was done for each profile at the different time steps to determine whether or not one could use a standard Gaussian or Lorentzian curve. One of the parameters checked by LMfit is the center of the curve, which is known from the data set, and the deviation from that. As the line center was known from the Doppler shifts and the data itself, the model with the closest fit to the actual line center was the best fit for the core of the spectral feature. Both the standard Gaussian and Lorentzian profiles fit the closest to the actual line center of the profiles.

Once the FWHM is known the relationship between the FWHM and microturbu-
To find the value of the microturbulent velocity in the atmosphere, one needs to know the entire emergent radiation field coming from the star. Once the profile is known, then the FWHM and the individual value for microturbulence can be calculated at each time step. Since this is not a plane parallel atmosphere, one also needs to know the averaged emergent profile across all six outward directions. Not all directions will have the same fraction of the total emergent profile: for example the total emergent radiation in the horizontal direction, m=6, will be a much smaller fraction of the total compared to the vertical direction. The other four directions that are offset by 60° will have close to the same fraction of the emergent profile, but less than that of the vertical direction. To find the values of the emergent radiation profile in all directions, one takes the fraction of the total emergent radiation field in that direction. To find the actual value of the microturbulence, one has to match the profile of

\[
\Delta \nu_{FWHM} = 1.665(u_0^2 + 2\xi^2)^{\frac{1}{2}}
\]  

(5.2)

where the subscripts correspond to the given direction. This shows that most of profile is from the vertical direction, a negligible fraction of the profile is from the horizontal direction, and equal portions of the emergent profile come from the off angle directions. The amount of emergent radiation coming from each of the six directions, it is a ratio of the total surface area of a sphere to a rhombic dodecahedron. Since stars are spheres and the radiation field is coming from all directions, the amount of the continuum in each direction is the fraction of that.

To find the actual value of the microturbulence, one has to match the profile of
the different models by adding in pseudo-microturbulence field to the models until the two profiles match the FWHM. This is done by first running the model with the appropriate temperature and surface gravity but with no added turbulence and adding different velocity values to see what the actual value would be. Once run, these were fitted in the same method using LMfit to find the FWHM, and checked against the Doppler shifted FWHM at each time step. The added velocity value that matched the FWHM of the Doppler shifted model is the given microturbulence value in the atmosphere.

5.5 Values of Microturbulence in the Atmosphere

As seen in the prior two sections, the Doppler shifts produce a larger equivalent width compared to that of the same temperature and surface gravity without the Doppler shifts. With this fact, the values for the microturbulence can be determined from the emergent profiles fitting the FWHMs. Out of the three models, the 3538 is the only one that the exact value of the microturbulence can be determined at every single time step. This model the spectral profile is fairly close to being symmetric in shape compared to the other two profiles. The other two models one can find the microturbulent velocities for most of the time steps but there are quite a few time steps that due to the shape of the profile and the limited frequency bins that the profiles of the Doppler shifted models cannot be matched completely to a non Doppler shifted model with added microturbulence.

As seen in the previous section, there is a definite increase in the equivalent width of the spectral feature compared to the same model with no Doppler shifts added into the profile feature. The reason for not finding an actual value of the microturbulent velocity comes back to the idea of the Doppler shifts themselves. Since the Doppler shifts can move the emergent profile line center, the line center for the Doppler shifted
Figure 5-6: Microturbulent velocities for 3538 over the entire time interval. The overall period for the shape of the microturbulent curve is approximately 50 time steps. The figure on the left shows the overall pattern of the microturbulent velocities over the entire time frame. The figure on the left gives the same microturbulent velocity graph with the inclusion of the location of the average velocity and one standard deviation from the average.

profiles are not centered at the original line center. The FWHM calculations for the non Doppler shifted models are centered about line center and are completely symmetric.

For the other star, the 3538 the value for the microturbulence can be determined at each time step. Since the turbulence can vary, the microturbulence will also change over the entire time period. The values of microturbulence range anywhere between 1-25 km/s over the course of time. The overall average value of microturbulence is 10.69 km/s. As seen in Figure 5-6, the values follow a sinusoidal wave which is to be expected since the velocity in the atmosphere has a similar shape. The FWHM for the values follow this similar pattern over the course of all time steps with a similar shape. The values for the FWHM increase and decrease over time with a fairly regular periodic shape.

