Stellar Abundances in the Solar Neighborhood

by

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ABSTRACT

The only elements that were made in significant quantity during the Big
Bang were hydrogen and helium, and to a lesser extent lithium. Depending
on the initial mass of a star, it may eject some or all of the unique, newly
formed elements into the interstellar medium. The enriched gas later collapses
into new stars, which are able to form heavier elements due to the presence
of the new elements. When we observe the abundances in a stellar regions,
we are able to glean the astrophysical phenomena that occurred prior to its
formation.

I compile spectroscopic abundance data from 49 literature sources for
46 elements across 2836 stars in the solar neighborhood, within 150 pc of the
Sun, to produce the Hypatia Catalog. I analyze the variability of the spread in
abundance measurements reported for the same star by different surveys, the
corresponding stellar atmosphere parameters adopted by various abundance
determination methods, and the effect of normalizing all abundances to the
same solar scale. The resulting abundance ratios [X/Fe] as a function of [Fe/H]
are consistent with stellar nucleosynthetic processes and known Galactic thin-
disk trends.

I analyze the element abundances for 204 known exoplanet host-stars.
In general, I find that exoplanet host-stars are not enriched more than the
surrounding population of stars, with the exception of iron. I examine the
stellar abundances with respect to both stellar and planetary physical prop-
erties, such as orbital period, eccentricity, planetary mass, stellar mass, and
stellar color. My data confirms that exoplanet hosts are enriched in [Fe/H]
but not in the refractory elements, per the self-enrichment theory for stellar
composition.
Lastly, I apply the Hypatia Catalog to the Catalog of Potentially Habitable Stellar Systems in order to investigate the abundances in the 1224 overlapping stars. By looking at stars similar to the Sun with respect to six bio-essential elements, I created maps that have located two “habitability windows” on the sky: \((20.6^h, -4.8^\circ)\) and \((22.6^h, -48.5^\circ)\). These windows may be of use in future targeted or beamed searches.
DEDICATION

I dedicate my dissertation to the three most important people in my life:
my parents and my Caleb.

Without your love, support, and advice, I would not be who I am today. You
have made me a better person by giving me your strengths and helping me
to overcome my weaknesses. Thank you with all of my heart.

Also, this dissertation is in loving memory of my grandmother, Lorraine – a
strong woman who loved chemistry so much she might have even read the
entirety of Chapter 3.

"Though the sex to which I belong is considered weak, you will nevertheless
find me a rock that bends to no wind."

~Elizabeth I
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4.4 Similar to Fig. 4.3 but for [N/Fe], plotted with respect to [Fe/H] (left) and relative frequency (right). The majority stars in both the full Hypatia catalog and the known exoplanets have an abundance of [N/Fe] between -1.0-0.0 dex. While a higher relative population of stars within all of Hypatia show larger [N/Fe] abundances, the known exoplanets have [Fe/H] predominantly above solar.

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Chapter 1

INTRODUCTION

One of the primary tools to understand the history of the solar neighborhood, and more generally the Milky Way, is the chemical composition of stars (Arnett, 1996, and references therein). Elements created within the interiors of stars are produced and ejected in a variety of ways, depending on the star. Stars are formed from massive gas clouds that collapse due to gravitational instabilities within the cloud. A collapsing region becomes a star when it reaches a sufficient density and temperature for nuclear fusion to begin. The fusion creates new elements out of those already present from the original gas cloud and releases energy to support the star via hydrostatic equilibrium. As lighter elements are converted into heavier elements, the fusion and energy decrease until the star is no longer able to maintain hydrostatic equilibrium. The end result of a star is dependent on its initial mass. A lower mass star may expand and contract as internal pressure and gravitational forces vary dramatically, releasing chemically enriched gas into the nearby environment. If a star is sufficiently massive, its core collapses and triggers a supernova explosion, where the shockwave is able to propel its internal material to large distances. The enriched gas is later integrated into massive clouds. When new stars are formed, heavier elements are formed due to the presence of the higher metallicity material. Observation of specific element enrichment can signify a particular astrophysical event and, as the cycle repeats, the history of a stellar environment may be ascertained.
From the initial efforts of Russell (1929), Suess & Urey (1956), and Bidelman (1960), to the more recent works of Anders & Grevesse (1989), Edvardsson et al. (1993), Bensby et al. (2005), Valenti & Fischer (2005), Asplund et al. (2009), and Lodders et al. (2009), compilations of stellar abundances provide an overall picture of the chemical evolution of our solar neighborhood. Notable results obtained over the past few decades include correlations of metallicity with age and galactocentric distance, and whether the Sun is suitably “average” (Eggen et al., 1962; Twarog, 1980; Feltzing et al., 2001; Robles et al., 2008a,b). Trends in the elemental abundances, as well as a limited number of isotopic abundances, relative to iron have also been observed to have a large range of metallicities within the plane of the Galactic disk (Venn et al., 2004; Soubiran & Girard, 2005). For example, oxygen and the other $\alpha$-chain elements, relative to iron, vary systematically from being overabundant at high metallicities ($[\text{Fe/H}] \lesssim 1.0$ dex) to roughly solar at solar metallicities, or $[\text{Fe/H}] \approx 0.0$. This decrease is widely taken to be caused by the contributions of supernovae Type Ia (SN Ia) in a mean, well-mixed interstellar medium (Truran & Cameron, 1971; Tinsley, 1980; Matteucci & Greggio, 1986; Lamberts, 1989; Wheeler et al., 1989; Timmes et al., 1995; Goswami & Prantzos, 2000; Gibson et al., 2003; Kobayashi et al., 2006; Krumholz et al., 2007; Prantzos, 2008; Romano et al., 2010; Kobayashi & Nakasato, 2011).

Another tool to help interpret the history of the solar neighborhood is the theory of stellar evolution, nucleosynthesis, and chemical evolution. By quantifying the ejecta from stars, this history can be reconstructed using theoretical models (Burbidge et al., 1957; Cameron, 1957; Woosley & Weaver, 1995; Thielemann et al., 1996; Meynet & Maeder, 2002a; Siess et al.,
2002; Ventura et al., 2002; Limongi & Chieffi, 2003; Karakas & Lattanzio, 2007; José & Iliadis, 2011). The models account for the initial mass function, star formation rate, stellar yields, and inherited composition from the local interstellar medium (ISM). Their results help quantify the formation of stars and provide important constraints on chemical evolution of the solar neighborhood, the Galactic disk, and other galaxies.

Stellar abundances have also been analyzed with respect to extrasolar planets, or exoplanets. Since the detection of the first exoplanet orbiting a main-sequence star by Mayor & Queloz (1995), there have been a number of questions regarding the stellar and planetary criteria under which a star may harbor a planet. Studies conducted by Bond et al. (2008, 2006); Fischer & Valenti (2005); Gálvez-Ortiz et al. (2011); Gilli et al. (2006); Gonzalez & Laws (2000); Gonzalez (1997); Laws et al. (2003); Reid (2002); Santos et al. (2004, 2001); Sousa et al. (2011) examine the correlation between the metallicity of the host-star and the presence of an exoplanet, within both volume- and magnitude-limited samples. The independent conclusions of these analyses is that stars with orbiting giant exoplanets are more metal rich than non-host stars.

The general metallicity of the host-star has been studied with respect to other planetary characteristics as well. Stars that host multiple exoplanets tend to be more metal rich (Fischer & Valenti, 2005). Giant planets with short periods or smaller semi-major axes predominantly orbit metal-rich stars (Gonzalez, 1998b; Santos et al., 2006a, 2003; Sozzetti, 2004). In contrast to the giant planets, the same metallicity enhancement is not found within stars that host planets with Neptune-masses or below (Udry & Santos, 2007; Ghezzi et al., 2010; Sousa et al., 2011). Guillot et al. (2006)
found that the chemical composition of a host-star is related to the makeup of the giant exoplanet. Unfortunately, there have been no direct measurements of a planet’s composition and therefore, no ability to quantitatively correlate the respective abundances. However, under the assumption that planets and host-stars were formed out of the same molecular cloud, the composition at the stellar photosphere can act as a potential indicator for the abundances of the exoplanet.

Star forming molecular clouds comprised of elements and abundances different than our Sun will likely result in stars with a variety of atmospheric compositions and ranges in which they may be detected. Fortney (2012) detailed how various ratios of C/O, specifically when $0.8 < \text{C/O} < 1.0$ per the results given in Bond et al. (2010); Delgado Mena et al. (2010); Petigura & Marcy (2011), alter the types of molecules seen within stellar atmospheres. For example, in the atmospheres of dwarf stars, if C/O $< 1$ then we expect to see a predominance of CO and H$_2$O, with high opacity in the infrared. On the other hand, if C/O $> 1$, the photosphere is composed of CO, $C_2$, and CN which dominates the optical spectra. Assuming the star-planet abundance correlation, the composition of a star can affect the planet’s makeup, structure, and atmosphere (Bond et al., 2010). For example, isotopes such as $^{26}$Al and $^{60}$Fe have relatively short radioactive decay times, $\sim 10^6$ years. Through radioactive heating, they are able to increase the temperature of a planetesimal and boil off water or other volatiles (Lee et al., 1976; Grimm & McSween, 1989; Prialnik & Bar-Nun, 1990; MacPherson et al., 1995; Shukolyukov & Lugmair, 1993a,b; Krot et al., 2006; Schubert et al., 2007; Castillo-Rogez et al., 2007).
While the vast majority of the literature has concentrated on \([\text{Fe/H}]\) as a general stellar metallicity indicator, some have examined host-star metallicity with respect to individual, non-iron elements (e.g. Beirão et al., 2005; Brugamyer et al., 2011; Ecuvillon et al., 2004; Gilli et al., 2006; Neves et al., 2009). When searching for terrestrial, Earth-like planets, the presence of some elements is more consequential and informative than others. Elements such as H, C, N, O, Mg, Si, P, S, Mo, and Se are paramount for the atmosphere, structure, and biogeochemistry found on Earth and are generally deemed “bio-essential.” Therefore, the chemical composition of a host-star, assuming a correlation between the abundances in the host-star and the exoplanet, is important when considering the habitability of the exoplanet.

If exoplanets are to be habitable, in addition to the bio-essential elements, it is also believed that host-stars should exhibit properties similar to the Sun. This concept is described in Turnbull & Tarter (2003a) (and references therein) who classified a subset of stars in the solar neighborhood from the Hipparcos Catalog as being potential hosts to habitable exoplanets. Their determinations were based on stellar age, variability, multiplicity, kinematics, spectral type, which went into creating the Catalog of Potentially Habitable Stellar Systems (hereafter, HabCat). While HabCat contains ~17,000 stars, the catalog contains only one abundance measurement, \([\text{Fe/H}]\), which acts as an indicator for metallicity.

In addition to analyzing exoplanet host stars, the Hypatia Catalog may be used to find stellar abundance trends between thin and thick disk stars, slow and fast rotating stars, stars of different spectral types (or effective temperatures), exoplanet hosts versus stars confirmed to be without exoplanets (as opposed to background stars), or solar analog stars. Similar to
HabCat, Hypatia may also be used to supplement pre-existing surveys such as NASA’s Kepler mission, the ESA/NASA Herschel mission, or the Sloan Digital Sky Survey. Given that most of the abundance data within the catalog was determined in the visible band, the data may also be combined with abundances from other wavelengths. The breadth of information present within the Hypatia Catalog also makes it useful for gleaning new stellar information, such as stellar ages and the kinematics of the solar neighborhood.

It is difficult and rare for one survey to systematically observe a large number of nearby stars and provide abundance determinations for a wide variety of elements. For example, Valenti & Fischer (2005) reported the relative abundance in 1040 stars for only five elements, including iron. Alternatively, Reddy et al. (2003) analyzed spectra for 27 elements, but their study had only 181 stars. To achieve the most complete coverage of the solar neighborhood, the relative abundances from known literature sources must be combined. Such compilations have been undertaken by, for example, Venn et al. (2004) and Soubiran & Girard (2005), with the amalgamation of thirteen and eleven published catalogs, respectively.

As the number of spectroscopic surveys of stars in the solar neighborhood increases, it has become tradition for authors of abundance surveys or chemical evolution models to compare their relative abundances to benchmark data sets for verification or validation. Typically, this involves comparing to Edvardsson et al. (1993), Reddy et al. (2003), Bensby et al. (2005), or Valenti & Fischer (2005). However, the manner by which these comparisons are conducted varies drastically. Some authors provide statistical evaluations such as mean differences and standard deviations,
some compare a few “typical” stars, and others graphically juxtapose entire catalogs. While there are certainly correlations between published data sets, there has been little discussion of the nuances, random uncertainties, and systematic biases of the compared data sets. It is, however, these idiosyncrasies that make interpreting trends between abundance catalogs challenging.

The purpose of this dissertation is to present the Hypatia Catalog (hereafter, Hypatia) — a compilation of spectroscopic abundance determinations from 49 literature sources for 46 elements across 2836 stars within 150 pc of the Sun. In Chapter 2 we discuss the collation of the data, the inherent challenges in combining different data sources, and our attempts to mitigate some of the challenges. In Chapter 3, we present the stellar abundance trends of 46 elements found in the solar neighborhood. In Chapter 4, we analyze the Hypatia Catalog with respect to the known exoplanet host stars within 150 pc. In Chapter 5, we present an application of Hypatia with respect to the Catalog of Potentially Habitable Stellar Systems by Turnbull & Tarter (2003a). We summarize our conclusions in Chapter 6. Finally, in Appendix A we describe a prescription for determining the area and volume fraction cut by a plane within a multidimensional, hydrodynamic grid cell. The work discussed in Chapters 2, 3, and 5 is currently in review with the Astronomy & Astrophysics journal.
Numerous studies analyze the photospheres of stars in the solar neighborhood using photometric and spectroscopic techniques. Photometric investigations have treated a much larger number of stars relative to spectroscopic methods. However, photometric studies generally yield one global metallicity parameter, $[\text{Fe}/\text{H}] = \log \left( \frac{N_{\text{Fe}}}{N_{\text{H}}} \right)_* - \log \left( \frac{N_{\text{Fe}}}{N_{\text{H}}} \right)_\odot$, with units in dex, where $N_{\text{Fe}}$ and $N_{\text{H}}$ are the number of iron and hydrogen atoms per unit volume, respectively. Despite the smaller number of stars analyzed with spectroscopy, the additional element abundances allow assessment of not just the overall metallicity, but the full chemical compositional range and evolution. Therefore, we have chosen to focus on published spectroscopic abundance catalogs.

We compiled Hypatia with the spectroscopic abundance determinations of 46 element abundances for 2836 unique stars from published catalogs. Our exhaustive literature search considered all abundance determinations, of which we are aware, for main sequence F/G/K/M-type stars within 150 pc of the Sun. Per the definition given in Gilmore & Reid (1983), all of the stars within Hypatia reside in the thin disk. Table 2.1 shows a sample of the Hypatia Catalog which includes stellar HIP/HD/BD names, spectral type, distance, position, and the compiled abundances as given by each catalog, with reference. The complete catalog is given in the electronic version of our published paper. Efforts were made to include literature sources with abundance measurements for local stars; any
Table 2.1: Example of the Hypatia Catalog

| Star: HIP = 400 | HD = 225261 | BD = B+22 4950 | Spec Type = G9V | dist (pc) = 26.39 | RA/Dec = (1.23, 23.27) | NaH -0.35 [Valenti & Fischer (2005)] | SiH -0.25 [Valenti & Fischer (2005)] | TiH -0.28 [Valenti & Fischer (2005)] | FeH -0.44 [Valenti & Fischer (2005)] | NiH -0.43 [Valenti & Fischer (2005)] | OH 0.01 [Petigura & Marcy (2011)] | FeH -0.44 [Petigura & Marcy (2011)] |

exclusion was not intentional. Therefore, if a star within the solar neighborhood was measured for abundances other than iron, then it was incorporated into Hypatia. The data sets that are contained in Hypatia are listed in Table 2.2, along with the number of stars meeting the above criteria and the element abundances determined therein. Throughout the paper, we give a more detailed description of each literature source and their method for determining stellar abundances.

A histogram of the number of stars measured for each element in Hypatia is shown in Fig. 2.1. All 2836 stars have a spectroscopically determined [Fe/H]. However, due to the effects associated with combining multiple data sets discussed in §2.1, Fig. 2.1 shows 2792 stars for [Fe/H]. The next most frequently measured elements in Hypatia are Si (2189 stars), Ti and Ni (2107 stars each), and Na (1883 stars). There are only 32 stars in the solar neighborhood for which [Ru/H] has been measured and only 20 stars for [P/H]. Fig. 2.1 also shows the relative paucity of stars in the solar neighborhood that have had their bio-essential nitrogen, magnesium, and sulfur abundances determined. This is primarily due to having too few
absorption lines, or lines that are too weak to separate from the continuum in the optical spectrum.

2.1 Spread in the Combined Data

Collecting abundance determinations from multiple authors over about a 25 year time span means at least the following differences between data sets: instrument zero points, resolution of the spectra, signal-to-noise ratios, oscillator strengths, line lists, equivalent widths, number of ionization stages used, local thermodynamic equilibrium (LTE) or non-LTE analysis, converged solar atmosphere models, curve-of-growth or spectral fitting, curve-of-growth program used, and adopted solar abundances. All of these factors may introduce systematic and stochastic differences between data sets. For example, Fig. 2.2 (top) shows the abundance measurements for six elements within five Hypatia stars. The circles are as labeled with the element name while all triangles designate [Fe/H], each with respective errorbars from the catalog from which it was measured. The variation between catalogs per element, the largest of which we call the spread, is generally in the range of 0.1-0.15 dex.

Due to the large number of catalogs compiled to form Hypatia, we find there is an accumulation of systematic and stochastic differences in the abundance measurements. Other authors have noted the difficulties in comparing different catalogs (e.g. Feltzing & Gustafsson, 1998; Bond et al., 2006), but few have tried to overcome the challenges. We attempt to make the various catalogs in Hypatia more copacetic by putting all the different measurements on the same solar abundance scale. Normalization to the same solar scale is the only correction available to us that does not involve
<table>
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<th>Literature Reference</th>
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<th>Elements</th>
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<tr>
<td>Allen &amp; Porto de Mello (2011)</td>
<td>33</td>
<td>(Fe, Mn, Cu, Zn, Y, Ba, Nd, Eu, Ge, Dy)</td>
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<td>(C, O, Mg, Si, Ca II, Sc II, Ti II, Fe, Co, Ni, Cu, Zn, Y, Ba, Ce, Nd, Eu)</td>
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<td>Petigura &amp; Marcy (2011)</td>
<td>914</td>
<td>(Fe, C, O)</td>
</tr>
<tr>
<td>Ramírez et al. (2007)</td>
<td>523</td>
<td>(Fe, O)</td>
</tr>
<tr>
<td>Ramírez et al. (2009)</td>
<td>64</td>
<td>(Fe, C, O, Na, Al, Si, S, Ca, Sc, Ti, V, Cr, Mn, Ni, Cu, Zn, Y II, Zr II, Ba)</td>
</tr>
<tr>
<td>Reddy et al. (2003)</td>
<td>179</td>
<td>(Fe, C, N, O, Na, Mg, Al, Si, S, K, Ca, Sc II, Ti, V, Cr II, Mn, Co, Ni, Cu, Zn, Sr, Y II, Ba, Zr II, Ce, Nd, Eu)</td>
</tr>
<tr>
<td>Reddy et al. (2006)</td>
<td>171</td>
<td>(Fe, C, O, Na, Mg, Al, Si, Ca, Sc II, Ti, V, Cr II, Mn, Co, Ni, Cu, Zn, Y II, Ba, Ce, Nd, Eu)</td>
</tr>
<tr>
<td>Shi et al. (2004)</td>
<td>97</td>
<td>(Fe, Na)</td>
</tr>
<tr>
<td>Takeda &amp; Honda (2005)</td>
<td>159</td>
<td>(Fe, C, N, O, Na, Mg, Al, Si, S, Ca, Sc, Sc II, Ti, Ti II, V, V II, Cr, Cr II, Mn, Co, Ni, Cu, Zn)</td>
</tr>
<tr>
<td>and Takeda et al. (2007)</td>
<td>663</td>
<td>(Li, O, Na, Mg, Al, Si, Ca, Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Sr, Y, Zr, Mo, Ba, La, Ce, Nd, Sm, Eu)</td>
</tr>
<tr>
<td>Thevenin (1998)</td>
<td>663</td>
<td>(Li, O, Na, Mg, Al, Si, Ca, Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Sr, Y, Zr, Mo, Ba, La, Ce, Nd, Sm, Eu)</td>
</tr>
<tr>
<td>Trevisan et al. (2011)</td>
<td>64</td>
<td>(Fe, Ca, Si, Ti, C, Ni, O, Mg)</td>
</tr>
<tr>
<td>Valenti &amp; Fischer (2005)</td>
<td>1002</td>
<td>(Na, Si, Ti, Fe, Ni)</td>
</tr>
<tr>
<td>Zhang &amp; Zhao (2006)</td>
<td>31</td>
<td>(Fe, O, Mg, Si, Ca, Ti, Na, Al, Sc, V, Cr, Mn, Ni, Ba)</td>
</tr>
</tbody>
</table>
Figure 2.1: Number of stars in the Hypatia Catalog with measured abundances for 46 different element species.
recalculating the abundance determinations from every literature source. First, we denormalize by multiplying the derived relative abundance by the solar abundance used in the given catalog. For example, per Table 2.1, Valenti & Fischer (2005) reported HIP 400 to have [Ti/H] = -0.28 dex. In their paper, they cite Anders & Grevesse (1989) as the source of their solar abundances, where $\log \epsilon(Ti) = 4.99$. Therefore, to denormalize, we write $10^{(-0.28)} \times 4.99 = 2.62$. Second, we renormalize using the Lodders et al. (2009) solar abundances. In our example, $\log \epsilon(Ti) = 4.93$. Therefore, the final renormalized abundance is $[Ti/H] = \log (2.62/4.93) = -0.27$. We did not renormalize those catalogs that used a differential, line-by-line approach to normalize to the Sun. We also experimented with renormalizing to Asplund et al. (2009). For either renormalization, the mean and max spread of each element decreased only slightly. This result shows that the magnitude of the spread is not caused by the choice of solar abundances and is driven by other factors.

We find the stellar parameters $T_{\text{eff}}$ and $\log(g)$ vary substantially between catalogs, Fig. 2.2 middle and bottom respectively, and may be one reason for the different abundance levels reported. For $T_{\text{eff}}$, there is a spread of $\sim 200$ K, while $g$ can differs by a factor of $\sim 2$. The overall abundance determinations are sensitive to the adopted stellar values, especially $\log(g)$. Due to these variations, in addition to the range of other possible causes listed in §2.1, we have not included $T_{\text{eff}}$ and $\log(g)$ for the stars in Hypatia. We note, though, that 43 of the 49 catalogs within Hypatia used the curve-of-growth method to determine their abundances.

Many stars in Hypatia, as exemplified by Fig. 2.2, have multiple measurements of the same element from different catalogs. In these cases, so
Figure 2.2: The representative spread (left) from different catalogs in the re-normalized abundance determinations (see text) for 6 element ratios for 5 stars, with quoted catalog errors such that the quoted uncertainty of individual measurements is less than the spread. The element ratios [X/H] for a given star are denoted by circles and the corresponding [Fe/H] abundances are shown as triangles. In the middle, the effective temperature, $T_{\text{eff}}$, values for the same stars, surface gravity, $\log(g)$, values are on the right where $g$ differs by a factor of $\sim 2$ between literature sources.
as not to favor any catalog, the median value for those measurements is used. If the discrepancy between catalog measurements is too large, the median abundance value was unreliable. However, any star with a spread in \([X/Fe]\) > 1.0 dex was therefore not included. This cutoff value was used because it is much larger than the respective error and spread for any element. Rather than preferentially choose one catalog over another, we opted to eliminate those stars from our analysis. The number of stars that were excluded because of a large spread per element are listed in Table 2.3. The values given in Fig. 2.1 represent the total number of stars in Hypatia minus those stars with large spread. Hence, the following analysis consists of 2792 stars, consistent with the number of stars listed as having \([\text{Fe/H}]\) measurements in Fig. 2.1. For all Hypatia calculations hereafter, we retain all catalog abundance values using the Lodders et al. (2009) abundance renormalization.

Combining 49 data sets that span about 25 years means there will be a spread among reported values for any element in many stars. We have taken a few steps to address the issues to help make results generated with Hypatia meaningful and physical. We (a) attempt to minimize the spread by renormalizing the abundances to a standard solar abundance scale; (b) exclude stars with a large spread; and (c) choose to use the median value of the spread avoid specific catalog bias when representing the abundance of a star. In Chapter 3 we show the overall trends in \([X/Fe]\) vs. \([\text{Fe/H}]\) by binning the data, and therefore reducing the random errors. Quantifying systematic
errors that could result from instrumental, atomic database, or stellar atmosphere models is beyond the scope of this paper, but we encourage the community to undertake such verification and validation studies.

Finally, most of the catalogs that are incorporated into Hypatia published their line lists. While some catalogs measured only one ionization state when reporting an abundance determination, a number of catalogs combined the abundances from multiple ionization states. In Hypatia, an abundance of [$X/Fe$] means that a catalog measured the neutral state, a combination of neutral and ionized state(s), or it was not specified. Whenever a catalog specifically stated it was only measuring the singly ionized state, we write [$X\ II/Fe$].

### 2.2 Analysis of Hypatia

After compiling abundance information for stars in the solar neighborhood, we seek trends in the abundance patterns of each element. We took the median of the element abundances reported per star and plotted each element in the traditional [$X/Fe$] versus [$Fe/H$] plane in Figs. 3.1-3.28. Representative errorbars, compiled from the quoted observational uncertainties given by each literature source, for each element are placed in the upper right corners of each figure. We have also binned each element measurements into three [$Fe/H$] bins: $[-1.0, -0.5]$ dex, $[-0.5, 0.5]$ dex, and $[0.0, 0.5]$ dex. These binned values are represented by the blue triangles in each figure. The errorbars for the blue triangles are determined by $\sigma_{rep}/\sqrt{N}$, where $\sigma_{rep}$ is the quoted observational error in the [$X/Fe$] or [$Fe/H$] direction and $N$ is the number of points per bin. These errorbars are much smaller than the blue triangles.
We also analyze the data for trends in position, radial distance, and height above the Galactic plane. We have included a handful of these plots for a variety of elements to demonstrate that the trends are consistent with a mean, well-mixed ISM. There are also a small number of paired plots with abundances before and after the Lodders et al. (2009) renormalization. Literature sources that have contributed to the Hypatia Catalog are discussed throughout.

In §3.2 and §3.3, we will present the relative abundances for elements that are “bio-essential,” or paramount for terrestrial biogeochemistry. These elements, Fe, C, N, O, Mg, Si, S, P, and Mo, are also relevant for the discussion of an application of the Hypatia Catalog in Chapter 5.
Hydrogen, helium, and the lighter elements were the only elements synthesized in standard Big Bang nucleosynthesis (Wagoner et al., 1967; Fields & Olive, 2006; Coc et al., 2012). With the formation of subsequent generations of stars came the creation of additional elements (e.g., Heger & Woosley, 2010, and references within). The principle energy sources for most stars are hydrogen burning via the pp-chain or the CNO-cycle, or $\alpha$-chain burning. These energy sources underlie the processes through which most of the naturally occurring elements are created (Burbidge et al., 1957; Cameron, 1957; Woosley & Weaver, 1995; Arnett, 1996; Thielemann et al., 2002; José & Iliadis, 2011). We succinctly summarize the astrophysical origin site of every element listed in Hypatia, and the biogeochemical applications of some elements, in the following sections. In addition, we examine a number of the elements with respect to radial distance, z-height above the galactic disk, and directionality with respect to the galactic center and anti-center.

3.1 Abundance Measurement Standard (Fe)

The tenth most abundant element by number in the solar composition is iron, which is $\sim$82% more abundant than silicon (Clayton, 2003). Both SN Ia and core-collapse supernovae (SN II, SN Ib/c) produce iron, on different timescales as well as in different and debated amounts (Chiappini et al., 1997; Thielemann et al., 2007; Prantzos, 2008). The dominant $^{56}$Fe isotope is produced primarily from the radioactive decay chain $^{56}$Ni $\rightarrow$ $^{56}$Co $\rightarrow$ $^{56}$Fe.
The progenitor, $^{56}\text{Ni}$, is produced in hydrostatic silicon burning as well as both explosive oxygen and silicon burning, where the forward and backward rates are nearly equal and abundances can be determined by a minimization of the free energy (Hix & Thielemann, 1996; Meyer et al., 1998; Hix & Thielemann, 1999). In either thermonuclear or core-collapse supernovae this generally occurs in conjunction with alpha-rich freezeout, when all of the $\alpha$ particles do not have the time to fuse into heavy nuclei (Woosley et al., 1973; Arnett, 1996).

Figure 3.1: Median $\text{[Fe/H]}$ ratio for all stars in Hypatia as a function of radial distance from the Sun. Horizontal errorbars along the top corresponding to the error in parallax angle used to calculate the distances. There is a large scatter in $\text{[Fe/H]}$ at any distance for F, G, K, and M-type stars in the solar neighborhood.

Iron is relatively easy to measure within stars, and because the mean trend of iron increases monotonically in time within the ISM, it can act as a
chronological indicator of nucleosynthesis (Wheeler et al., 1989; Pagel, 1997; Vangioni et al., 2011). Therefore, as [Fe/H] increases, so does the general timeline of chemical evolution – where we expect to see contributions from core-collapse supernovae for low values of [Fe/H] and the effects from SN Ia at higher values (Wheeler et al. 1989, Matteucci & Recchi 2001, Gibson et al. 2003, Chiappini 2011). However, stars can migrate or scatter into or out of the solar neighborhood, and different galactic populations can have different star formation histories. In this case, [Fe/H] does not necessarily represent the same timeline, which may introduce some ambiguity in using [Fe/H] as a chronometer (Wielen et al., 1996; Gratton et al., 1996; Sellwood & Binney, 2002; Haywood, 2008; Prantzos, 2011).

Fig. 3.1 shows the median values of [Fe/H] reported for 2792 stars in Hypatia, excluding those with a spread in [Fe/H] > 1.0 dex (see §2.1), with respect to the radial distance from the Sun. The horizontal errorbars along the top are 0.32 pc at 20 pc, 5.1 pc at 80 pc, and 16.3 pc at 140 pc. They show how the fractional uncertainty in parallax angle affects the uncertainty in the distance calculation. Within our solar neighborhood’s radius of 150 pc, there is a relatively large scatter in [Fe/H] at any distance, which may be due to the variability in stellar origin. The scatter in [Fe/H] spans ≈ 3.5 dex, although the vast majority of the stars lie within [-1.0, 0.5] and are mostly centered around the solar value of [Fe/H]. Given that 150 pc is small on galactic scales, near-solar values might be expected, and we restrict the [Fe/H] range in Figs. 3.2-3.28 to [-1.0, 0.5].
CNO nuclei are among the most abundant elements in the solar neighborhood (Anders & Grevesse, 1989; Lodders et al., 2009; Asplund et al., 2009). They are important in stellar interiors as opacity sources (Iglesias & Rogers, 1996), as energy producers through the CNO cycle (Bethe & Critchfield, 1938), and are essential building blocks of terrestrial biochemistry (Pace, 2001). Observations of the CNO abundances are thus valuable for recording what types of stars have been responsible for CNO nucleosynthesis, and for detection of terrestrial exoplanets.

The element carbon is dominated by its $^{12}$C isotope, which is a product of hydrostatic helium burning in stars. Its overall production is governed by the competition between the triple-$\alpha$ rate and destruction by the $^{12}$C($\alpha, \gamma$)$^{16}$O rate (Iben, 1991; Wallerstein et al., 1997; Busso et al., 1999; Langanke et al., 2007; José & Iliadis, 2011; Bennett et al., 2012). The $^{12}$C isotope is underproduced in the non-rotating solar metallicity massive star models by about a factor of three (Woosley & Weaver, 1995; Rauscher et al., 2002; Kobayashi et al., 2006; Ekström et al., 2011). Hence, explanation of the solar system abundance of $^{12}$C is consistent with the proposed origin in dredged-up material from helium shell flashes and incomplete carbon burning in intermediate-mass stars on the giant branches (Iben, 1991; Herwig & Austin, 2004; Carigi et al., 2005; Karakas & Lattanzio, 2007; Cescutti et al., 2009; Romano et al., 2010).

Evolution of [C/Fe] as a function of [Fe/H] for the 1466 stars in Hypatia is shown in Fig. 3.2 (left). A representative error bar derived from the quoted observational uncertainties is shown in the upper right. The green
Figure 3.2: [C/Fe] (left) and [N/Fe] (right) ratio for stars in Hypatia as a function of [Fe/H], with a representative observational errorbar in the upper right. Each abundance value is colored by the radial distance of the host-star and the blue triangles show the average abundance ratio value from all abundance values, not just the median, for three [Fe/H] bins: < 0.2 dex, [0.2, 0.3] dex, and > 0.3 dex (the errorbar for each triangle is smaller than the size of the triangle).

The abundance of [C/Fe] is generally constant with radial distance away from the Sun, and maintains a negative slope as [Fe/H] increases, while there is a rather large scatter in [N/Fe] to [Fe/H], as well as radial distance.
circles indicate stars with distances from the Sun less than 30 pc, yellow circles designate distances between 30 pc and 60 pc, and red circles specify distances larger than 60 pc. When different abundance determinations for the same star exist, we have plotted the median value as discussed in Chapter 2.

The [C/Fe] ratio in halo and disk dwarfs has been observed to be roughly constant for a long time (Sneden, 1974; Tomkin & Lambert, 1984). A solar and relatively flat [C/Fe] ratio is interesting because two competing sources come into play at [Fe/H] ≃ -0.8 dex. Intermediate and low mass stars begin depositing large amounts of carbon but no iron, while SN Ia start injecting significant amounts of iron but no carbon. The blue triangles in Fig. 3.2 (left), which represent binned abundance values, indicate a decrease in [C/Fe] with increasing [Fe/H], suggesting SN Ia have been injecting more iron than the intermediate and low mass stars have been injecting carbon over the range -0.8 < [Fe/H] < 0.4. Fig. 3.2 (left) indicates a scatter of ≈ 0.8 dex in [C/Fe] at any [Fe/H] shown, with a larger scatter at [Fe/H] ≤ -0.4 dex.

Isotopes of nitrogen are produced in stars by the CNO cycle (Arnett, 1996). Primary nitrogen is usually produced as a convective helium burning shell mixes into a hydrogen shell, where C and O nuclei form nitrogen with nearly explosive consequences (Talbot & Arnett, 1974; Meynet & Maeder, 2002a; Ekström et al., 2008; Karakas, 2010). Secondary nitrogen production is dependent on the present abundance of carbon and oxygen. Regardless of being primary or secondary, 14N is the main end product of the CNO reactions and dominates the elemental nitrogen abundance.

Fig. 3.2 (right), shows [N/Fe] with respect to [Fe/H]. There are ~5.5 times fewer stars for which [N/Fe] has been measured as compared to the [C/Fe] ratio in the Hypatia Catalog, making it a priority measurement for
future observations. Despite the fewer [N/Fe] abundance determinations, the
trend is for a near-solar values for [N/Fe]. This suggests $^{14}$N was produced as
a primary element, since [N/Fe] is relatively constant with [Fe/H] (Laird,
1985; Carbon et al., 1987). The scatter in [N/Fe] is $\approx 0.8$ dex, with larger
scatter present near the solar value of [Fe/H]. This trend also implies that
SN Ia have been injecting comparable amounts of iron as intermediate and
low mass stars have been injecting nitrogen over the range $-0.4 < [\text{Fe/H}] < 0.4$.

Laird (1985) determined carbon and nitrogen abundances in dwarf
stars using intermediate resolution ($\Delta \lambda = 1$ Å) image tube spectra of the
3300-5250 Å band features of molecular CH and NH. All of these stars are in
the Hypatia Catalog. Effective temperatures were found from calibrated
R-I, b-y and V-K color indices. Surface gravities were derived from the
spectra and Strömgren photometry, supplemented with gravities based on
parallax data and estimated masses. A differential analysis was adopted, and
equivalent widths of the Fe I lines were used to determine the iron
abundances. Since no individual CH or NH lines could be detected in the
spectra, local thermodynamic equilibrium (LTE) synthetic spectra
determined the final abundances. An analysis of the [C/Fe] ratio as a
function of the effective temperature indicated a systematic offset, so a
correction factor of 0.10 dex was applied to all the [C/Fe] ratios and 0.20 dex
for [N/Fe]. This correction factor was not used in the Hypatia Catalog.

Oxygen is a product of hydrostatic He, C, and Ne burning, with $^{16}$O
being the dominant isotope (Clayton, 1968; Arnett, 1996; Thielemann et al.,
2002; Ekström et al., 2011). Three different oxygen features in the visible
spectrum are used to determine oxygen abundances: the O I triplet at 7700Å
Figure 3.3: Same as Fig. 3.2 but for [O/Fe] as a function of [Fe/H]. There appears to be no trend between [O/Fe] and radial distance, but a strong, $\alpha$-element characteristic, negative slope with increasing [Fe/H].

, the [O I] doublet, or the OH lines. Oxygen abundances determined from the excitation feature (9.15 eV) O I triplet at 7700Å are known to be sensitive to the temperature structure of the model atmosphere, as well as being affected by non-LTE corrections and convective inhomogeneities. Nevertheless, all 1672 stars in Hypatia for which [O/Fe] was determined use the O I triplet. Most catalogs applied various empirical corrections by undertaking non-LTE calculations or providing an agreement with [O I] doublet determined abundances (e.g., Edvardsson et al., 1993; Brugamyer et al., 2011).

Fig. 3.3 shows [O/Fe] versus [Fe/H] for the stars in Hypatia. The binned trend, shown by the blue triangles, is classic $\alpha$-element, starting from core-collapse supernovae depositing large amounts of oxygen but no iron and
later on SN Ia injecting significant amounts of iron but no oxygen (Gratton & Ortolani, 1986; Brewer & Carney, 2006; Marcolini et al., 2009; Kobayashi & Nakasato, 2011). While the scatter in [C/Fe] is larger at the high and low ends of [Fe/H], [O/Fe] maintains a scatter of $\approx 0.7$ dex throughout the range of [Fe/H]. The majority of stars with [Fe/H] $> 0.0$ dex also have a radial distance greater than 60pc from the Sun.

3.3 Additional Bio-Essential Elements (Mg, Si, S)

Magnesium is an $\alpha$-element whose dominant isotope $^{24}$Mg is formed during hydrostatic carbon burning when a $^{12}$C+$^{12}$C reaction creates the seed for $^{23}$Na($p, \gamma$)$^{24}$Mg, and during hydrostatic neon burning via $^{20}$Ne($\alpha, \gamma$)$^{24}$Mg (Limongi & Chieffi, 2003; Karakas et al., 2006). The less abundant $^{25,26}$Mg isotopes are formed from the release of neutrons from $^{22}$Ne when temperatures are high enough (Gay & Lambert, 2000). Fenner et al. (2003) noted that mean galactic chemical evolution models generally underestimate the $^{25,26}$Mg/$^{24}$Mg ratios, signaling a potential additional production site. Their inclusion of $^{25,26}$Mg yields from intermediate-mass asymptotic giant branch (AGB) stars, along with the contributions from core-collapse supernovae, more closely matched observations.