Even though the values for the microturbulence is not found directly from the velocity in the atmosphere it would have a fairly similar shape to the velocity itself as that is what is causing the Doppler shifts. The overall period for the microturbulence
is 50 time steps and then it settles down lower towards the end of the run closer to
the average of 10-11 km/s. This is expected as the larger changes in the velocity
occur in the earlier portion of the run even with the star reaching an equilibrium,
the larger spread in microturbulent velocities would indicate a larger turbulent time
frame in the earlier stages of the run. At the end of the run when the velocities are
closer to the average the standard deviation of the velocities is 6.83 km/s which is
within the standard range of error for microturbulence within the 5-20 km/s seen in
the literature (Cantiello 2009).

5.6 Mass Loss Due to Winds

Since there is a nonzero velocity in the upper portion of the atmosphere this means
that material can be blown off in terms of a stellar wind. Positive upward velocities
means that the material is moving up and off the star. There are also points in the
time evolution of the atmosphere that material is moving downwards. While there is
no constant stream of material off of the star, one can see how the material and the
formation of the wind behaves over the course of time and estimate the amount of
mass that would be lost from the atmosphere.

To find see how much mass would be lost due to the stellar wind one needs to find
\( \dot{M} \), which is the mass loss rate given by:

\[
\dot{M} = \rho v dA
\]

(5.4)

where \( dA \) is the surface area of a cell:

\[
dA = \frac{ds^2}{2\sqrt{2}}
\]

(5.5)

with \( ds \) related back to the scale height of the atmosphere. As the model has off
diagonal velocities that will contribute to the amount of mass blown off due to a wind, the directions m=2,3,4,5 include a factor of \( \frac{1}{2} \) included because of the 60° from the vertical.

Not all of the cells at a given depth will contribute to the mass loss; only the cells at the upper boundary will be the ones that have any material leaving the atmosphere. These cells and directions are shown in Figure 5-7. The directions of the upper cells with no arrows do not contribute any to the stellar wind as those would be connected to cells included in the model.

The mass loss is actually calculated at the upper surface of depth \( l=3 \) for all three different models involved. This depth was chosen instead of \( l=1 \), so that the upper boundary condition had less influence but close enough to the top of the atmosphere that the material would be able to escape the atmosphere.

During the first 1000 steps with the smaller grid size the amount of mass that is lost is more dynamic at the beginning compared to after the star comes close to an equilibrium. During this period of time the star is still adjusting to the perturbations occurring with the Doppler shifts and because of this sees the most significant
Figure 5-8: Mass gain and loss over time for both sets of iteration for 3538. The left figure is the model run with the 10 cell grid while the figure on the right corresponds to the 102 cell model. Negative values indicate that the atmosphere is gaining material at that depth from the depth above, while positive values indicate that there is a loss of material at that depth.

Table 5.4: Overall mass gain or loss for the three models over the first 1000 time steps.

<table>
<thead>
<tr>
<th>Star</th>
<th>Average Mass Loss ($M_{\odot}$/yr)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3535</td>
<td>8.381x10^{-6} (loss)</td>
</tr>
<tr>
<td>3538</td>
<td>1.24x10^{-6} (loss)</td>
</tr>
<tr>
<td>4038</td>
<td>1.68x10^{-6} (loss)</td>
</tr>
</tbody>
</table>

Even though there is mass gain and loss over the course of the time intervals used, the integrated amount of gain and loss is a mass loss. As seen in Tables 5.4 and 5.5, which describe the mass change over the course of the total time including both the initial time and the later time intervals, the last column has a positive value which indicates the total amount of mass change is a loss. This is due to the positive
Star Average Mass Loss ($M_\odot$/yr)
3535 $2.97 \times 10^{-3}$ (loss)
3538 $5.15 \times 10^{-8}$ (loss)
4038 $4.74 \times 10^{-5}$ (loss)

Table 5.5: Overall mass loss for the three models over the second set of time steps.

velocities pushing the material outwards. If one looks at the values from Table 5.5, which is the larger resolution the values correspond to the amount of material expected for the temperature and surface gravities of hot stars. The standard amount of mass loss from winds for stars of $T=30,000$ K, is $10^{-9} M_\odot$/yr (Abbott 1981). While stars with temperatures around $35,000$ K have mass loss due to stellar winds of $10^{-4}-10^{-5} M_\odot$/yr. The value for the 3538 falls within the range of what would be expected for the temperature and surface gravities of the stars. The other two stars values are outside of the range seen in Abbott and are either much higher or lower than what would be expected for the two stars. This may be related to the amount of time steps ran for all of the different models. In both cases these stars were ran for less time steps compared to the 3538 model so the overall average may be skewed because of this. The other reason is this may not be a stellar wind and something else is going on completely due to the boundary conditions causing an artificial mass loss.