Fig. 3.4 shows [Mg/Fe] as a function of [Fe/H] prior to renormalizing (left) and afterward to Lodders et al. (2009) (right). While there are some small changes, the overall effect of renormalization is not significant, which is consistent with the other elements within the Hypatia Catalog. This suggests that other factors, such as the adopted temperature scale to which the derived abundances are very sensitive, as noted by Gonzalez (2006), are cause for the spread in the data (see section Chapter 2). Similar to the other
α-elements, there is a general decrease in the [Mg/Fe] abundance in Fig. 3.4 (right) as [Fe/H] increases, due to the late injection of iron from SN Ia, and a flattening of [Si/Fe] at super-solar metallicities (Matteucci & Greggio, 1986; Gibson et al., 2003; Romano et al., 2010; Kobayashi & Nakasato, 2011). However, the slope of [Mg/Fe] with [Fe/H] is shallower than the other α-elements, as indicated by the different y-axis scales. The average scatter is \( \sim 0.4 \text{ dex} \) in [Mg/Fe], becoming slightly larger for [Fe/H] > -0.2 dex, supporting the multiple productions sites predictions of (Fenner et al., 2003).

Silicon is the second most abundant element in the earth’s crust (Walker et al., 2008) and the third most trace element within the human body (Sripanyakorn et al., 2005). Despite it being a controversial “essential” element, an increasing number of studies have found silicon to be important to both plant and human biology (Walker et al., 2008). For example, silicon is vital to connective tissue, for example bones, skin, tendons, the aorta, and the trachea, (Sripanyakorn et al., 2005, and references therein). Silicon is also critical for the presence of plants on the Earth given the dependency of plant nutrients on the silicon-rich soil (Epstein, 1994). In addition, silicates play an important role in the formation of land masses and the subsequent transference of the other bioessential elements onto the planet’s surface (Leger et al., 2004). Therefore, we have deemed it a bio-essential element.

The dominant \(^{28}\text{Si}\) isotope is produced by hydrostatic and explosive oxygen burning in massive stars (Arnett, 1996). The final yield of \(^{28}\text{Si}\) in supernova ejecta is sensitive to a variety of factors, including convection in the progenitor stars (Meakin & Arnett, 2007; Arnett et al., 2009; Arnett & Meakin, 2011). The secondary and less abundant \(^{29,30}\text{Si}\) isotopes may have risen to their solar values from intermediate-mass AGB star contributions.
Figure 3.4: Similar to Fig. 3.2 but for magnesium, showing the data as measured by the literature sources (left), and renormalized to (Lodders et al., 2009). The evolution trend in either case is similar to the other α-elements but with a shallower slope.
(Clayton & Timmes, 1997; Zinner et al., 2006). Fig. 3.5 (left) shows silicon is a classic α-chain element, but with a distinct flattening of [Si/Fe] for [Fe/H] ≥ 0.0, which is not typically associated with the α-chain elements. The [Si/Fe] ratio has the most entries in the Hypatia Catalog, being measured for 2189 stars. There is a scatter ≈ 0.3 dex about the mean trend (blue triangles) at any given [Fe/H].

The three most abundant sulfur isotopes are $^{32}S$, $^{34}S$, and $^{33}S$, respectively, with ratios of 22.5:1:0.18 in the solar system (Anders & Grevesse, 1989; Chin et al., 1996; Lodders et al., 2009). Sulfur is produced within massive stars, via hydrostatic and explosive oxygen and burning (Clayton, 1968; Heger et al., 2000; Rauscher et al., 2002; Limongi & Chieffi, 2003). On average, a typical core-collapse supernovae ejects about 10 times more $^{32}S$ than a SN Ia, and occurs about five times more frequently than SN Ia (van den Bergh & Tammann, 1991; Tammann et al., 1994; Cappellaro et al., 1999; Botticella et al., 2008; Maoz et al., 2011).

There are relatively fewer stars, 482 in Hypatia, for which sulfur has been measured, as shown in Fig. 3.5 (right). This is due to absorption lines being too weak in the visible spectrum or blended to separate from the continuum, making it difficult to determine an accurate abundance (Francois, 1987). Takeda et al. (2005) reports significant, ≈ 0.2 dex, non-LTE corrections affecting several lines used in the determination of S and Zn abundances in F, G, and K stars. Like other α-elements, there is decrease in [S/Fe] as [Fe/H] increases from ≈ -1.0 dex to ≈ 0.4 dex. The scatter in [S/Fe] is ≈ 0.4 dex over the entire [Fe/H] range shown, but several outliers have a larger scatter.
Figure 3.5: Same as Fig. 3.2 but for silicon (left) and sulfur (right). [Si/Fe] is one of the most common measurements in Hypatia (2189 stars), with less entries for [S/Fe] (482 stars).
Luck & Heiter (2005) reported the abundances for Mg, Si, and S, as well as for 25 other elements, in 114 F, G, K, M stars within 15 pc of the Sun. Table 2.2 shows 110 of these stars are in the Hypatia Catalog. Their high signal-to-noise spectra (in excess of $\approx 150$ per spectral pixel) were taken between 1997 and 2003 using the Sandiford Cassegrain Eschelle Spectrograph attached to the 2.1 m telescope at McDonald Observatory. They determined the solar flux spectrum by using differential analysis, with Callisto as the reflector. The model atmospheres were determined by MARCS75 (Gustafsson et al., 1975). Photometry was acquired through the General Catalogue of Photometric Data (Hauck & Berthet, 1991). Surface gravities log $g$ values and Fe abundances were obtained by iterating until the [Fe/H] value from both Fe I and Fe II were equal. Overall abundance uncertainties for [X/Fe] were determined on a per element basis.

### 3.4 Challenging Bio-Essential Elements (P & Mo)

The abundance of phosphorus is the most challenging to determine of the bio-essential elements; there are just 20 stars in Hypatia with measured phosphorous abundances. Struve (1930) pointed out that while phosphorous is one of most abundant element on the Earth, there are no P I lines in the optical spectrum of main-sequence stars. There are a few P I lines in the infrared and P I, II, and IV lines in the ultra-violet range which are observed in spectra of hot B stars (Caffau et al., 2007; Hubrig et al., 2009). The dominant phosphorus isotope is $^{31}$P and is likely created by neutron-capture onto neutron-rich $^{29}$Si or $^{30}$Si seed nuclei. It is perhaps also produced to a lesser extant by $^{31}$S $\rightarrow$ $^{31}$P $+ e^+ + \nu_e$ and $^{28}$Si($\gamma, p$)$^{31}$P during carbon and neon shelling burning in massive stars (Caffau et al., 2011).
Caffau et al. (2011) reported phosphorus abundances in 20 G and F dwarfs by observing infrared lines with CRIRES detectors at the Very Large Telescope. They centered their observations on 10595 Å to detect four of the strongest P I lines, with the 10681 Å and 10813 Å lines being out of the range of the detectors. Their atmospheric models were computed with ATLAS12, and the abundances were determined from the measured equivalent width using WIDTH (Kurucz, 2005). Sensitivity studies to $T_{\text{eff}}$ ($\pm 100K$) and $\log g$ ($\pm 0.2$) suggested the abundance changes were smaller than the cited uncertainty of 0.1 dex.

Evolution of [P/Fe] with [Fe/H] is shown in Fig. 3.6. As discussed by Caffau et al. (2011), it might be expected that [P/Fe] should increase with [Fe/H] since there are more neutron-rich seed nuclei available. Instead, the observed trend is similar to an $\alpha$-element with [P/Fe] decreasing with increasing [Fe/H] (Kobayashi et al., 2006; Cescutti et al., 2011). However, caution is advised as the number of stars is small.

Molybdenum is an key constituent of certain enzymes that catalyze redox reactions: the reduction of molecular nitrogen and nitrate in plants and oxidation of purines and aldehydes in animals (e.g., Raymond et al., 2004; Anke & Seifert, 2007). Owing to these diverse functions, molybdenum is bio-essential element for terrestrial biogeochemistry. However, a scarcity of molybdenum in the Earth’s early oceans may have been a limiting factor in the evolution eukaryotes for nearly two billion years (Scott et al., 2008).

Molybdenum is formed by a number of processes. It is created by proton capture on heavier seed nuclei formed via the r-process (Woosley et al., 1994; Fryer et al., 2006; Wanajo, 2007), for which $^{100}$Mo is the dominant isotope (Woosley & Hoffman, 1992; Wanajo & Ishimaru, 2006).
Figure 3.6: Similar to Fig. 3.2 but for phosphorus (left) and molybdenum (right). There are few measurements for [\text{P/Fe}] or [\text{Mo/Fe}], due to the difficulty in measuring UV or IR spectral lines from ground-based telescopes.
Neutrino-irradiated outflows in core-collapse supernovae can also form molybdenum, for which $^{92}$Mo and $^{94}$Mo are the dominant isotopes. Finally, the s-process primarily produced $^{96}$Mo and $^{98}$Mo (Hoffman et al., 1996; Meyer et al., 2000; Fröhlich et al., 2006; Fisker et al., 2009). Fig. 3.6 shows the [Mo/Fe] ratio has no consistent trend with [Fe/H]. [Mo/Fe] is relatively larger at low metallicity, although there is a scatter of ≈ 1.0 dex. For [Fe/H] ≥ −0.2 dex, the blue triangles suggest [Mo/Fe] may decrease with [Fe/H], but again the scatter is large in [Mo/Fe] and the trend difficult to discern. Table 2.2 shows only Feltzing & Gustafsson (1998); Galeev et al. (2004) and Thevenin (1998) have measured molybdenum, which is likely due to the small number of lines in the optical spectrum, $\text{M I at 5570.39 Å}$ (Feltzing & Gustafsson, 1998).

3.5 Additional $\alpha$-Elements (Ca & Ti)

Calcium is the 13th most abundant element in the solar composition (Lodders et al., 2009) and the 5th most abundant element in the Earth’s crust (McDonough, 2001) and most terrestrial biochemical systems (Nordin, 1976; White & Broadley, 2003). Calcium has four major functions in terrestrial biochemistry: structural in skeletons or exoskeletons, electrophysiological in carrying charge across membranes, intracellular regulator, and as a cofactor for extracellular enzymes and regulatory proteins (Martin, 1983).

Calcium is an $\alpha$-element whose dominant, double magic isotope $^{40}$Ca is produced by oxygen burning in massive stars (Woosley & Weaver, 1995). The isotope $^{42}$Ca is also produced in oxygen burning, while $^{43,46}$Ca are made in neon and carbon shells (Rauscher et al., 2002; Limongi & Chieffi, 2003).
In contrast, $^{44}\text{Ca}$ is mostly made as radioactive $^{44}\text{Ti}$, and usually accompanied by large amounts of $^{56}\text{Ni}$ (Woosley & Weaver, 1995). The decay of $^{44}\text{Ti}$ and $^{56}\text{Ni}$ has significant observational consequences for the light curves of core-collapse supernovae (Arnett et al., 1989; Timmes et al., 1996; The et al., 1998; Renaud et al., 2006; Young et al., 2006; Hoffman et al., 2010), isotopic patterns measured in primitive meteorites (Wadhwa et al., 2007) and presolar grains (Zinner, 1998), and anomalies in the deep-sea crust (Knie et al., 2004). The origin of $^{48}\text{Ca}$, also double magic and unusually neutron-rich for such a light nucleus, usually requires special conditions and has long been mystery (e.g., Meyer et al., 1996).

Fig. 3.7 (left) shows how $\frac{[\text{Ca}]}{[\text{Fe}]}$ exhibits the same trend with $[\text{Fe}/\text{H}]$ as other $\alpha$-elements. However, the shallow slope over the $[\text{Fe}/\text{H}]$ range suggests that calcium production by massive stars is more closely balanced by iron production from SN Ia. There is $\approx 0.4$ dex scatter in $[\text{Ca}/\text{Fe}]$ for all values of $[\text{Fe}/\text{H}]$, but there are some distinct outliers. While the blue triangles seem to indicate that $[\text{Ca II}/\text{Fe}]$ decreases with increasing $[\text{Fe}/\text{H}]$, seen in Fig. 3.7 (right), there are few stars for which this species has been measured. Scatter in $[\text{Ca II}/\text{Fe}]$ is $\approx 0.4$ dex for the range of $[\text{Fe}/\text{H}]$.

While most of the catalogs within Hypatia determined their calcium abundances through $\text{Ca I}$, two catalogs (Allende Prieto et al., 2004; Gebran et al., 2010) used $\text{Ca II}$ lines, shown in Fig. 3.7 (right). Allende Prieto et al. (2004) compared the derived abundances from the neutral and ionized lines, and reported the abundance for $\text{Ca I}$ and $\text{II}$ differed by 0.25 dex due to the broadening of the wings in the line profiles. These dissimilarities could be mollified by a change in the surface gravity and $T_{\text{eff}}$, at the expense of weakening the $\text{Ca I}$ line. Therefore, their final abundances were derived from
Figure 3.7: Same as Fig. 3.2 but for neutral (left) and ionized (right) calcium. The measurements for [Ca/Fe] show tighter correlations with [Fe/H] than other $\alpha$-elements. Unlike neutral calcium, there doesn’t appear to be any correlation between [Ca II/Fe] and [Fe/H].
the Ca II 8662 Å line, since this was less blended than the Ca II 8498 Å line, and are shown for 98 stars in Fig. 3.7 (right). While there is significant scatter in [Ca II/Fe] with respect to [Fe/H], we note the scale change between the left and right figures. The abundances for [Ca II/Fe] vary between [-0.1, 0.3] dex for the range of [Fe/H] considered and follows the trend of [Ca/Fe].

Titanium is produced in massive stars by explosive burning processes in core-collapse supernovae (Woosley et al., 1973; Arnett, 1996; Limongi & Chieffi, 2003). There are five stable isotopes: $^{48}\text{Ti}$, $^{46}\text{Ti}$, $^{47}\text{Ti}$, $^{49}\text{Ti}$, and $^{50}\text{Ti}$, that have relative terrestrial abundances, in descending order, of 73.4: 7.9: 7.7: 5.5: 5.3 (Seaborg & Perlman, 1948; McDonough, 2001). The dominant $^{48}\text{Ti}$ isotope is made as $^{48}\text{Cr}$ during explosive silicon burning (Clegg et al., 1979; Wallerstein et al., 1997; José & Iliadis, 2011).

Like calcium, titanium abundances have been determined with two ionization states as shown in Fig. 3.8. Since there are a large number of spectral lines for Ti I and Ti II in the optical spectrum, titanium is one the more commonly measured elements in Hypatia (see Fig. 2.1). While a number of catalogs measured abundances using both the Ti I and Ti II lines (Bond et al., 2008; Gratton et al., 2003; Neves et al., 2009; Takeda et al., 2007), Bergemann (2011) found that abundances can vary by 0.1 dex or larger when comparing pure Ti I and Ti II line determinations. Most catalogs, though, used the Ti I lines alone.

The [Ti/Fe] binned trend with [Fe/H], shown by the blue triangles in Fig. 3.8 (left), suggests an evolution similar to the other $\alpha$-elements. While the rise in [Ti/Fe] with decreasing [Fe/H] has been long observed (Wallerstein, 1962), massive star models have difficulty producing this trend (Kobayashi et al., 2006; Romano et al., 2010). There is a $\approx$ 0.6 dex scatter in
Figure 3.8: Same as Fig. 3.2 but for neutral (left) and ionized (right) titanium. The abundances of $\text{[Ti/Fe]}$ to $\text{[Fe/H]}$ are correlated, with similar scatter for all $\text{[Fe/H]}$ values. Significant outliers with larger $\text{[Ti/Fe]}$ at smaller $\text{[Fe/H]}$ are located at distances less than $\sim 30$ pc; $\text{[Ti II/Fe]}$ shows several of the same features.
[Ti/Fe] over the entire range of [Fe/H]. For [Fe/H] < -0.4 dex, stars at larger distances tend to show solar [Ti/Fe], while stars at smaller distances tend to exhibit larger [Ti/Fe]. The binned trend for [Ti II/Fe] is similar to [Ti/Fe], Fig. 3.8 (right). However, blue triangles indicate that the slope of [TiII/Fe] becomes more shallow as [Fe/H] increases, which may be a result of smaller-number statistics. There are significantly fewer stars with [Ti II/Fe] determinations at distances greater than 60 pc.

Fig. 3.9 (left) shows [Ti/Fe] as a function of distance, with errorbars similar to Fig. 3.1. On the left, the stars are colored according to their height above the Galactic plane, \( z \). Stars with heights greater than 15 pc are shown in purple, less than -15 pc in blue, and between ± 15 pc in orange. [Ti/Fe] shows little dependence on height above the plane, and the majority of stars in Hypatia that have [Ti/Fe] abundance measurements are located within 60 pc of the Sun. Stars with a radial distance greater than 100 pc are show more scatter, \( \approx 0.6 \) dex. Fig. 3.9 (right) shows those same stars, but colored according to their position toward the galactic center (green), toward the anti-center (purple), and in-between (blue). Stars that are towards the galactic anti-center have predominantly near solar abundances, with \( \approx 0.2 \) dex scatter.

Fig. 3.10 shows [Na/Ca] (left) and [Si/Ca] (right) as a function of [Fe/H]. The [Na/Ca] evolution, an odd-Z element to an \( \alpha \)-element ratio, shows a change in slope of [Na/Ca] at [Fe/H] \( \approx 0.0 \) dex (Marcolini et al., 2009). Production of sodium and calcium were roughly equivalent at smaller [Fe/H], but sodium dominates calcium as [Fe/H] increases. This trend may be due to SN Ia or intermediate- to low-mass stars injecting additional sodium relative to calcium at later times, although the \( \approx 0.7 \) dex scatter in
Figure 3.9: $[\text{Ti}/\text{Fe}]$ with respect to distance, where the abundance trend are shown with respect to height above the Galactic plane (left) and direction to the Galactic center and anti-center (right). Errorbars are similar to Fig. 3.1.
[Na/Ca] for [Fe/H] > 0 is rather large. In contrast, the flat and solar trend in
[Si/Ca] with [Fe/H], with ≈ 0.4 dex scatter, shows silicon and calcium are
α-elements dominated by contributions from massive stars.
Figure 3.10: Similar to Fig. 3.2 but for [Na/Ca] (left) and [Si/Ca] (right). At larger values of [Fe/H], [Na/Ca] increases as sodium injections dominates calcium creating a concave-up trend. [Si/Ca] is relatively constant with [Fe/H], consistent with both Si and Ca behaving as $\alpha$-elements.
3.6 Odd-Z Elements (Li, Na, Al, K, Sc)

Lithium occurs naturally as two stable isotopes, $^6$Li and $^7$Li, the latter being much more abundant (92.5%) in the solar composition (Anders & Grevesse, 1989; Lodders et al., 2009). Lithium is found in trace amounts in many organisms, with levels being lower in vertebrates (Kabata-Pendias & Pendias, 2001; Eisler, 2009). The precise role of lithium in natural biological systems is unknown. The isotope $^7$Li is formed during Big Bang nucleosynthesis from $^4$He($^3$H,γ)$^7$Li and $^3$He($^4$He, γ)$^7$Be(e+,$\nu_e$)$^7$Li (Fields & Olive, 2006; Fields, 2011; Kusakabe et al., 2008; Coc et al., 2012). The latter reaction can also be a net producer of $^7$Li in AGB stars (Spite & Spite, 1982; Ventura et al., 2000; Herwig, 2005; Meléndez et al., 2010), as well as the $\nu$-process in core-collapse supernovae (Woosley et al., 1990; Yoshida et al., 2006). The less abundant $^6$Li isotope is primarily formed by spallation reactions on CNO nuclei in the ISM (Reeves et al., 1970; Reeves et al., 1990; Ramaty et al., 1997; Kawanomoto et al., 2009).

The abundance ratio [Li/Fe] versus the [Fe/H] ratio is shown in Fig. 3.11 (left) for the 154 stars in the Hypatia Catalog, which derive from four literature sources: Galeev et al. (2004); Gonzalez et al. (2001); Thevenin (1998). While the majority of the [Li/Fe] measurements are above solar, there is also a scatter of $\approx 5.0$ dex over the entire range of [Fe/H], reflecting the strong sensitivity of lithium to its main production and destruction channels (e.g., Matteucci et al., 1995). The average [Li/Fe] in three [Fe/H] bins, represented by the blue triangles, suggests a decreasing [Li/Fe] with increasing [Fe/H], however, the large scatter in [Li/Fe] indicates caution is necessary in interpreting this trend.
Figure 3.11: $[\text{Li/Fe}]$ ratio (left) and $[\text{Al/Fe}]$ (right) as a function of $[\text{Fe/H}]$, with the same format as Fig. 3.2. There is an $\approx 5.0$ dex scatter for $[\text{Li/Fe}]$ - see text for discussion. $[\text{Al/Fe}]$ is clustered around solar with a scatter on the order of $\approx 0.5$ dex.
Aluminum, whose only stable isotope is $^{27}$Al, is mainly synthesized in hydrostatic carbon and neon burning (Arnett & Thielemann, 1985; Thielemann & Arnett, 1985; Woosley & Weaver, 1995; Limongi & Chieffi, 2006) and is the third most abundant element in the Earth’s crust (Rudnick & Gao, 2003). Despite its abundance, aluminum has no essential role in any terrestrial biological system, making it a very poor metal co-factor Exley et al. (e.g., 2007).

Evolution of [Al/Fe] with [Fe/H] is shown in Fig. 3.11 (right) for the 1350 stars in the Hypatia Catalog. The three blue triangles suggest [Al/Fe] values near solar with a shallow concave-up trend, consistent with the trends seen in data studies over a larger metallicity range (Peterson, 1981; Magain, 1989; Fulbright, 2000; Brewer & Carney, 2006). Curiously, there is a relative paucity of [Al/Fe] measurements for stars with [Fe/H] $\leq$ -0.5 dex and within 30 pc of the Sun. Most of the individual abundances determinations are within $\pm$ 0.2 dex of solar. Fig. 3.12 shows [Al/Fe] with respect to radial distance, colored to show height above the Galactic plane (left) and directionality towards or away from the galactic center (right). Stars within 60 pc span a larger range of [Al/Fe], -0.25 $\leq$ [Al/Fe] $\leq$ 0.4, than stars at larger distances. Additionally, stars in Hypatia whose height below the galactic plane is larger than -15 kpc and stars that are towards the galactic anti-center (purple circles in both plots) tend to have a smaller scatter in [Al/Fe] values than stars with height above the galactic plane larger than 15 kpc (blue circles).

Sodium and potassium play a key role in terrestrial biochemistry. Usually the concentration of potassium ions inside many cells is greater than that of sodium. This concentration difference is maintained by the “sodium
Figure 3.12: $[\text{Al}/\text{Fe}]$ ratio as a function of radial distance, similar to Fig. 3.9. There is more scatter for stars with a radial distance less than $\sim 30$ pc and stars with $z > 15$ pc tend to be nearer to the solar value of $[\text{Al}/\text{Fe}]$. Similarly, stars towards the anti-center are also closer to the solar value of $[\text{Al}/\text{Fe}]$. 
pump”, a process whose energy is supplied by the hydrolysis of adenosine triphosphate (Skou, 1997; Roberts et al., 2003).

The only stable isotope of sodium, $^{23}\text{Na}$, is produced mainly in carbon-burning in massive stars, whose final abundance is sensitive to the overall neutron enrichment (Woosley & Weaver, 1995; Chieffi & Limongi, 2004). Some $^{23}\text{Na}$ is produced in the hydrogen envelope as a result of the neon-sodium cycle (Denisenkov & Ivanov, 1987; Langer et al., 1993; Andrievsky, 2002; José & Iliadis, 2011), while additional $^{23}\text{Na}$ is also produced by neutron capture onto $^{22}\text{Ne}$ during helium burning (Mowlavi, 1999; Jonsell et al., 2005; Bond et al., 2008; Charbonnel & Lagarde, 2010). The abundance ratio [Na/Fe] as a function of the [Fe/H] ratio is shown in Fig. 3.13 (left) for the 1983 stars in the Hypatia Catalog. The three blue triangles, which give the average [Na/Fe] in the three [Fe/H] bins, shows a concave-up evolution (Edvardsson et al., 1993; Bensby et al., 2003, 2005), with the minimum occurring near solar [Fe/H]. This suggests that stars of all masses are injecting more sodium than core-collapse and thermonuclear supernova are depositing iron for [Fe/H] > 0. The magnitude of the scatter about the mean [Na/Fe] values is consistent with the scatter seen in other elements, and there are no distinct trends with distance. Fig. 3.13 (right) shows the effects of our attempts to put all the abundance determinations on a common solar abundance scale. While there are some changes, the change in the overall spread is not significant.

Three isotopes of potassium occur naturally: stable $^{39,41}\text{K}$ and the long-lived radioisotope $^{40}\text{K}$ which has a half-life of $1.248 \times 10^9$ yr (Tuli, 2005). The isotope $^{39}\text{K}$ accounts for about 93% of the solar abundance of potassium, with most of the remainder in $^{41}\text{K}$ (Clayton, 2003). The isotopes
Figure 3.13: [Na/Fe] ratio as a function of [Fe/H], similar to Fig. 3.2. Sodium is one of the more frequently measured elements in the Hypatia catalog with 1983 entries. The figure on the left shows [Na/Fe] as determined by the literature sources; the data on right has been re-normalized to Lodders et al. (2009).
$^{39,41}\text{K}$ are produced during oxygen burning, with $^{41}\text{K}$ made as $^{41}\text{Ca}$, but some $^{41}\text{K}$ is produced as itself during neon burning.

The abundance ratio $[\text{K/Fe}]$ versus the $[\text{Fe/H}]$ ratio is shown in Fig. 3.14 for the 218 stars in the Hypatia Catalog. Blending between the K I and atmospheric O$_2$ lines means potassium abundances are more difficult to determine (Gratton & Sneden, 1987), accounting for the relatively fewer number of stars with K abundance determinations. In addition, the low excitation energies of K I might be susceptible to non-LTE or strong hyperfine structure effects (Ivanova & Shimanskiĭ, 2000). Both individual stars and the average $[\text{K/Fe}]$ values, shown by the blue triangles, suggest $[\text{K/Fe}]$ decreases as $[\text{Fe/H}]$ increases between $[\text{Fe/H}] = [-1.0, 0.2]$ with at least a $\approx 0.5$ dex scatter at any $[\text{Fe/H}]$. In addition, stars more distance than 60 pc (red circles) are nearly three times as enriched in $[\text{K/Fe}]$ than stars closer to the Sun.

A number of abundance determinations from Reddy et al. (2003) are used in Fig. 3.13 (right) and Fig. 3.14. They investigated 27 elements, including sodium and potassium, in 181 F and G dwarfs from a differential LTE analysis of high-resolution ($\Delta \lambda/\lambda \approx 60,000$) and high signal-to-noise (S/N=300-400) spectra from the Smith 2.7 m telescope at McDonald Observatory. Of these 181 stars, 179 are in Hypatia. Effective temperatures were adopted from an infrared flux calibration of St"romgren photometry. Surface gravities and stellar ages were determined from stellar evolution tracks and Hipparcos Catalogue parallaxes. The 6154.23 Å and 6160.75 Å lines of Na I and the 7698.98 Å line of K I were used in the analysis, with oscillator strengths taken from Lambert & Warner (1968).
Figure 3.14: $[\text{K/Fe}]$ ratio as a function of $[\text{Fe/H}]$, similar to Fig. 3.2. Potassium is one of the less frequently measured elements in the Hypatia Catalog with 218 stars. Despite the scatter, there is a trend of decreasing $[\text{K/Fe}]$ abundance with increasing $[\text{Fe/H}]$.

Naturally occurring scandium is composed of one stable isotope $^{45}\text{Sc}$ and one radioactive $^{46}\text{Sc}$ isotope, which has the longest half-life, 83.8 days, of the unstable scandium isotopes (Tuli, 2005). Scandium was predicted to exist by Mendeleev (1869) eight years before two grams of scandium oxide were isolated (Nilson, 1879) and 46 years before the pure metal was produced (Fischer et al., 1937). The isotope $^{45}\text{Sc}$ is made as itself and as radioactive $^{45}T$ (Tuli, 2005) in hydrostatic and explosive oxygen-burning and in alpha-rich freezeouts in core-collapse events (Rauscher et al., 2002; Limongi & Chieffi, 2003; Ekström et al., 2011)
The abundance $[\text{Sc/Fe}]$ versus $[\text{Fe/H}]$ is shown in Fig. 3.15 for the 847 stars in the Hypatia Catalog with Sc I based abundance determinations (left) and the 1045 stars with Sc II based abundance determinations (right). $[\text{Sc/Fe}]$ ratios determined from Sc I lines are near solar or larger, where few stars have abundances much less than solar. The three blue triangles show a shallow trend of decreasing $[\text{ScI/Fe}]$ with increasing $[\text{Fe/H}]$. In contrast, $[\text{Sc II/Fe}]$ ratios follow a more concave-up trend with $[\text{Fe/H}]$ (Thevenin, 1998; Zhang & Zhao, 2006). The $\approx 0.4$ dex scatter in $[\text{Sc II/Fe}]$ is much smaller than the $\approx 0.7$ dex scatter in $[\text{Sc I/Fe}]$.

Feltzing & Gustafsson (1998) explored scandium abundances in 47 G and K dwarf stars with $-0.1 \text{dex} < [\text{Fe/H}] < 0.42 \text{dex}$ using a differential LTE analysis with respect to the Sun of high-resolution ($\Delta \lambda/\lambda \approx 100,000$) and high signal-to-noise ($S/N \approx 200$) spectra. Of these 47 stars, 45 are in Hypatia (see Table 2.2). The 5484.64 Å line is used for Sc I and the 5239.82 Å 5318.36 Å 6300.69 Å 6320.84 Å lines are used for Sc II. Noting that single line abundance determinations should be viewed with caution, Feltzing & Gustafsson (1998) base their scandium abundance determinations on Sc II and discuss the apparent overionization and other non-LTE effects that may effect most of the abundance determination, including scandium. Zhang et al. (2008) performed a non-LTE study of scandium in the Sun and find strong non-LTE abundance effects in Sc I due to missing strong lines. Thus, scandium abundances determined from single line LTE determinations are generally unsafe and abundances based on multiple Sc II lines in non-LTE are preferred.
Figure 3.15: $\text{[Sc/Fe]}$ ratio as a function of $\text{[Fe/H]}$, and the figure has the same format as Fig. 3.2. Scandium abundances based on Sc I are on the left and abundances determined from Sc II are shown on the right.
3.7 Iron-Peak Elements (V, Cr, Mn, Co, Ni)

The elements V, Cr, Mn, Co, and Ni are formed by the same nuclear processes that create iron in core-collapse and thermonuclear supernova, in varying degrees (Thielemann et al., 2002; Limongi & Chieffi, 2003; Thielemann et al., 2007). Vanadium is dominated by the isotope $^{51}$V, which is produced as $^{51}$Cr and $^{51}$Mn during explosive oxygen burning, explosive silicon burning, and $\alpha$-rich freezeouts in core-collapse supernovae (Clayton, 2003). The less dominant $^{50}$V is produced as itself during explosive oxygen burning and explosive neon burning. Chromium, essentially $^{52}$Cr, is formed as a result of radioactive decay from $^{52}$Fe during quasiequilibrium explosive silicon burning (Arnett, 1996; Dauphas et al., 2010). Manganese – dominated by $^{55}$Mn from the radioactive decay of $^{55}$Co, cobalt – dominated by $^{59}$Co from the radioactive decay of $^{59}$Cu, and nickel – dominated by $^{58}$Ni made as itself, are all generally the result of quasiequilibrium reactions during explosive silicon burning (Woosley & Weaver, 1995). Because of these elements’ proximity to iron (see §3.1), most of the abundance evolutions track iron.

Vanadium is the least abundant of the iron group elements. Chemical evolution models of vanadium generally underproduce the solar abundance by about a factor of two (Timmes et al., 1995; Romano et al., 2010), although vanadium has also historically presented challenges to massive star models. The solar abundance of the dominant isotope, $^{51}$V, may have additional contributions from incomplete helium detonations on white dwarfs, either as SN Ia models (Bildsten et al., 2007) or subluminous models for SN Ia (Woosley et al., 1986; Nomoto et al., 2003; Rosswog et al., 2009; Raskin et al., 2010).
Figure 3.16: Same as Fig. 3.2 but for neutral (left) and ionized (right) vanadium. The abundances of [V/Fe] are flat and solar with respect to [Fe/H], although the scatter is large and biased towards super-solar values of [V/Fe]. Abundances determined from [V II/Fe] are consistent with a flat and solar evolution, and show a smaller scatter.
Vanadium plays a number of limited roles in terrestrial biochemistry (Sigel & Sigel, 1995; Tracey et al., 2007) and is more important in ocean environments than on land (Chasteen, 1990). For example, bromine compounds in some marine algae are generated by vanadium dependent bromoperoxidase (Michibata et al., 2002). In addition, vanadium nitrogenase is used by some nitrogen-fixing organisms (Rehder, 2000), where vanadium replaces the more common molybdenum or iron, and gives the nitrogenase slightly different properties (Lee et al., 2010),

Of the 15 literature sources in the Hypatia Catalog that determined vanadium abundances, only Feltzing & Gustafsson (1998) and Takeda (2007) determined vanadium abundances from both ionization states. Both surveys reported the lines for the neutral and ionized species were limited to only one or two lines in the optical spectrum, or too weak to separate out from the spectrum. Zhang et al. (2008) reported the vanadium abundances using V I, for 32 mildly metal poor stars using spectra with a signal-noise ratio of about 150 per pixel at 6400 Å and a resolving power of about 37,000. Solar abundances, calculated from the daylight spectrum were used to derive stellar abundances relative to the Sun. The effective temperature was determined from the b-y and V-K color indices; surface gravities were calculated from Hipparcos parallax. They reported that V I follows Fe very closely, with no offset between thin and thick disk stars.

The ratio \([V/Fe]\) versus \([Fe/H]\) is shown in Fig. 3.16 for the 1278 stars in the Hypatia Catalog with V I based abundance determinations (left) and the 142 stellar abundances determined with V II (right). The average \([V/Fe]\) trend, shown by the blue triangles, indicates a flat and solar trend, which may be due to vanadium produced by \(Z \geq 0.1 Z_\odot\) from core-collapse
supernovae being balanced by iron produced from SN Ia. However, there is a significant \( \approx 0.8 \) dex scatter over the entire [Fe/H] range. Most of this scatter is biased towards super-solar values of [V/Fe]. Curiously, the largest values of [V/Fe] are found at distances of 60 pc or less. For [Fe/H] \( > 0 \), V is slightly underproduced, with some stellar abundances significantly below solar [V/Fe]. While the number of stars for which V II was measured is \( \sim 9\% \) that of V I, the blue triangles in Fig. 3.16 (right) still indicate a flat and solar trend for [V II/Fe]. The scatter in [V II/Fe] is about half of what was seen in [V/Fe], \( \approx 0.4 \) dex for [Fe/H] \( < -0.3 \) dex. Above [Fe/H] \( = -0.3 \) dex, the dispersion in [V II/Fe] reaches \( \approx 0.5 \) dex. There is a paucity of stars with a radial distance greater than 60 pc which have [V II/Fe] abundance determinations.

Fig. 3.17 shows [V/Fe] ratios versus radial distance, colored to show the height above the Galactic plane (left plot) and directionality towards or away from the galactic center (right plot). There is a slight prevalence of stars with [V/Fe] near solar to be at a z-height greater than 15 pc. There is also a large scatter of \( \approx 1.0 \) dex in [V/Fe] for those stars with a distance less than \( \sim 40 \) pc and \(-15 \) pc \( < z < 15 \) pc (orange open circles). The large scatter in [V/Fe] at radial distances less than 40 pc is most likely due to the increased number of stars that have been measured closest to the Sun. At distances larger than \( \sim 40 \) pc, the dispersion drops to \( \approx 0.4 \) dex, as abundances become more difficult to measure accurately. All stars towards the Galactic anti-center tend to cluster around solar [V/Fe].

Evolution of [Cr/Fe] with [Fe/H] is shown in Fig. 3.18 for the 1171 stars in the Hypatia Catalog with Cr I based abundance determinations (left) and the 915 stars with Cr II based abundance determinations (right).
Figure 3.17: Similar to Fig. 3.9 but for vanadium. Stars with \( z > 15 \) pc or that are towards the galactic anti-center cluster more strongly around solar. Stars within 40 pc have more scatter in [V/Fe] than stars at larger distances.
Eighteen catalogs within Hypatia report abundances using Cr I lines, while six used both features or just the Cr II lines: Feltzing & Gustafsson (1998); Gratton et al. (2003); Neves et al. (2009); Reddy et al. (2003, 2006); Takeda (2007). For example, Neves et al. (2009) present a survey 12 elements whose abundances are derived from spectra obtained with the HARPS spectrograph on the ESO 3.6 m telescope. The Cr I lines 4588.20 Å and 4592.05 Å along with the Cr II line of 4884.61 Å were used in a differential LTE analysis relative to the Sun to determine the abundance levels. Of the 451 stars in the Neves et al. (2009) survey, 443 are in the Hypatia Catalog. Initial estimates of the oscillator strengths were taken from the Vienna Atomic Line Database and refined using a semi-empirical, inverse analysis with the MOOG2002 (Sneden, 1973). Effective temperatures, surface gravity, microturbulence, and metallicity were taken from Sousa et al. (2008). Neves et al. (2009) reported that abundance levels determined from neutral states are more sensitive to effective temperature changes, whereas abundances derived from ionized states are more sensitive to changes in surface gravity. Abundances from ionized elements are also more sensitive to metallicity changes than the neutral elements, although the sensitivity is not as significant as for the effective temperature or surface gravity.

While most of the stars in Fig. 3.18 for both ionization states are near solar, the trend for [Cr II/Fe] is distinctly below solar. As discussed in Neves et al. (2009), [Cr II/Fe] may also have a weak downward trend with increasing [Fe/H], with a corresponding weak trend for [Cr/Fe]. The scatter in [Cr/Fe] is ≈ 0.2 dex over the entire [Fe/H] range, while the scatter in [Cr II/Fe] is ≈ 0.4 dex for [Fe/H] < 0 and ≈ 0.5 dex for [Fe/H] > 0. These differences may be the result of weak, blended Cr II lines (Neves et al.,
Figure 3.18: Same as Fig. 3.2 but for neutral (left) and ionized (right) chromium. The majority of individual stars cluster around solar values of [Cr/Fe] and sub-solar values for [Cr II/Fe].
2009), different surface gravities for the two ionization states (Reddy et al.,
2003; Gratton et al., 2003), or overionization from Cr II (Feltzing &
Gustafsson, 1998). Both ionization states show some stars with unusually
large chromium to iron ratios.