There is a definite difference in the amount of mass loss between the low resolution model and the high resolution model with the time steps. This is an interesting and surprising result since the mass loss over time are all fairly similar for all three models used but for the higher resolution the values vary significantly. This may be related to the fact that all three of the low resolution models ran for a significantly more time steps compared to any of the individual high resolution models on the order of at least five times more time steps ran. Because of this, the overall average is smoothed out over a longer time frame and settles down to match within reason to expected values of mass loss for the temperature and surface gravities. If one looks at a smaller
portion of the low resolution model the values are consistent with each other.

### 5.7 Velocities in the Atmosphere

As seen with the initial input of the Doppler shifts, there is a periodic pattern to the velocity in the atmosphere. At the scale of the models here, the addition of the Doppler shifts causes the atmosphere itself to move in terms of plane waves instead of individual hot and cool cells in the atmosphere. This means that the entire horizontal surface moves up and down as a whole. The models show similar periodic patterns in the velocity. The velocities in several different layers should be moving up and down and switching directions. As the upper layers move downwards with a negative velocity, deeper layers move up with a positive velocity, and vice versa.

As one goes through the entire cycle of the iterations, there are a few points at specific depths where the velocities are no longer constant with small deviations across the horizontal surface. During these time steps the upper layers of the atmosphere have a larger dispersion, as seen in Figure 5-10. All three of the models show the same pattern in the velocities, so it is not a special feature for one surface gravity or temperature. In Figure 5-10, the right figure is zoomed in to show the distinct differences in the velocity, but even when zoomed out there is distinct separation in the layers. In each case, after a few time steps the velocity returns to close to an almost completely flat horizontal surface again.

At the same time, not all of the depths have this feature. For certain depths closer to l=20 and lower the velocity stays close to the flat horizontal surface seen in Figure 5-9. This is related back to the depth of the atmosphere itself. Since this is only occurring at specific depths, it indicates that there is something else going on during these iterations at the depths in question that is causing this difference in velocity across the surface.
Figure 5-9: Velocity versus cell position for all three models used. Top left is 3535, top right is 3538, and bottom left is 4038. Notice that for the most part all three of the models’ velocities are fairly constant and that there is no large variation in the velocities across the surface for each depth.
Figure 5-10: Velocities for two different time steps for star 3538. The figure on the right is during one of the time periods where the velocities for the 4 chosen depths disperse and are no longer a completely flat surface. The figure on the left is two time steps before.

One cause of this behavior with the velocity for certain depths could be that it is a by-product of how the time steps are done. Even with the discussion of different algorithms tested to speed up the computational portion of the model, to run a large grid for long intervals takes a great deal of time. To decrease the time involved, there was a factor added to the code to increase the time step for each iteration. This allowed for a run of half the number of iterations in the same amount of time. Although the time steps chosen still are under the Courant limit for the maximum size of the time step to not exceed the time for sound to travel to the next grid cell, the fact that some of the velocities start to have a greater spread and reorient themselves a few steps later causes some concern.
Chapter 6

Conclusions and Future Work

6.1 Conclusions

6.1.1 Microturbulence

The main goal of this work was to see whether or not adding Doppler shifts into the spectral profile of a hot star itself would cause a microturbulent velocity field to appear without having to add any additional factors to the model itself. As seen with both the actual value of the microturbulence for the 3538 model, and the discussion with the equivalent widths for all three models, this was a success. For all of the steps the value of the equivalent width for the Doppler shifted atmospheres were larger than the same atmospheres with no Doppler shifts. A larger equivalent width implies that the spectral feature is broadened by more than just thermal motions and natural broadening alone. Though the actual value of the microturbulence could not be determined directly for two of the models used, this still allows for proof that the Doppler shift idea can cause a microturbulence field without having to add in additional terms. The value for the one star that the microturbulent velocity could be calculated directly, 3538, is within the range expected empirically for hotter stars. The value for the microturbulence trends to larger values for hotter stars compared to the same surface gravity with a lower temperature.
Seen in the 3538 model the microturbulent velocity is not a single value throughout the entire time iteration. This value ranged anywhere between 1 km/s- 24.4 km/s. This implies that it may not be that accurate to use one value for the microturbulent velocity in hot stars as seen in Steffen et al’s (2013) work. Though the microturbulent velocities for the most part fall into the standard range of errors within 5-10 km/s, there is still enough variation to need to find the exact value of the microturbulence for each time step. This could change how stellar atmosphere models include microturbulence for spectra matching with observations. To make certain that the values for hot stars match empirical models it would be best to run other star temperature and surface gravities in the O, B, and A ranges.

6.1.2 Stellar Winds

One of the surprising consequences for the inclusion of Doppler shifts in the stellar atmosphere was the formation of a wind in the upper layers of the atmosphere. As discussed in the last chapter, the overall mass loss and gain from the movement of the atmosphere at one of the subsurface depths is an overall loss for all three models. This implies that the mass is leaving the atmosphere at a rate near what is found in typical hot main sequence stars (Abbott 1981). The origin of stellar winds has not been well understood, and this finding could be the cause of the winds that are observed. Without the inclusion of the Doppler shifts there is no mass loss in the upper layers of the atmosphere and as soon as the Doppler shifts are included into the atmosphere there is an overall net amount of material leaving the star. This is seen both in the initial perturbation and then again in the second set of runs using the larger grid size. This is a preliminary finding that needs more exploration to see whether or not longer time steps may cause the mass loss to be within the generally accepted range.

If same behavior happens in stars at a lower temperature but still considered hot
stars then this may very well be the origin for winds in all hot stars. In this case, not only can the Doppler shifts naturally cause a microturbulent velocity with any level of metallicity, this can also naturally explain where stellar winds come from.

6.1.3 Overall Structure of the Atmosphere

Normally one would expect at the horizontal surface at any depth that there would be "cool" and "hot" bubbles moving up and down in the atmosphere, so that at any given depth the velocities would not all be the same. This was not the case as seen looking at all the information for the temperature, density, pressure, and velocity across the surface. All of those values at any given depth have similar values and the atmosphere moves up and down in a plane wave rather than some of the cells move up while other cells move down. Since all of the velocities are similar value in the same direction, the temperature and density also flat across the horizontal surface at any depth. One of the consequences of this is seen from the stellar winds. All of the cells in the entire depth will either be gaining of losing material at that point instead of some of the cells losing material at any given point. This causes the overall atmosphere to have a coherent motion instead of a turbulent motion that would generally be expected to have at any given point with the inclusion of the Doppler shifts.

While the overall atmosphere moves up and down, there were certain points that the velocity started to disperse over a range of velocities for a few time steps and then resume the pattern of a flat velocity surface. The time step increase was not the cause of this reaction, otherwise the velocity would flatten again across the horizontal surface within a few time steps. The emergent profiles did not show anything happening out of the normal with the values for the microturbulent velocity before or after this occurred, but it would be worth letting the model run for a longer time frame to see if this happens on a regular basis every few cycles or not.
6.2 Future Work

In this thesis, the models used were for a small range of both temperatures and surface gravities to analyze the value for microturbulence. In reality hot stars have a large range of both temperatures and surface gravity to include for all O, B, and A spectral type stars. This thesis show that the values found for the models in question follow the general trend for values of microturbulence for hot stars but to fully explore this, a larger range of temperatures and surface gravities is needed. In the future one could look at stars with temperature range from 15,000 K to 45,000 K to make certain that the values for these stars match what is expected and found from observations such as the FLAMES survey. There was a very narrow range of surface gravities used in the three model atmospheres which could be expanded out to a range of log $g$ from 2.0 to 4.4, covering the entire hot star range. Including a wider variety of hot stars not only will be able to match the microturbulent velocities with the empirical values for the upper range, or actual values for the stars at the lower range it will also allow to see whether or these stars also have a formation of a stellar wind at a large range of temperatures.

Along with increasing the range of the temperature and surface gravity, one could increase the time steps further than to track the continual evolution of the microturbulence. As seen, the microturbulence in the middle of the atmosphere fits a similar shape for the change of the value of microturbulence with changes due to the change of velocity, so further study of this evolution, one would need to increase the number of time steps out to longer durations. Increasing the number of time steps allow to see if the trend for the values follow the track and gives better information on the emergent profile of the atmosphere.

The cell grid used for this thesis was a 102 cell grid with 45 depths at the upper portion of the atmosphere. The larger the cell grid the greater resolution for the
change in velocities and other general properties of the star, such as temperature, density, and electron pressure at each cell point in the atmosphere. It is ideal to have the best resolution possible to fully see the extent of the physics, therefore it would be advantageous to increase the cell grid size by at least a factor of two or greater. Increasing the cell grid by a factor of two would allow to see in finer detail the overall trend of microturbulence. At the same time, increasing the depth of the atmosphere would also allow to see how the microturbulence behave at even greater depths. As different spectral features appear at different depths in a real stellar atmosphere, depending on the optical depth of the atmosphere at that point, increasing the depth would allow for the simulation of other spectral features and to see the behavior of the microturbulence at that depth.
References


C. Hunter et al., 2013, ”The VLT-FLAMES survey of massive stars: Evolution of surface N abundances and effective temperature scales in the Galaxy and Magellanic Clouds”, A&A 7838