Variation of the [Mn/Fe] ratio with [Fe/H] for the 1260 stars in
Hypatia is shown in Fig. 3.19 (left). Unique elements in the iron group is
shown by the increasing [Mn/Fe] with [Fe/H] for [Fe/H] > -1.0 dex (Helfer
et al., 1959; Gratton, 1989; Goswami & Prantzos, 2000; Feltzing et al., 2007).
The scatter in [Mn/Fe] is ≈ 0.4 dex over the entire range of [Fe/H] shown,
although there are significant outliers at any [Fe/H]. The increasing trend,
coupled with notable abundance corrections from hyperfine splitting effects
in strong lines, has made the rise in [Mn/Fe] with [Fe/H] challenging to
decipher whether manganese from core collapse supernovae or SN Ia
dominate the trend for [Fe/H] > -1.0 dex (Chen et al., 2000; Prochaska &
McWilliam, 2000; McWilliam et al., 2003; Bergemann & Gehren, 2007;
Feltzing et al., 2007; Bergemann & Gehren, 2008). The single stable isotope
of manganese, $^{55}$Mn, is produced during explosive silicon burning, freeze-out
from nuclear statistical equilibrium in massive stars (Thielemann et al., 2002;
Seitenzahl et al., 2008; Thielemann et al., 2011) and SN Ia (Thielemann
et al., 1986; Iwamoto et al., 1999; Townsley et al., 2009), and possibly as part
of the $\nu$-process in massive stars (Woosley et al., 1990; Yoshida et al., 2006;
Heger & Woosley, 2010). Woosley & Weaver (1995) found their exploded
solar metallicity massive star models produced a factor of 5 times more $^{55}$Mn
than smaller initial metallicity models.

Fig. 3.20 shows [Mn/Fe] ratios versus radial distance, colored to show
the height above the Galactic plane (left plot) and directionality towards or
Figure 3.19: Same as Fig. 3.2 but for manganese (left) and cobalt (right). There is a steady increase in [Mn/Fe] with increasing [Fe/H], and a shallow concave-up feature for [Co/Fe] compared to [Fe/H] with the minimum near solar [Fe/H].
Figure 3.20: Like Fig. 3.9 but for manganese. Both plots show much scatter, especially for those stars with a radial distance below 40pc.
away from the galactic center (right plot). There is significant scatter in
[Mn/Fe], ≈ 0.5 dex, out to at least ∼ 100 pc. Stars around the solar value of
[Mn/Fe] are not as clustered, especially stars that have z > 15pc and towards
the galactic anti-center, as for most other elements.

Variation of the [Co/Fe] ratio with [Fe/H] is shown in Fig. 3.19
(right). The average [Co/Fe] ratio in three [Fe/H] bins, shown by the blue
triangles, indicates a slight concave-up trend. Aspects of this feature is noted
by several authors (Reddy et al., 2003; del Peloso et al., 2005; Reddy et al.,
2006; Neves et al., 2009), and is similar to the trend seen for sodium in Fig.
3.13. For [Fe/H] below solar, [Co/Fe] decreases from ≈ 0.1 dex to ≈ 0.0 dex,
with a scatter of ≈ 0.3 dex. When [Fe/H] is above solar, [Co/Fe] increases
from ≈ 0.0 dex to ≈ 0.1 dex, with a scatter of ≈ 0.4 dex. In either regime,
there are outliers with significant super-solar [Co/Fe] ratios.

The single stable isotope of cobalt, $^{59}$Co, is produced by a variety of
processes in several sources. It is produced during the s-process that takes
place during helium burning in massive stars (Umeda & Nomoto, 2002) and
AGB stars (Busso et al., 1999; Herwig, 2005), during the α-rich freezeout in
massive stars (Heger & Woosley, 2010) and SN Ia (Iwamoto et al., 1999),
and possibly as part of the $\nu$-process in massive stars (Woosley et al., 1990).
As a result, there is no consensus on the overall trend of cobalt in halo and
thin/thick disk stars, nor a generally accepted origin site for the production
of cobalt (Bergemann et al., 2010).

Nickel has the most measurements of any element within the iron
group in Hypatia; twenty-eight literature sources are listed with [Ni/Fe]
abundances in Table 2.2. This is because nickel has a similar ionization
potential and atomic structure as iron and is relatively easy to measure in
Figure 3.21: Similar to Fig. 3.10 but for the α-chain elements [Ni/Ca] (left) and [Ni/Si] (right) plotted against [Fe/H]. There is no correlation between [Ni/Ca] and radial distance while the increase of [Ni/Ca] with [Fe/H] follows the trends expected from mean galactic chemical evolution models. Similarly, there does not seem to be a correlation between [Ni/Si] and radial distance, but there is slight increase in [Ni/Si] with [Fe/H] and minimal scatter.
the optical spectrum. For example, Gilli et al. (2006) measured the abundances nickel (and 11 other elements) for 101 stars in the solar neighborhood, 93 of which are known to be host-stars to exoplanets. A total of 98 of their stars are in the Hypatia Catalog. Their spectra was acquired using five different spectrographs that, in total, spanned the range of 3800 Å to 10000 Å, with significant overlap in wavelength coverage between the spectrographs. The maximum resolution was $\lambda / \Delta \lambda \approx 110000$ and minimum resolution of $\lambda / \Delta \lambda \approx 48000$. A standard LTE analysis, with respect to the solar abundances determined by Anders & Grevesse (1989), was done for all elements using MOOG (Sneden, 1973) and the ATLAS9 atmospheres (Kurucz, 2005). Effective temperatures, surface gravities, microturbulence, and metallicity $[\text{Fe/H}]$ were all determined by Santos et al. (2005, 2004). The spectral lines that were used for refractory elements matched those within Bodaghee et al. (2003), while the lines for the other elements are from Beirão et al. (2005). Gilli et al. (2006) estimate an overall uncertainty of of $\sim 0.10$ dex for all abundance determinations.

Elemental nickel in the solar composition is dominated by the $^{58}\text{Ni}$ (68.0%) and $^{60}\text{Ni}$ (26.2%) isotopes (Lodders et al., 2009). Both isotopes are made in freeze-outs from nuclear statistical equilibrium (Woosley et al., 1973; The et al., 1998) in massive stars and standard paradigm deflagration SN Ia (e.g., José & Iliadis, 2011). However, $^{60}\text{Ni}$ can also have a significant contribution from the s-process during helium burning (Busso et al., 1999; Herwig, 2000; Karakas, 2010).

Fig. 3.21 shows the evolution of $[\text{Ni/Ca}]$ (left) and $[\text{Ni/Ca}]$ (right) with $[\text{Fe/H}]$. Both show positively sloped trends with $[\text{Fe/H}]$, indicating the injection of the iron-peak nuclei from SN Ia for $[\text{Fe/H}] > -1.0$ dex. The
scatter of \([\text{Ni/Ca}]\) is \(\approx 0.2\) dex for \([\text{Fe/H}] < 0\) and increases to \(\approx 0.4\) dex above solar \([\text{Fe/H}]\). In comparison, \([\text{Ni/Si}]\) has a scatter of \(\approx 0.2\) dex for all \([\text{Fe/H}]\). Evolution of the \([\text{Ni/Fe}]\) ratio with \([\text{Fe/H}]\) for the 2107 stars in Hypatia is shown in Fig. 3.22 (left). Most stars cluster around a solar value of \([\text{Ni/Fe}]\) over the entire \([\text{Fe/H}]\) range shown. The scatter is \(\approx 0.2\) dex, except for the region \(-0.2\) dex \(\leq [\text{Fe/H}] \leq 0.2\) dex where the scatter is \(\approx 0.3\) dex.

3.8 Beyond the Iron-Peak (Cu, Zn, Sr, Y, Zr)

Nuclei above the iron peak have large Coulomb barriers, making charged-particle interactions unlikely at temperatures that would not photodissintegrate the nuclei. Elements beyond the iron-peak have fewer spectral lines in the optical regime, resulting in fewer abundance determinations for these elements as shown in Fig. 2.1.

Copper has two stable isotopes, \(^{63}\text{Cu}\) and \(^{65}\text{Cu}\), both of which contribute to the solar element abundance, 69.2% and 31.8%, respectively. The more common isotope, \(^{63}\text{Cu}\), is mostly created as radioactive \(^{63}\text{Ni}\) via the s-process during hydrostatic helium burning in massive stars and intermediate mass AGB stars. It is also produced as radioactive \(^{63}\text{Zn}\) from the \(\alpha\)-rich freezeout in massive stars (Travaglio et al., 1999; Bisterzo et al., 2004; Mashonkina et al., 2007; Käppeler et al., 2011). The isotope \(^{65}\text{Cu}\) is mostly formed as itself during the s-process and as radioactive \(^{65}\text{Zn}\) during quasiequilibrium explosive burning (Busso et al., 1999; McWilliam & Smecker-Hane, 2005; Bonifacio et al., 2010). The evolution of \([\text{Cu/Fe}]\) with \([\text{Fe/H}]\), as shown in Fig. 3.22 (right), is mostly flat and solar with \(\approx 0.5\) dex scatter at any \([\text{Fe/H}]\), although with some significant outliers (Gonzalez &
Figure 3.22: Same as Fig. 3.2 but for nickel (left) and copper (right), where $[\text{Ni}/\text{Fe}]$ is one of the most frequently measured abundances (see Fig. 2.1) in Hypatia. Both elements are mostly flat and solar with respect to $[\text{Fe}/\text{H}]$, with $[\text{Ni}/\text{Fe}]$ having a smaller scatter, $\approx 0.2$ dex, than $[\text{Cu}/\text{Fe}], \approx 0.5$ dex. The average trend in three $[\text{Fe}/\text{H}]$ bins, shown by the blue triangles, suggest a slight concave-up trend in $[\text{Cu}/\text{Fe}]$. 
Laws, 2007; Romano & Matteucci, 2007; Ramírez et al., 2009; Nissen & Schuster, 2011; Allen & Porto de Mello, 2011). The average [Cu/Fe] in three [Fe/H] bins, shown by the blue triangles, is consistent with a slight concave-up feature at larger [Fe/H] but caution is warranted in interpreting this feature due to the scatter in [Cu/Fe].

Figure 3.23: Same as Fig. 3.2 but for zinc. The [Zn/Fe] ratio decreases slightly with [Fe/H], although the scatter ≈ 0.5 dex is larger than for most other elements for [Fe/H] > 0.

Zinc is the 25th most abundant element in Earth’s crust (Rudnick & Gao, 2003) and has 5 naturally occurring isotopes. The isotope $^{64}$Zn is the most abundant, providing 48.6% of the total solar element abundance (Lodders et al., 2009). It is made as radioactive $^{64}$Ge in the s-process during hydrostatic helium burning (Couch et al., 1974; Iben, 1982; Busso et al., 1999; Käppeler et al., 2011) and in α-rich freezeouts from massive stars.
(Woosley et al., 1973; Hix & Thielemann, 1996), but consensus on the origin site has not yet been reached (Hoffman et al., 1996; Umeda & Nomoto, 2002; Chen et al., 2004; Mishenina et al., 2011). The second and third most abundant isotopes are $^{66}$Zn (27.9%) and $^{68}$Zn (18.7%), respectively, which are both produced as themselves in the s-process (Clayton, 2003). The evolution of $[\text{Zn/Fe}]$ with $[\text{Fe/H}]$, as shown in Fig. 3.23, has a shallow negative trend over the $[\text{Fe/H}]$ range shown (Roederer et al., 2010; Kobayashi & Nakasato, 2011). Near $[\text{Fe/H}] = -1.0$ dex the scatter is $\approx 0.3$ dex, whereas for $[\text{Fe/H}] > 0.2$, the scatter is $\approx 0.5$ dex, with some significantly enhanced $[\text{Zn/Fe}]$ stars for $[\text{Fe/H}] > 0$ dex.

A total of 64 stars within the Hypatia Catalog have copper and zinc abundances determined by Ramírez et al. (2009). Their spectra has a resolution of $\lambda/\Delta\lambda \approx 60000$ over the range 3800–9125 Å and high signal-to-noise ($S/N \approx 200$ per spectral pixel) for the solar twins and analog stars. They determined the solar flux spectrum by using differential analysis from asteroid spectra. Effective temperatures, surface gravities, and microturbulent velocities were obtained by iterating until the difference in $[\text{Fe/H}]$ values from both Fe I and Fe II approached zero. Model LTE atmospheres from Kurucz (2005) and MOOG (Sneden, 1973) were used to determine all element abundances. The reported uncertainties for the abundance measurements is $[\text{X/Fe}] \approx 0.03$ dex.

There are multiple processes that produce strontium, yttrium, and zirconium. According to Arlandini et al. (1999), 85% of strontium in the solar composition is from the r-process and 15% from the s-process. Similarly, 92% of yttrium and 83% of zirconium is through the r-process while 8% and 17%, respectively, is from the s-process. While the relative
Figure 3.24: Same as Fig. 3.2 but for neutral (left) and ionized (right) strontium. There is a large scatter in [Sr/Fe], with respect to both the radial distance and [Fe/H]. The errorbar for these measurements is also larger than most of the other elements, $\sim 0.5$ dex.
contributions from each process depend on the initial enrichment and the age of the stellar system, there are unaccounted contributions at low metallicities (Thielemann et al., 2007). These abundance remainders might be due to primary production of strontium, yttrium, and zirconium within massive stars, possibly through neutrino-proton interactions (Arnould et al., 2007).

Elemental strontium is dominated by $^{88}\text{Sr}$ (82.6%), followed by $^{86}\text{Sr}$ (9.9%). Six literature sources within Hypatia measured strontium for 274 stars: Galeev et al. (2004); Luck & Heiter (2005); Mashonkina et al. (2007); Reddy et al. (2003); Thevenin (1998). Due to the limited number of available lines in the optical spectrum, a number of these literature sources quoted high uncertainties from blended, weak lines. The abundance of [Sr/Fe] as a function of [Fe/H] is shown in Fig. 3.24 (left). The scatter in [Sr/Fe] is $\approx 1.5$ dex over the entire range of [Fe/H], which may be indicative of multiple origin sites (Lai et al., 2007). The blue triangles, representing the average [Sr/Fe] in three [Fe/H] bins, indicate a flat and solar trend (McWilliam, 1997). Stars in Hypatia with a distance less than 30 pc have a larger [Fe/H] abundance, the majority of which are above solar. There are 58 stars in the Hypatia Catalog which have strontium abundances determined from Sr II, as shown in in Fig. 3.24 (right). The scatter in [Sr II/Fe] is $\approx 2.0$ dex with no clear clustering near solar, unlike [Sr/Fe]. However, stars closer than 30 pc to the Sun have a [Sr/Fe] ratios closer to solar.

Many catalogs within Hypatia made the distinction between measuring neutral or singly ionized yttrium, although only Feltzing & Gustafsson (1998) measured both Y I and Y II. Evolution of [Y/Fe] as a function of [Fe/H] for 423 stars is shown in Fig. 3.25 (left) while [Y II /Fe] versus [Fe/H] for 774 stars is shown on the right. The more numerous Y II
Figure 3.25: Same as Fig. 3.2 but for neutral (left) and ionized (right) yttrium. The scatter in [Y/Fe] is large, both with respect to radial distance and [Fe/H], although there is a clumping of stars with [Y/Fe] ≈ 0.0 dex. On the other hand, [Y II/Fe] is relatively flat and solar over the [Fe/H] range shown, although there is a scatter of ≈ 0.4 dex.
measurements are due to rather weak and blended lines available for Y I in the optical spectrum. The average [Y/Fe] abundances, represented by the blue triangles, suggest a flat and solar trend (Qian & Wasserburg, 2008; Roederer et al., 2010), but with a dispersion of \( \approx 1.2 \) dex for all [Fe/H]. There are relatively few stars with a radial distance greater than 60 pc and the majority of stars exhibit solar or larger [Y/Fe] abundances. Comparatively, the evolution of yttrium studies with [Y II/Fe] shows a solar and flatter trend for all values of [Fe/H]. The scatter in [Y II/Fe] is \( \approx 0.4 \) dex. A few stars with distances between 30 pc and 60 pc show enrichment in [Y II/Fe].

Zirconium abundances in Hypatia are similar to those of yttrium, in that the singly ionized state was preferentially measured due to blending of weak neutral lines in the optical spectrum. Evolution of [Zr/Fe] as a function of [Fe/H] for the 256 stars in Hypatia is shown in Fig. 3.26 (left), and [Zr II/Fe] versus [Fe/H] for 535 stars is given in Fig. 3.26 (right). There is a large scatter in [Zr/Fe], on the order of 1.5 dex or more, over the entire range of [Fe/H]. While the general trend indicated by the blue triangles is centered on solar (Qian & Wasserburg, 2008; Kashiv et al., 2010), the large scatter makes any dependence on [Fe/H] difficult to discern. Comparatively [Zr II/Fe], like [Mn/Fe], shows a shallow concave-down trend. The scatter in [Zr II/Fe] is consistently \( \approx 0.5 \) dex over the range of [Fe/H], although for [Fe/H] = [-0.6, 0], there are a number of stars at larger distances from the Sun that appear to be highly enriched in ionized zirconium. Similarities between the patterns seen in [Zr II/Fe] and [Y II/Fe] with respect to [Fe/H] suggests similar origin sites.

Bond et al. (2006) determined Y II and Zr II abundances in of 144 G-type stars, all of which are in Hypatia, using high resolution (\( \lambda/\Delta \lambda \approx \).
Figure 3.26: Same as Fig. 3.2 but for neutral (left) and ionized (right) zirconium. There is a large scatter in [Zr/Fe] both with radial distance and [Fe/H]. Comparatively, [Zr II/Fe] shows a shallow concave-down feature with [Fe/H] based on the blue triangles.
80000), high signal-to-noise ratio (S/N \approx 250 per pixel) spectra of the 5380.32 Å and 6587.62 Å lines of C I. Oscillator strengths and excitation energies for each line were obtained from the NIST Atomic Spectra Database. Effective temperatures were determined from the stellar colors listed in the Hipparcos Catalogue, which is different from similar studies that utilize the spectra for an effective temperature value, and resulted in a mean $T_{\text{eff}}$ uncertainty of $\pm 100$ K. An LTE analysis using WIDTH6 (Kurucz, 2005) in conjunction with a grid of Kurucz (2005) ATLAS9 atmospheres was used to determine the elemental abundances. Surface gravities $\log g$ values and Fe abundances were obtained by iterating until the [Fe/H] value from both Fe I and Fe II was the same. The microturbulence parameter $\zeta$ which minimized the correlation coefficient between $\log \zeta$ for Fe I and $\log (W_\lambda/\lambda)$ was selected with an estimated uncertainty of $\pm 0.25$.

3.9 Neutron-Capture Elements (Ru, Ba, La, Ce, Pr, Nd, Sm, Eu, Gd, Dy, Pb)

The heavy neutron capture elements have the majority of their lines in the extreme blue and UV part of the spectrum, making it challenging to measure these elements (Spite & Spite, 1978; Sneden et al., 2008). As a result fewer catalogs report these abundances (see Fig. 2.1) and the observational uncertainties in the abundance ratios are generally larger for the neutron capture elements. For example, Galeev et al. (2004) measured the Ru, Ba, La, Ce, Pr, Nd, Sm, and Eu abundances for 15 stars in the solar neighborhood, all of which are in the Hypatia Catalog, using the 2 m reflector at Terskol Observatory in the northern Caucasus. Their high resolution spectra ($\lambda/\Delta \lambda \approx 45000$) covered 4000 - 9000Å with a
signal-to-noise ratio of 150-200 per spectral pixel. They determined the solar flux spectrum via differential analysis, using solar light scattered off of the Earth’s atmosphere. An LTE analysis with WIDTH6 (Kurucz, 2005) is used, in conjunction with oscillator strengths from the VALD database (Kupka et al., 1999), to determine the final elemental abundances. An accuracy of 0.10 dex is assigned to their [Fe/H] measurements. We elect not to discuss Ru, La, Pr, Sm, Gd, Dy and Pb in this paper, although these elements are listed in Hypatia, focusing on those elements with more measurements: Ba, Ce, Nd, and Eu.

Elemental barium is dominated by three isotopes: $^{135}$Ba, $^{137}$Ba, and $^{138}$Ba, the majority of which are made in the s-process (Arlandini et al., 1999; Travaglio et al., 1999; Mashonkina & Gehren, 2000; Carlson et al., 2007). The lines of barium are strongly affected by hyperfine splitting (Mashonkina & Gehren, 2000; Mashonkina et al., 2007). Variation of [Ba/Fe] with [Fe/H] for the 948 stars in Hypatia is shown in Fig. 3.27 (left). The blue triangles, representing the mean [Ba/Fe] ratio in three [Fe/H] bins, suggest a slight concave-down trend over the range of [Fe/H]. Otherwise, the evolution is consistent with a flat and solar [Be/Fe] ratio with a scatter of $\approx$ 0.5 dex (Thevenin, 1998; Reddy et al., 2006). Similar to [Zr II/Fe], some stars are highly enriched in barium and are at a radial distance of 60 pc or more away from the Sun (Allen & Porto de Mello, 2011).

Cerium is also predominantly (77%) made by made by the s-process as either $^{140}$Ce or $^{142}$Ce Arlandini et al. (1999); Simmerer et al. (2004); Käppeler et al. (2011). Only eight catalogs within Hypatia measure cerium, due to only one or two lines in the optical spectrum that were not strongly affected by blending (Luck & Heiter, 2005). Fig. 3.27 (right) shows a
Figure 3.27: Same as Fig. 3.2 but for barium (left) and cerium (right). Both elements show a flat and trend over the $[\text{Fe/H}]$ range shown, but there are some significant outliers.
predominantly solar and flat trend of [Ce/Fe] with respect to [Fe/H], also noted by Brewer & Carney (2006), for the 622 stars in Hypatia. The scatter in [Ce/Fe] is $\approx 0.5$ dex for all [Fe/H], although some stars show very large [Ce/Fe] ratios. Unlike previously discussed elements with this pattern, some of the [Ce/Fe] rich stars are within 30 pc of the Sun.

The seven stable isotopes of neodymium are made by both the r- and the s-processes (Roederer et al., 2008), with $^{142}\text{Nd}$, $^{143}\text{Nd}$, $^{144}\text{Nd}$, and $^{146}\text{Nd}$ being the most abundant isotopes. For example, $^{142}\text{Nd}$ is made primarily by the s-process, $^{148,150}\text{Nd}$ are mostly synthesized by the r-process, and the other four isotopes are composed as a combination of the two neutron capture processes (Arlandini et al., 1999; Simmerer et al., 2004; Andreasen & Sharma, 2006; Kratz et al., 2007). Due to blending with nearby lines, there are only one or two lines in the optical spectrum from which [Nd/Fe] is measured (Galeev et al., 2004; Bond et al., 2008). The average [Nd/Fe] trend, shown by the blue triangles, indicates a downward trend of [Nd/Fe] with [Fe/H], particularly for [Fe/H] $\geq 0.2$ dex. Otherwise, the evolution is consistent with a flat and solar [Nd/Fe] ratio (Thevenin, 1998; Reddy et al., 2003), where the scatter is $\approx 0.7$ dex over the range of [Fe/H] shown. There is a cluster of stars with distance greater than 60 pc that have large [Nd/Fe] ratios in the -0.6 dex $\leq$ [Fe/H] $\leq$ -0.2 dex range (Thevenin, 1998; Allen & Porto de Mello, 2011).

There are only two stable isotopes of europium: $^{151}\text{Eu}$ (47.8%) and $^{153}\text{Eu}$ (52.2%) (Roederer et al., 2008; Lodders et al., 2009). About 91% of europium is estimated to be from the r-process (Cameron, 1982; Arlandini et al., 1999) and is often used as a standard against a predominantly s-process element, such as [Ba/Eu] (McWilliam, 1997; Travaglio et al., 1999;
Figure 3.28: Same as Fig. 3.2 but for neodymium (left) and europium (right). There is a slight decrease of [Nd/Fe] with increasing [Fe/H], although the scatter is large. While [Eu/Fe] has significant scatter, there is a trend for decreasing [Eu/Fe] with [Fe/H].
Mashonkina & Gehren, 2000). There are thirteen literature sources within Hypatia that measured \([\text{Eu/Fe}]\) using one or two lines in the optical spectrum. Like neodymium, the trend of \([\text{Eu/Fe}]\) with respect to \([\text{Fe/H}]\) has a negative slope for \([\text{Fe/H}]\) (Thevenin, 1998; Reddy et al., 2003; Galeev et al., 2004; Bond et al., 2008; Allen & Porto de Mello, 2011), as shown in Fig. 3.28 (right). However, the overall scatter is relatively large, \(\approx 0.9\) dex over the range of \([\text{Fe/H}]\) shown. Stars with distances greater than 60 pc tend to be clustered at \([\text{Eu/Fe}] \approx 0.1\) dex and \([\text{Fe/H}] \approx -0.3\) dex (Thevenin, 1998; Allen & Porto de Mello, 2011).

The extent of the abundance information for solar neighborhood stars within the Hypatia Catalog makes it useful for a number of applications. Stellar abundance trends may be found for stars with similar physical or kinematic properties. The data may also be used to supplement or compare against similar catalogs that employed different methods, wavelengths, or instruments. Given that the evaluation of the data described in Chapter 2 was for the purpose of our analysis alone, and is not present within the published catalog, it is also possible to compare the abundance data from specific surveys incorporated into the Hypatia Catalog. In Chapter 4 we present an application of the Hypatia Catalog to known exoplanet host stars, analyzing their compositions with respect to each other as well as the physical characteristics of the stellar systems. We present a second application of Hypatia in Chapter 5 to HabCat, in order to find regions on the sky that may be potentially habitable.
APPLICATION TO KNOWN EXOPLANETS

Before the discovery of the first exoplanet, our only understanding of planets was based on the Solar System, where the smaller terrestrial planets orbit closer to the Sun than the giant gas planets. However, this all rapidly changed with the observation of “hot Jupiters” or planets with masses on the order of Jupiter that orbit very close to their host star. Soon after the initial discovery (Mayor & Queloz, 1995), new theories were formulated to explain the formation of these new stellar systems (Lin et al., 1996). And as the number of exoplanets continued to increase, the stellar hosts also became a target of investigation (Gonzalez, 1997). To date, +500 extrasolar planets have been positively identified (Wright et al., 2011), with another ∼2300 candidates observed by Kepler (Borucki et al., 2011; Batalha et al., 2012).

The slew of new data has instigated a number of surveys of the physical and chemical properties for both the exoplanets and their hosts. The ultimate questions of the planetary studies concern formation and possible migration. These studies try to determine in what ways the planet and star interact, both physically (e.g. orbit) and chemically (e.g. accretion). Analyses of the stellar hosts seek to understand the differences between stars with planets (or SWPs) and stars without (or background disk stars). In other words, how do the characteristics of a star relate to the star hosting an exoplanet. The examination of multiple stellar and planetary properties give new insight into mechanisms that are currently only theoretical.
In §4.1, we will compare the element abundances for a subset of 204 SWPs from the Hypatia Catalog to the remaining 2632 stars within the catalog. We find that SWPs have higher iron abundances as compared to the stars in the full Hypatia Catalog. However, this enrichment does not extend to any of the other elements. We will also analyze some of the more important elemental abundances with respect to the physical properties of the planetary system in §4.2. For example, we find potential biases in the data with respect to orbital period, multi-planet systems, and systems with less massive planets (< 0.1 M_J). These are corroborated by planetary characteristic trends already observed in the literature (§4.2.3). Given the breadth of elements within Hypatia, as discussed in §3, we are able to examine a number of both volatile and refractory elements. These specific groups of elements give insight into the compositional implications of stellar hosts (§4.3) as well as planetary formation (§4.4).

4.1 Abundance Trends for Known Host-Stars

As the number of exoplanets have increased, so has spectroscopic resolution and the ability to discern the weaker or blended lines within stellar atmospheres. This has made abundances for elements other than iron more easily measured within host-stars, and with smaller errorbars. A histogram of the number of stars measured for each element in the SWPs is shown in Fig. 4.1. All 204 SWPs have a spectroscopically determined [Fe/H], the other 42 elements have the total number of stars for which they were measured labeled respectively. The most frequently measured elements are Si (187 stars), Ti (168 stars), Ni and Na (166 stars each), and O (165 stars) – similar to Fig. 2.1. We will discuss Si, Ni, and Na more in §4.2.2. Fig. 4.1
also shows the relatively few stars for which the elements beyond the iron peak and those created by neutron-capture have been measured.

In this section will we examine the relative frequency of planets with respect to elemental abundances in the host star. We will begin with iron and bio-essential elements in detail, due to their importance, and then discuss some of the more frequently measured elements en-mass.

4.1.1 Iron Abundance in Exoplanet Hosts

Since the initial report by Gonzalez (1997), there have been numerous studies on the planet-metallicity correlation, typically with respect to background disk stars. The vast majority of the surveys have found that iron is preferentially enriched within exoplanet hosts, namely Fischer & Valenti (2005); Fuhrmann et al. (1997); Bond et al. (2006); da Silva et al. (2011); Ghezzi et al. (2010b); Gonzalez et al. (2001); Gonzalez (1998b, 1997); Heiter & Luck (2003); Laws et al. (2003); Murray & Chaboyer (2002); Neves et al. (2009); Queloz et al. (2000); Rojas-Ayala et al. (2010); Sadakane et al. (2002); Santos et al. (2005, 2004, 2001, 2000); Valenti & Fischer (2008). In Fig. 4.2, we show a relative frequency histogram for the [Fe/H] abundance in both SWPs (solid orange) and the full Hypatia Catalog (dashed red), binned in 0.1 dex intervals. The exoplanets hosts peak $\sim 0.2$ dex higher than the background disk stars, a difference that is larger than the typical 0.05 dex error for [Fe/H] (see §3.1 Asplund, 2005). Comparing the two stellar populations, 77% of the exoplanet hosts lie above the solar value of [Fe/H] while only 54% of the background Hypatia stars are above [Fe/H] = 0.0 dex. In terms of units of dex, the difference between both sets of stars in [Fe/H] is higher any other element ratio [X/Fe] studied in this paper, with the
Figure 4.1: Number of exoplanet host-stars in the Hypatia Catalog with measured abundances for 43 different element species.
Figure 4.2: A histogram of the relative frequency for $[\text{Fe}/\text{H}]$ in both SWPs and the full Hypatia Catalog, where the exoplanet hosts are shown as solid orange and the entire Hypatia Catalog as dashed red. The exoplanets a much higher enrichment in $[\text{Fe}/\text{H}]$ than the full catalog.

exception of sulfur (see §4.1.3). We have also employed a Kolmogorov-Smirnov (KS) test as a non-parametric comparison to determine if the two observed distributions are drawn from the same parent sample. The probability of the two distributions being from the same parent distribution, or p-value, is $4.8 \times 10^{-18}$. In other words, there is significant confidence that the $[\text{Fe}/\text{H}]$ metallicity distribution for the SWPs is different than that of the background stars. Please note that this does not indicate that SWPs are preferentially enhanced in metals, merely that the two populations are different. Given the number of independent studies that have confirmed the iron enrichment in SWPs with respect to background stars in both
magnitude- and volume-limited samples, we find that the planet-metallicity trend has been confirmed with the data. The iron enrichment is therefore not an observational bias.

4.1.2 C, N, O Abundances in Exoplanet Hosts

Evolution of [C/Fe] as a function of [Fe/H] for 1466 stars in the Hypatia Catalog (see Fig. 2.1) are shown in Fig. 4.3 (left), with 142 SWPs overlayed in blue. A representative error bar derived from the quoted observational uncertainties is shown in the upper right. For the disk stars, as is shown in Fig. 3.2, green circles indicate stars with distances from the Sun less than 30 pc, yellow circles designate distances between 30 pc and 60 pc, and red circles specify distances larger than 60 pc. While both sets of stars follow the same trend, the exoplanet host-stars mainly occupy the region with higher [Fe/H] and lower [C/Fe]. On the right, the histogram shows the relative frequency of [C/Fe] abundance for both sets of data, similar to Fig. 4.2. The shapes of both distributions are similar, peaking at [C/Fe] between -0.1–0.0 dex. However, 58% of the SWPs with carbon measurements have [C/Fe] abundances below solar, while 51% of the full Hypatia Catalog stars lie above solar. A KS-test with respect to [C/Fe] between the two populations finds a significant difference with 99.96% confidence, or a p-value of $3.7 \times 10^{-4}$.

Originally, Gonzalez & Laws (2000) claimed that [C/Fe] was slightly lower in SWPs than the abundance within disk stars. After reevaluation of the manner in which they combined their data with others, offsets were applied in Gonzalez et al. (2001). In the latter paper, the SWPs were found to exhibit slightly higher [C/Fe] compared to disk stars, although the

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Figure 4.3: On the left, $[\text{C}/\text{Fe}]$ ratio as a function of $[\text{Fe}/\text{H}]$ for the entire Hypatia catalog (green, yellow, and red open circles), with the known exoplanet host abundances overlayed as solid blue circles. Blue triangles show the average abundance ratio value from all abundance values for three $[\text{Fe}/\text{H}]$ bins: $<-0.5$ dex, $<-0.5,0.0>$ dex, and $>0.5$ dex (see text). On the right, a histogram of the relative frequency of $[\text{C}/\text{Fe}]$ for both sets of stars, where the exoplanet hosts are shown as solid orange and the entire Hypatia catalog as dashed red.
differences were not significant. The SWP [C/Fe] trends found in Gonzalez & Laws (2007) don’t appear significantly different from other stars. Similarly, Takeda & Honda (2005), Luck & Heiter (2006), da Silva et al. (2011), and Ecuvillon et al. (2004) did not find a noticeable difference between the SWPs and the non-plant-hosting stars. The measurements determined by Bond et al. (2006) were divided into subgroups depending on V-band magnitude, V < 7.5 and V > 7.5. A noticeable mean difference in [C/H] between host- and non-host-stars was found for those stars with V < 7.5: 0.15 ± 0.03 dex and -0.01 ± 0.02, respectively.

Compared to the other bio-essential elements, nitrogen abundances have been measured in relatively few stars, about 1/3 as many SWPs, due to weak N I lines. As a result, the trends seen in [N/Fe] with respect to [Fe/H] are rather diffuse with a scatter in [N/Fe] ≥ 1.0 dex, see Fig. 4.4 (left) and Fig. 3.2. Similar to carbon, the [N/Fe] ratios for the SWPs are generally low in contrast to the disk stars, but with [Fe/H] ratios lie predominantly above solar. Fig. 4.4 (right) shows a bi-modal distribution, which peaks between [N/Fe] between -1.0–0.0 dex, with a secondary peak within 1.0-2.0 dex. The stars in the full Hypatia Catalog also peak between -1.0–0.0 dex, with a more gradual decline towards the positive abundances. Of the total number of SWPs with [N/Fe] measurements, 64% were below the solar value. In comparison, 59% of the background stars had [N/Fe] > 0.0 dex. A KS-test between the SWPs and the background Hypatia stars yields a p-value of 2.7 × 10⁻³, meaning that the two [N/Fe] distributions are significantly different, although with less confidence than was seen for [Fe/H] and [C/Fe]. The [N/Fe] abundances determined by Takeda & Honda (2005) for 27
Figure 4.4: Similar to Fig. 4.3 but for [N/Fe], plotted with respect to [Fe/H] (left) and relative frequency (right). The majority stars in both the full Hypatia catalog and the known exoplanets have an abundance of [N/Fe] between -1.0-0.0 dex. While a higher relative population of stars within all of Hypatia show larger [N/Fe] abundances, the known exoplanets have [Fe/H] predominantly above solar.
planet-host stars found that there was no statistical difference between them and the disk stars.

There are a number of spectral lines that have been used to determine stellar oxygen abundances: the near-IR O I triplet at 7700Å, the forbidden [O I] doublet at 6300Å and 6363Å, and the near-UV OH lines at 3100Å. Ecuvillon et al. (2006) studied the observational differences encountered when determining the [O/Fe] ratio with all three indicators for both exoplanet hosts and non-hosts. The general trend in [O/Fe] with [Fe/H] were relatively consistent between the three oxygen indicators, in that a least-squares fit for all three resulted in a slope of $-0.50 \pm 0.04$. While the measurements from the OH and doublet lines were similar, Ecuvillon et al. (2006) noted some slight discrepancies in the abundance determinations. For example, the O I triplet abundances were more of an upper bound determination, while NLTE corrections resulted in measurements that were consistently too low. For any indicator, the authors did not find any significant differences between SWPs and the disk stars.

All of the [O/Fe] measurements in the Hypatia Catalog were determined with the O I triplet. Many of the catalogs applied corrections by matching to abundances determined with the [O I] doublet or by undertaking non-LTE calculations (e.g., Brugamyer et al., 2011). Given the discussion by Ecuvillon et al. (2006), if the oxygen abundances within Hypatia are inconsistent with actual stellar abundances, they are likely offset similarly. Fig. 4.5 (left) shows [O/Fe] versus [Fe/H] for both SWPs and the full Hypatia Catalog, similar to Fig. 3.3. Both sets of stars display a classic $\alpha$-element evolution (see §3.2), where the SWPs lie predominantly in the $[\text{Fe/H}] > -0.1$ dex regime. The [O/Fe] abundances for the SWPs are
markedly lower than the disk stars, as illustrated by Fig. 4.5 (right). While the host- and non-host-stars both peak at [O/Fe] between -1.0–0.0 dex, the distribution of the disk stars is skewed towards abundances above solar, with 54% above solar. The SWP distribution is relatively sub-solar, where 59% of the total number of stars have [C/Fe] < 0.0 dex. A KS-test between the SWPs and the Hypatia stars has determined that the distributions did not come from the same parent sample, such that p = 1.6 × 10⁻⁹.

The studies conducted by Brugamyer et al. (2011), Takeda & Honda (2005), and Luck & Heiter (2006) did not find any statistical differences between the [O/Fe] abundances found in SWPs and disk stars. The [O/Fe] to [Fe/H] plots presented in both papers are noticeably similar to Fig. 4.5 (left), in that [Fe/H] is enriched for SWPs while [O/Fe] is not. Bond et al. (2008) analyzed the oxygen abundances with respect to both hydrogen and iron and also found no difference between SWPs and disk stars. The same trend was found by Gonzalez et al. (2001) and Gonzalez & Laws (2007). The overall conclusion from this and other studies is that planet-hosting stars follow the same chemical abundance trends as other non-hosting stars, with the possible exception of [C/Fe] in SWPs with V < 7.5 (Bond et al., 2008).

Per the discussion of Fortney (2012, and references therein), there have been multiple studies with respect to both carbon and oxygen, as well as their respective ratio, within stellar photospheres. Due to the observational errors associated with each element, and despite attempts to rule out biases, it is possible to over estimate the fraction of stars with high C/O ratios. For example, while Bond et al. (2010); Delgado Mena et al. (2010) and Petigura & Marcy (2011) predict C/O > 1.0 for 1-5% of FGK stars, only 0.04% carbon-stars were actually observed in a joint
Figure 4.5: Similar to Fig. 4.3 but for [O/Fe], plotted with respect to [Fe/H] (left) and relative frequency (right). Similar to both carbon and nitrogen, the known exoplanet hosts exhibit higher ratios of [Fe/H], while maintaining similar majority abundances of [O/Fe] between -1.0–0.0 dex. The stars in the entire Hypatia catalog exhibit higher [O/Fe] ratios.
SDSS-2MASS survey of ~ 10,000 stars (Covey et al., 2008). Reasons for this over-estimation may include systematic errors from [O I] and CI lines, the choice in solar-reference abundance, adopted stellar parameters, and choice of stellar atmospheric models (Fortney, 2012).

4.1.3 Mg, Si, S Abundances in Exoplanet Hosts

Like carbon and oxygen, magnesium is an α-element (see §3.3). As a result, the [Mg/Fe] abundances exhibit a similar trend with respect to [Fe/H]. The [Mg/Fe] measurements linearly decrease with increasing [Fe/H], see Fig. 4.6 (left) and Fig. 3.4. However, the slope is slightly more shallow compared to the other α-elements, as shown by the change in y-axis scale. While the number of stars with [C/Fe] or [O/Fe] measurements steeply drops around [Fe/H] ≈ -0.1, the transition to lower [Fe/H] ratios is more steady in [Mg/Fe]. There is also no obvious cluster of stars towards higher [Fe/H] metallicity. The same is also true with regard to [Mg/Fe], see Fig. 4.6 (right). The distribution of SWPs, which peaks at 0.0-1.0 dex, is only slightly more heavily populated for [Mg/Fe] values below solar (52%). In contrast, the stars in the full Hypatia Catalog are strongly towards [Mg/Fe] values above solar (72%), also with a maximum value at 0.0-1.0 dex. The two stellar populations are not from the same parent distribution, given that the KS-test yields a p-value of $5.2 \times 10^{-8}$.

Neves et al. (2009), Bond et al. (2008), Beirão et al. (2005), and Gilli et al. (2006) all found that SWPs have an overabundance of [Mg/H] with respect to stars without planets, where the latter two authors reported a bimodal distribution in relative frequency of [Mg/H] abundances. Due to the widely agreed upon iron enrichment seen in SWPs, the findings of these four
Figure 4.6: Similar to Fig. 4.3 but for [Mg/Fe], plotted with respect to [Fe/H] (left) and relative frequency (right). The majority stars in both the full Hypatia catalog and the known exoplanets have an abundance of [Mg/Fe] between 0.0-1.0 dex. While a higher relative population of stars within all of Hypatia show larger [Mg/Fe] abundances, the known exoplanets have [Fe/H] predominantly above solar, although there are a few outliers.
authors do not necessarily negate the trend reported here, since an increased iron abundance would lower the [Mg/Fe] ratio. The final conclusion from both Neves et al. (2009) and Beirão et al. (2005) was that SWPs follow the same abundance trend in [X/Fe] vs. [Fe/H] as the non-host stars. And while Gonzalez et al. (2001) determined that [Mg/Fe] was generally smaller in SWPs as compared to disk stars, Gonzalez & Laws (2007) found that the [Mg/Fe] ratios were comparable using a combined data set. In general, other studies agree with our findings that there is no magnesium enrichment in stars hosting exoplanets.

Silicon is the element most measured within both the full Hypatia Catalog and the exoplanet host-star subset, totaling 2189 stars and 187 stars, respectively (see Fig. 2.1 and 4.1). The [Si/Fe] trend seen in Fig. 4.7 (left) is similar to the other α-chain elements, however, there is a flattening of [Si/Fe] for [Fe/H] ≥ 0.0 dex. The flattening is most noticeable in the SWPs, whose range in [Si/Fe] is very narrow compared with the other bio-essential elements (right). The majority of the SWPs for which [Si/Fe] was measured are within the range of -1.0–1.0 dex, where the peak of the distribution lies in the sub-solar bin. However, the number of host stars for which [Si/Fe] was measured are evenly distributed about solar. The majority of disk stars, which also exhibit a narrow distribution, lie within 0.0-1.0 dex for [Si/Fe] and have 67% of their population with [Si/Fe] abundances above 0.0 dex. The background stars and the SWPs have a p-value of $1.7 \times 10^{-10}$ via the KS-test, meaning that they do not come from the same original distribution.

The literature for [Si/Fe] abundances in stars with and without planets is polarized. Robinson et al. (2006) find that planet-host stars within the data presented by Valenti & Fischer (2005) are enriched with [Si/Fe].
Figure 4.7: Similar to Fig. 4.3 but for [Si/Fe], plotted with respect to [Fe/H] (left) and relative frequency (right). The majority stars in both the full Hypatia catalog and the known exoplanets have an abundance of 0.0-1.0 dex for [Si/Fe]. While a higher relative population of stars within all of Hypatia show larger [Si/Fe] abundances, the known exoplanets have [Fe/H] predominantly above solar, although there are a few outliers.
Similarly, the study conducted by Brugamyer et al. (2011) found that their SWP population was enriched in [Si/Fe]. Bond et al. (2006) determined that SWPs with $V < 7.5$ exhibited a mean 0.15 dex increase in [Si/Fe] compared to the non-hosts. However, stars with $V > 7.5$ did not show such a large variation: 0.08 dex. Neves et al. (2009) reports an overabundance of [Si/H] in SWPs compared to the disk stars, but no noticeable difference in [Si/Fe]. Finally, Gonzalez et al. (2001), Gonzalez & Laws (2007), Bodaghee et al. (2003), and Fischer & Valenti (2005) did not find significant difference between the populations. Given the narrow distribution in [Si/Fe] for both hosts and non-hosts, along with the average $\pm 0.05$ dex error associated with those abundances, we believe that the results are not as conclusive in this case as with the other bio-essential elements.

Due to weak and/or blended lines in the visible spectrum, only 93 SWPs in the Hypatia Catalog have been measured for [S/Fe]. Like the other $\alpha$-elements, Fig. 4.8 (left) shows a decrease in [S/Fe] with increasing [Fe/H], but with much more scatter in [S/Fe]. Again, the SWPs occupy the low-[S/Fe], high-[Fe/H] region of the plot. The relative frequency histogram (right) depicts a distinct difference in [S/Fe] abundance between host and non-host stars, where the former peaks between -0.2 – -0.1 dex and the latter between 0.0-0.1 dex. This 0.2 dex difference in population abundances is the largest for all the bio-essential elements. The [S/Fe] abundances for the SWPs lie almost predominantly below solar (87%), while the disk stars are roughly symmetric about the peak (57% above solar). A KS-test has determined that the two populations of stars are significantly different, with a p-value of $7.2 \times 10^{-16}$. The studies conducted by both Gonzalez & Laws (2007) and Ecuvillon et al. (2004) did not find any sulfur enrichment in
Figure 4.8: Similar to Fig. 4.3 but for [S/Fe], plotted with respect to [Fe/H] (left) and relative frequency (right). The known exoplanet hosts show a marked difference between the full Hypatia catalog. The make-up the majority of stars with [Fe/H] above solar while their [S/Fe] ratios are below solar, in contrast to the other bio-essential elements.
SWPs, such that the [S/Fe] abundances were indistinguishable between stars with and without planets.

4.1.4 Additional Elements

Figures 4.9-4.11 shows the relative frequency histograms for fifteen elements as [X/Fe] ratios. We wished to analyze those elements prevalent enough to compare our results with literature. The elements shown were measured within a statistically significant number of SWPs found in the Hypatia Catalog, above 33% of the SWP sample or within +70 stars (see Fig. 4.1).

Out of the 15 elements shown, only in four cases did the distributions for SWPs and background stars (“All Hypatia”) peak in different bins. Exoplanet host-stars exhibited a slightly lower abundance in [Ca/Fe] and [Ti/Fe] than the disk stars. The majority of SWPs lie between -0.1–0.0 dex and the disk stars between 0.0-1.0 dex, in both cases (see Fig. 4.9). The SWP distribution in [Ca/Fe] is more towards sub-solar values, with 80% of the stellar abundances below [Ca/Fe] = 0.0 dex. Comparatively, the relative frequency in [Ti/Fe] for SWPs is more symmetric around the solar value, with only 52% above [Ti/Fe] = 0.0 dex. The KS-test p-values were $1.5 \times 10^{-25}$ and $7.9 \times 10^{-5}$, respectively, meaning the stellar populations did not come from the same parent sample for either element. In contrast, the [Mn/Fe] and [Cu/Fe] abundances in SWPs appear more enriched than their non-host counterparts (Figs. 4.10 and 4.11, respectively). The distribution for both elements peak at 0.0-1.0 dex. The distribution in the exoplanet hosts for [Mn/Fe] is relatively symmetric, such that only 54% of stars with [Mn/Fe] abundance measurements have values above 0.0 dex. The [Cu/Fe]
SWP distribution is perfectly symmetric about the peak 0.0–0.1 dex bin, such that there are an equal number of stars on either side of the maximum. In comparison to the non-host stars, the [Mn/Fe] and [Cu/Fe] distributions are significantly different, with KS-test p-values of $1.5 \times 10^{-15}$ and $1.5 \times 10^{-11}$, respectively. These two iron-peak element ratios, in addition to [Fe/H], are the only instances where the exoplanet hosts have significantly higher abundance measurements than the background stars. However, given that the error for [Mn/Fe] and [Cu/Fe] are 0.056 dex and 0.8 dex, respectively, the $\sim 0.1$ dex difference between the two stellar populations falls within error of the abundance measurements.

The background stars and exoplanet hosts have relative frequency histograms that peak in the same range for the remainder of the elements. For the SWPs, the distributions about the solar abundance for [Na/Fe], [Ni/Fe], and [Zn/Fe] are all relatively symmetric, with 58%, 43%, and 55%, respectively, of the total measured stars above solar. The distribution about the respective peaks of [ScII/Fe], [Cr/Fe], and [Co/Fe] are also relatively symmetric, with only 8%, 4%, and 18%, respectively, more stars below the peak as above. The abundances for [CrII/Fe] and [Al/Fe] are more skewed more towards sub-solar values. Both element ratios peak in a bin below solar and the former has 41% more stars lying the below peak while the latter has 80%. Similarly, [Sc/Fe] and [V/Fe] are both skewed to values above solar, where both distributions peak above solar. There are 30% and 90% more stars above the peak than below, respectively. The KS-tests for [Al/Fe], [V/Fe], [Cr/Fe], [CrII/Fe], and [Co/Fe] signified that the two stellar populations were from different parent distributions. The p-values were between 0.03 ([V/Fe]) and $9.6 \times 10^{-9}$ ([Cr/Fe]) in all cases. The remaining
element ratios shown in Figs. 4.9-4.11, namely: \([\text{Na/Fe}]\), \([\text{Sc/Fe}]\), \([\text{ScII/Fe}]\), \([\text{TiII/Fe}]\), \([\text{Ni/Fe}]\), and \([\text{Zn/Fe}]\), did not show significant difference between the SWPs and the non-host, background stars. The p-values in these instances were all greater than 0.05, or below the 95% confidence level.

There have been a number of authors who have measured abundances in exoplanet host-stars other than the bio-essential elements: Beirão et al. (2005); Bodaghee et al. (2003); Bond et al. (2006, 2008); Ecuvillon et al. (2004); Fischer & Valenti (2005); Gilli et al. (2006); Gonzalez et al. (2001); Gonzalez & Laws (2007); Luck & Heiter (2006); Neves et al. (2009); Robinson et al. (2006); Sadakane et al. (2002); Santos et al. (2000); Schuler et al. (2011b); Valenti & Fischer (2005). A review of the literature leads to the general conclusion that \([X/Fe]\) element ratios in SWPs are indistinguishable from non-host, disk stars. A few authors cite a few exceptions to the trend, for example Gonzalez et al. (2001) noted that SWPs had less \([\text{Na/Fe}]\), \([\text{Mg/Fe}]\), and \([\text{Al/Fe}]\) as compared to non-hosts, as did Gilli et al. (2006) and Gonzalez & Laws (2007) in the case of \([\text{Al/Fe}]\). Gilli et al. (2006) also found that planet-hosts had less \([\text{V/Fe}]\). Comparatively, some slight overabundances were also observed in SWPs: Robinson et al. (2006) for \([\text{Ni/Fe}]\), Gilli et al. (2006) with respect to \([\text{Mg/Fe}]\) and \([\text{Co/Fe}]\), and Gonzalez & Laws (2007) for \([\text{Ti/Fe}]\). Bond et al. (2008) found overabundances in planetary hosts for all ten elements measured, the mean difference with non-hosts ranging from 0.05-0.11 dex and the median variation between 0.05-0.16 dex. Similarly, Bond et al. (2006) observed an enrichment in the average SWP population for all elements observed therein. However, their sample was divided into two subgroups, those stars with magnitude in the V-band > 7.5 and V < 7.5.
Our results indicate that exoplanet hosts have identical, if not deficient, abundances for almost all elements with respect to background stars. Of the 22 element ratios that were measured in a statistically significant number of exoplanet host stars, 17 of those abundance ratio distributions were found to be from a different stellar population than the background stars, with a confidence of 97% or above. Out of those 17 [X/Fe] distributions, the SWPs had higher abundances than the non-host stars for only three element ratios, all of them iron-peak or beyond: [Fe/H], [Mn/Fe], and [Cu/Fe]. Our findings are in accordance with the trends noted by other authors using both magnitude- and volume-limited stellar populations.
Figure 4.9: The relative frequency of [X/Fe] ratios for Na, Al, Ca, Sc, ScII, and Ti. These elements were measured in 70 or more known exoplanet hosts and were not shown in Figs. 4.3-4.8. In all but four cases, the majority of stars in both sets of stars peaked in the same [X/Fe] bin (see text).
Figure 4.10: The relative frequency of [X/Fe] ratios for TiII, V, Cr, CrII, Mn, and Co. These elements were measured in 70 or more known exoplanet hosts and were not shown in Figs. 4.3-4.8. In all but four cases, the majority of stars in both sets of stars peaked in the same [X/Fe] bin (see text).
Figure 4.11: The relative frequency of [X/Fe] ratios for Ni, Cu, and Zn. These elements were measured in 70 or more known exoplanet hosts and were not shown in Figs. 4.3-4.8. In all but four cases, the majority of stars in both sets of stars peaked in the same [X/Fe] bin (see text).
4.2 Abundances With Respect to Stellar and Planetary Properties

The underlying cause for the enrichment of exoplanet host-stars in iron, if nothing else, is not well understood. While there are a number of theories as to the source of the compositional anomalies, such as self-enrichment, migration, or a primordial influence, these theories are still under debate (see §4.3). By analyzing the properties common to the verified exoplanets and their host-stars, more information may be gleaned that may help the understanding of exoplanets, their formation, and their relationship to their host-star.

We analyze the bio-essential elements with respect to a number of stellar (mass, \(\text{B–V}\), \(V\) magnitude, \(\log(g)\), \(T_{\text{eff}}\), rotational velocity) and planetary (mass, eccentricity, semi-major axis, multiple/single systems, orbital period) properties. The rotational velocity of the star is given by: \(V \sin(i)\), with \(i\) as the inclination of the star’s axis. Similarly, planetary mass is defined using the lower-bound estimate: \(M_p \sin(i)\) where \(i\) is the angle of inclination of the planet’s orbit relative to Earth. We find there are a number of properties that measure the same (\(\Rightarrow\)) or similar characteristics (\(\sim\)), such as: stellar mass \(\Rightarrow\) \(B – V\) \(\Rightarrow\) \(T_{\text{eff}}\), orbital period \(\Rightarrow\) semi-major axis (or SMA), and \(T_{\text{eff}} \sim \log(g)\). However, our aim is to analyze the multiple stellar and planetary properties with respect to the stellar abundances and compare our results with those seen in the literature (see §4.2.3). And since the correlations are not precise, we chose to retain stellar mass, \(B – V\), period, SMA, and \(\log(g)\) as separate parameters.

There are a number of standard parameter plots present within the exoplanet field. In order to verify and expound upon the trends found by
other authors, it would be extraordinarily redundant to visualize those
parameters with respect to every element. Therefore, the elemental
abundances within SWPs are presented in two ways: as an average between
the bio-essential elements measured within a host-star and as individual
element ratios, $[\text{X}/\text{Fe}]$ for a few elements. We average the abundances by
taking the unlogged sum of the bio-essential elements measured within a
star, dividing by the total number of those elements (which varies on a
star-by-star basis, with a maximum of 6), and then re-logging the average.
Mathematically, for a star with C, O, and Si abundances, this appears as:

$$\text{Avg. } [\text{X}/\text{Fe}] = \log \left[ \frac{10^{(\text{C}/\text{Fe})} + 10^{(\text{O}/\text{Fe})} + 10^{(\text{Si}/\text{Fe})}}{3} \right].$$

(4.1)

So as not to lose any information, we also present some of the stellar and
planetary physical properties with respect to abundance ratios for a few
elements that are “representative” of common nucleosynthetic origins (see
§3). We analyze the $[\text{X}/\text{Fe}]$ ratios for Si ($\alpha$-element), Ni (iron-group
element), and Na (odd-Z element) in §4.2.2. In the case of planetary mass,
we also chose to present the data on different scales between plots.

4.2.1 Averaged Bio-Essential Abundances with Physical Properties

Fig. 4.12 shows the average bio-essential element abundances with
respect to $[\text{Fe}/\text{H}]$. The stars are color coded to designate approximate
planetary mass, where red is indicative of exoplanet masses greater than 1.0
$\text{M}_J$, purple is for masses smaller than 0.1 $\text{M}_J$, and yellow is in between. In
the case of multiple planets within one system, the most massive planet was
used. The stars indicated by purple are highlighted in this plot because their
exoplanet’s mass is on the order of Neptune, or 0.054 $\text{M}_J$. The average mass
of these low-mass planets is 0.045 $M_J$, where the lowest mass exoplanet is 0.01 $M_J \approx 3.2 M_\oplus$, of which there are three. The stars hosting the low mass planets predominantly occupy the region of the figure with higher, super-solar average bio-essential abundances, but relatively lower, sub-solar $[\text{Fe/H}]$ ratios. This is, in general, opposite to the trend seen for the majority of SWPs, which exhibit high $[\text{Fe/H}]$ and low bio-essential abundances, as was seen in Figs. 4.3–4.8. However, more abundance measurements for stars hosting single, low-mass planets are needed to confirm this trend more reliably. A fuller range of planetary masses is more thoroughly examined in §4.2.2.

Stellar color, via $B-V$, versus planetary mass is illustrated in Fig. 4.13, where the most massive planet was used for multi-planet systems. The average abundances of all bio-essential elements measured within the host-star were binned, such that higher abundances, above 0.5 dex, are shown in green and lower abundances, below -0.5 dex, in blue. Stars with average abundances between 0.5 dex and -0.5 dex are in orange. The planetary orbit eccentricity corresponds to the ellipticity of the symbols, such that planets with circular symbols have nearly circular orbits and ellipsoidal symbols are for highly eccentric orbits. There is no obvious trend with eccentricity and stellar color or planet mass.

Stellar mass, in units of $M_\odot$, versus planetary orbital period, measured in Earth days, for the known SWPs is shown in Fig. 4.14 (left). The averaged bio-essential abundances are shown in color, similar to Fig. 4.13, where red designates high abundance ratios, purple is centered on solar, and blue for low abundances. Systems with only one planet orbiting the host-star are shown using the • symbol, whereas multi-planet systems are
Figure 4.12: The average abundance of all bio-essential elements within a host-star as a function of [Fe/H]. The colors depict the mass of the exoplanet (in the case of multiple planets within one system, the most massive planet was used), where purple highlights smaller-mass planets where $M < 0.1 \, M_J$. While the majority of exoplanet host-stars have a lower average abundance and higher [Fe/H] ratio, those with smaller planets show a somewhat opposite trend.

given by the $\times$ symbol. Stars with masses less than $1.0 \, M_\odot$ show a prevalence for a higher averaged abundance of the bio-essential elements, as confirmed in Fig. 4.12. They also seem to be correlated with single planet systems. The largest planet in multiple-planet systems have orbital periods predominantly longer than 100 days. Only 9% of the larger planets have an orbital period shorter than 100 days. We note, also, the lack of systems that have been observed with a large stellar mass ($> 1.4 \, M_\odot$) and small planetary period (< 100 days). While this trend may be an observational bias, we discuss it more with respect to the literature in §4.2.3.
Figure 4.13: Exoplanet mass (in the case of multiple planets within one system, the most massive planet was used) with respect to stellar color, B-V. The average abundances were binned (see figure legend) and shown with respect to color. The orbit eccentricity is demarcated by the shape of the points, where a more elliptic point corresponds to a more eccentric orbit and a circle point, a more circular orbit.

Figure 4.14 (right) show the planetary SMA (AU) with respect to the stellar log(g). Similar to Fig. 4.13, the averages abundances within the SWPs are binned and color-coded, such that higher average abundances are in green, near-solar abundances are in orange, and lower, sub-solar average abundances are in gray. The \( \times \) symbol designates a \( V_{mag} < 7.5 \) for the host-star, and the \( \bullet \) corresponds to \( V_{mag} > 7.5 \), similar to the cutoffs used in Bond et al. (2006). Due to the sensitivity of the stellar models on both \( T_{eff} \) and \( \log(g) \), it is expected that the majority of SWPs have similar
Figure 4.14: Variation of the average bio-essential element abundance (in color, see figure legends) with stellar and planetary characteristics. On the left, the logged planetary period with respect to stellar mass, where the circles denote a single planetary system, the x’s designate that there is more than one planet around the host-star. On the right, logged planetary semi-major axis versus log($g$) where the circles show those stars with rotational velocity greater than 3 km/s, diamonds have rotational velocity less than 2 km/s, and x’s are in between.
log(g) values that lie within a narrow range, or between 4.0-4.5. The SMA is greater than 1 AU for the majority of SWPs, which corresponds to having a larger orbital period, shown on the left. Stars with $V_{\text{mag}}$ below 7.5 are also correlated to these larger SMAs. The average abundances for the bio-essential elements seem homogeneous with respect to both stellar log(g) and the SMA of the orbiting planet. A gap similar to the one in Fig. 4.14 (left) is also observed.

Looking more closely at stellar abundances with respect to $V_{\text{mag}}$, we wish to examine the SWPs with respect to the full Hypatia Catalog. We exclude, of course, the exoplanet hosts within Hypatia and those stars for which no bio-essential elements have been measured. The mean and the median of the average bio-essential abundance within stars with $V_{\text{mag}} > 7.5$ is 0.07 dex and 0.02 dex, respectively. Similarly, for stars with $V_{\text{mag}} < 7.5$: 0.06 dex and 0.03 dex, respectively. Comparatively for the exoplanet host stars with $V_{\text{mag}} > 7.5$, the mean and median average abundance is -0.02 dex for both. Exoplanet hosts with $V_{\text{mag}} < 7.5$ give a mean and median of 0.01 dex and -0.02 dex, respectively. While we do not find that disk stars exhibit higher average bio-essential abundance ratios as a function of $V_{\text{mag}}$, as observed in Bond et al. (2006), we do note that the discrepancies found by the authors between the two populations of stars were not significant to negate our results (Bond et al., 2010).

4.2.2 Representative Abundances with Physical Properties

We now analyze a few individual element abundances, as opposed to the average of the bio-essential elements, with respect to the stellar and planetary properties. We have chosen three elements that are representative
of specific nucleosynthetic origins, namely Si (α-element), Ni (iron-group element), and Na (odd-Z element). See §3 for more discussion of these elements.

Fig. 4.15 shows $[\text{Si}/\text{Fe}]$ with respect to stellar mass ($M_\odot$) on the left. The coloring denotes B–V stellar color, where $B–V > 0.8$ is red, $B–V < 0.65$ is blue, and purple lies between. As mentioned before, while stellar color tracks stellar mass such that bigger stars are bluer, it is not a perfect correlation. There are some larger stars, with masses above $1.4 M_\odot$, that are more red and purple in color. Additionally, the majority of SWPs for which $[\text{Si}/\text{Fe}]$ has been measured have $[\text{Si}/\text{Fe}] > -0.1$ dex; all blue SWPs are above $-0.1$ dex. The symbols represent the varying rotational velocities, $v$, of the star, where $\bullet$ refers to those stars with $v \leq 3$ km/s and $\times$ is for stars rotating at speeds greater than 3 km/s. Smaller SWPs with $M < 1.2 M_\odot$ have velocities above 3 km/s. Also, slower rotating SWPs have determinations of $[\text{Si}/\text{Fe}] > -0.1$ dex.

The right plot in Fig. 4.15 shows $[\text{Si}/\text{Fe}]$ versus planetary mass ($M_J$), where the most massive planet was used in the instance of multiple planets in one stellar system. Note that the planetary mass scale incorporates some of the larger-mass planets, as compared to Fig. 4.14. The eccentricity of the planetary orbit is placed into three bins and denoted by color, where high eccentric orbits with $e > 0.3$ are green, more spherical orbits with $e < 0.15$ are purple, and those in between are orange. Planets with high eccentricity show slightly lower $[\text{Si}/\text{Fe}]$ abundances in the host star, such that few stars are above 0.1 dex in comparison to the other eccentricity bins. Overall, more massive planets have higher eccentricity orbits and $[\text{Si}/\text{Fe}]$ near solar. The $\bullet$ symbol is representative of those planets with orbital periods greater than or
Figure 4.15: Dependence of star mass and planet mass on [Si/Fe]. On the left, the x-axis is stellar mass, colors denote stellar color, and the shapes show rotational velocity. On the right, the x-axis is planet mass (similar to Fig. 4.14 but on a different scale), shapes give orbital period, and the size of the shapes distinguish between single and multi-planetary systems.
equal to 300 days, and × shows those planets with periods less than 300
days. The majority of exoplanets with \( M < 1.5 \, M_J \) also have orbital periods
less than 300 days; the larger periods are predominantly associated with
larger mass planets. Finally, the size of the symbol is indicative of number of
planets orbiting the star, where a small symbol is for a single planet and a
large symbol means a multiple-planet system. Multi-planet systems mostly
occur when the more massive planet has a mass less than 4.0 \( M_J \) and the
stellar host [Si/Fe] abundance lies between -0.1–0.25 dex.

Similar to silicon, Fig. 4.16 gives the [Ni/Fe] abundance with respect
to stellar mass (\( M_\odot \)) on the left and planetary mass (\( M_J \)) on the right. The
majority of SWPs exhibit abundance ratios for the iron-group element within
-0.1–0.1 dex, similar to the \( \alpha \)-element silicon. In this case, the slower, bluer
stars are not wholly above -0.1 dex (see left) and a few faster rotating stars
are below -0.2 dex. To the right, higher mass planets in the multiplanet
systems tend to have periods greater than 300 days and [Ni/Fe] abundances
centered around 0.0 dex. Of the 17 planets that do not have [Ni/Fe] within
-0.1–0.1, 13 of them have periods greater than 300 days. Multi-planet
systems have host stars with [Ni/Fe] abundances closely centered on solar (> 0.01 dex).

The [Na/Fe] abundances measured within the SWPs show a much
broader scatter than for either the silicon or nickel ratios, spanning
-0.35–0.35 dex, shown in Fig. 4.17. The majority of SWPs with [Na/Fe]
abundances lie within -0.2–0.2 dex, including all but one of the bluer, slower
rotating stars (see left). Only the SWPs with \( v > 3 \, \text{km/s} \) span the entire
abundance range. On the right, planets with higher eccentric orbits are more
scattered with respect to [Na/Fe] than the other two representative element
Figure 4.16: Similar to Fig. 4.15 but for [Ni/Fe]. On the left, the slower, bluer stars exhibit slightly more scatter in [Ni/Fe] as compared to [Si/Fe]. On the right, the host-stars of multi-planet systems exhibit [Ni/Fe] abundances centered on 0.0 dex.
Figure 4.17: Similar to Fig. 4.15 but for [Na/Fe]. Stars for which sodium has been measured show a much larger scatter in [Na/Fe] than the other two elements discussed, such that the majority of SWPs lie within -0.2–0.2 dex, including the slower, blue stars. The right shows that multiple-planet systems within -0.1–0.3 dex.
ratios. The higher mass planets in the multiple-planet systems have predominantly longer periods. Also, planets with higher mass have, for the most part, stellar host [Na/Fe] abundances near solar. The multi-planet systems show [Na/Fe] abundances above 0.01 dex.

4.2.3 Comparison to Literature

There have been a number of authors who have analyzed the physical and chemical characteristics of exoplanets and their host stars, oftentimes within a specific volume- or magnitude-limited survey. Given that Hypatia is not such a “well-defined” survey, we wish to analyze the trends noted in §4.2.1 and §4.2.2 with respect to the literature.

The SWP enrichment in [Fe/H] has been confirmed and reconfirmed by a number of studies (see §4.1.1). However, the analysis of additional elements is still relatively tentative due to the admittedly difficult task of comparing catalogs with different stellar parameters, line-lists, stellar models, etc. and the errors associated with the catalogs (e.g. §2 ; Bond et al., 2006; Ramírez et al., 2009). Despite typical error with [X/Fe] abundances having a lower bound of 0.05 dex (Asplund, 2005), overarching trends in the chemical make-up of SWPs are apparent. For example, Santos et al. (2003) observed that metal-poor stars are not as likely to host high-mass exoplanets. And, as shown here, stars hosting giant planets exhibit similar chemical abundances as background, disk stars.

The majority of exoplanets discovered are giant planets, $M \gtrsim M_J$, where only 9% have Neptune-masses (0.054 $M_J$) or below. While this is largely due to observational bias, Udry & Santos (2007) and Sousa et al. (2011) observed a bimodal distribution present in the relative frequency of
planetary masses, centered on both Jovian and Neptunian masses. However, the smaller-mass planets do not exhibit the same metallicity enhancement within their hosts as the Jovians (e.g. Udry et al., 2006; Ghezzi et al., 2010b). This is also shown in Fig. 4.12, where 7% of the exoplanets shown have Neptune-masses or below.

Fischer & Valenti (2005) also showed that higher metallicity is correlated with total planet mass, which may be explained by theoretical models of planet formation and evolution (e.g. Lin & Ida, 2004; Mordasini et al., 2009). It was for this reason that we chose to use the highest mass planet in multiple-planet systems in our analysis. We found that multi-planet systems have [Si/Fe], [Ni/Fe], and [Na/Fe] abundances larger than single-planet systems, with abundance ratios consistently above 0.1 dex, shown in Figs. 4.15-4.17. A similar trend is also shown in Fig. 4.14 where stars with a higher average abundance of the bio-essential elements were more likely to host multi-planet systems. We will discuss further implications of high planet mass and metallicity in §4.3 and §4.4.

The eccentricity of the known exoplanets spans the full 0.0-1.0 range, making the physical cause behind planetary eccentricity an enigma. While Udry & Santos (2007) outlined some possible explanations for the eccentricities observed, their own analysis found only a variety of “small differences” between populations at different eccentricities that suggest potentially different origins. Marcy et al. (2005) showed that, despite larger inertial resistance needed to move massive exoplanets, most of the larger planets exhibit an eccentricity greater than the smaller exoplanets. Our analysis in Fig. 4.13 did not cover the full range of planet mass and,
therefore, we did not observe this discrepancy. Also, like Fischer & Valenti (2005), we did not find any correlation between metallicity and eccentricity.

Stars hosting exoplanets show a relatively bimodal distribution in period/SMA, as mentioned in both Udry & Santos (2007) and Marcy et al. (2005). A large number of exoplanets have periods less than \( \sim 5 \) days or greater than \( \sim 100 \) days, also shown in Fig. 4.14. There remains a gap in the distribution of orbital periods with respect to stellar mass such that no high stellar mass \(( > 1.4 \, M_\odot )\), short planetary period \(( < 100 \) days\) systems have been observed. In fact, Valenti & Fischer (2008) shows that half of the SWPs seen at that time had SMAs above 0.96 AU. Gonzalez (1998b); Queloz et al. (2000); Santos et al. (2006a, 2003) and Sozzetti (2004) all found that there were no planets with \( P \leq 5 \) days where the host star exhibited \([Fe/H] < 0\); meaning planets close to their host star (short periods and small SMAs) are more likely to be found around a metal-rich star. While similarly noted in Fig. 4.14 that planets with longer periods and SMAs have host-stars with a lower averaged bio-essential abundance, Fischer & Valenti (2005) did not find any correlation between metallicity and orbital period.

In Fig. 4.14 (left) we show that SWPs with masses below solar are more enriched in the averaged bio-essential abundances than more massive stars. This trend was also observed by Ghezzi et al. (2010a) who analyzed dwarf, subgiant, and giant SWPs with respect to metallicity. They observed that dwarfs and subgiants were more metal rich, with metallicity of 0.11 dex on average, while giants were more metal poor, averaging -0.06 dex. da Silva et al. (2011) also showed that dwarfs and subgiants were more enriched in \([C/Fe]\) than giants. Fischer & Valenti (2005) did observe a correlation between stellar mass, metallicity, and planet occurrence, however they
ultimately concluded that metallicity was more likely to affect planetary formation than stellar mass. Johnson et al. (2010) also confirm that planet occurrence increased with stellar mass. With respect to Figs. 4.15-4.17, higher-mass stars tend to have the respective [X/Fe] abundances near solar, while the lower mass stars exhibit more of a scatter, both above and below solar.

Since Barnes (2001) investigated the rotational velocities of SWPs, where there was no wholly conclusive difference between ~ 50 known host-stars and non-host stars, many new exoplanets have been discovered. Gonzalez (2011) and Gonzalez et al. (2010) have both carefully investigated the rotational velocity of SWPs, correcting for a number of biases that might have skewed the data. Their overwhelming conclusion is that planet-hosting stars have a much slower rotational velocity compared to non-hosting disk stars. We have found, shown in Figs. 4.15-4.17, that slower rotating SWPs tend to have higher abundances in [Si/Fe], [Ni/Fe], and [Na/Fe]. Alves et al. (2010) did not find any trend between rotational velocity and metallicity.

A higher log(g) corresponds to higher average abundances, see Fig. 4.14. Ghezzi et al. (2010b) did not find a difference in log(g) between SWPs and their control sample. Similarly, Ghezzi et al. (2010a) also looked at log(g) with respect to giant and subgiant stars. Despite finding that subgiants tended to occupy a much smaller range in log(g) than giants, they found no discrepancy between stars with and without planets in the two subgroups. Fischer & Valenti (2005) found no trend in T\textsubscript{eff}, which roughly corresponds to log(g), with respect to metallicity for their entire sample of main sequence stars or for their subgiant population. However, they did note the potential for large errors in log(g), given that it is coupled with the
T_{\text{eff}}$ determination, which may also explain the asymmetry between the left and right plots in Fig. 4.14.

Gonzalez (1997) hypothesized that enrichment would be the most evident in warmer, bluer dwarf stars. Gonzalez (2003) later determined that the number of SWPs increases with higher T_{\text{eff}}, or color, although they did not find the trend significant. Neither Luck & Heiter (2006) nor Valenti & Fischer (2008) found a trend in temperature/color with [O/Fe] and [C/Fe] or [Fe/H], respectively. Comparable to studies for log(g), Ghezzi et al. (2010b) and Ghezzi et al. (2010a) also did not find an obvious discrepancy between disk stars, SWPs, subgiants, or giants. From the data shown in Figs. 4.13, 4.15-4.17, we also did not see a trend in color with respect to metallicity. The only point of interest was that color did not always correlate with stellar mass and that bluer SWPs have higher abundances in [Si/Fe], [Ni/Fe], and [Na/Fe].

### 4.3 Stellar Compositional Implications

There are currently two main theories to explain the compositional anomalies and physical trends seen in SWPs. The first proposes that metal-rich material, such as comets, asteroids, and planets, has been accreted onto a star, altering the composition of the outer convective envelope. This method of self-enrichment was first discussed by Gonzalez (1997) and may be verified by looking for a trend in metallicity with respect to the convective zone mass or condensation temperature, as well as atypical lithium abundances (Gonzalez, 2003, 2006). A few studies on the convective zone mass have been conducted which showed positive evidence for the self-enrichment theory (e.g. Laws et al., 2003; Chambers, 2010; Ramírez
et al., 2011), while others were not in favor (e.g. Johnson et al., 2010).
Similarly ambiguous results have been found for condensation temperature as well, where enrichment in refractory (as opposed to volatile) elements is expected due to the evaporation of the lighter elements upon infall before accretion (Ramírez et al., 2011; Gonzalez, 2011; Schuler et al., 2011a,b; Hernández et al., 2010; Santos et al., 2006b; Sadakane et al., 2002; Takeda et al., 2001; Udry & Santos, 2007).
Self-enrichment may also be related to the possible causality between host metallicity and short planetary orbital periods (< 6 days), or shorter SMAs (Sozzetti, 2004). The migration scenario originally presented by Lin et al. (1996) may explain the few observed “hot Jupiters,” but the majority of planets that orbit close to their host star have smaller sub-Jupiter masses, see Figs. 4.15-4.17. As discussed in the review by Udry & Santos (2007, and references therein), planet migration might actually account for the dearth of high mass, short orbit stars due to partial or total accretion of mass from the giant planet onto the host star. But given that the current detection of exoplanets is biased towards those planets with close orbits, and the lack of understanding regarding multi-planet systems in this regime, it’s difficult to determine a conclusive origin of the orbital-period bias.

The second theory for host metallicity enhancement suggests that the initial star formation clouds were enriched and that the consequential higher density of metal-rich material in the protoplanetary disk later formed giant planet cores (Gonzalez, 1998a,b). The lack of evidence for self-enrichment, meaning metallicity trends as a function of convective zone mass or condensation temperature, tends to confirm the primordial hypothesis. However, the theory is also bolstered by its prediction that the number of
giant planets should increase with metallicity. While not wholly conclusive, this second theory is the preferred explanation for the enrichment seen in SWPs, cited by both literature reviews (Gonzalez, 2006, 2003; Santos et al., 2006a; Udry & Santos, 2007) and recent studies (da Silva et al., 2011; Garaud, 2011; Sousa et al., 2011).

From the histograms seen in Figs. 4.2-4.11, we find that there is no clear enrichment in the volatile or refractory elements for the SWPs any more than for the stars in the full Hypatia Catalog. If mass was accreted onto the star, we would expect to see some enrichment in the refractory elements since they would not have evaporated. Taking into account refractory settling times, the convection zones in cooler solar-type stars are deeper than hotter, more massive stars (Klein et al., 2011, and references therein). While the settling time for refractory elements are shorter than the lighter elements, the abundance variations for the heavier elements should only vary by $\sim 10\%$ below the convective zone and therefore have no affect on the spectroscopic observations (Vauclair, 1998). While there were three iron-peak or beyond elements that were enriched in the exoplanet hosts, the differences seen between the two populations for $[\text{Mn/Fe}]$ and $[\text{Cu/Fe}]$ are not strong and are within error of the data. In addition, this enrichment was not consistent for any of the other refractory elements, such as $[\text{V/Fe}]$, $[\text{Co/Fe}]$, or $[\text{Ni/Fe}]$.

We have undertaken a similar analysis of our data as Murray & Chaboyer (2002). Fig. 4.18 (left) gives the color-magnitude diagram for the full Hypatia Catalog in white with the known exoplanets overlayed in orange. The SWP population does not appear to be skewed with respect to the full catalog. To the right, we have binned the stellar masses of both stellar groups by $0.1 \, M_\odot$ and plotted the average $[\text{Fe/H}]$ metallicity within that bin.
Figure 4.18: On the left, the color magnitude diagram for the Hypatia Catalog and the known SWPs. On the right, the average \([\text{Fe/H}]\) per 0.1 \(M_{\odot}\) bin, as per Murray & Chaboyer (2002).
Similar to Murray & Chaboyer (2002), we have excluded those stars for which $B-V < 0.46$, which should not affect stars with $M < 1.1 M_\odot$ and does not affect any of the SWPs. Given the stellar range of the full Hypatia Catalog, we have also cut stars with $[\text{Fe/H}] < -0.5$ dex, leaving a total of 2288 stars in the catalog. The errorbars mimic those given by Murray & Chaboyer (2002): variance divided by the square root of number of stars within the bin minus one. According to Murray & Chaboyer (2002) and the models they produced, the steep increase of metallicity with stellar mass for the SWPs, not observed for the disk stars, suggests that iron-rich material must have been accreted onto the stellar-hosts once they were on the main sequence. Johnson et al. (2010) have done a similar test and argue against convective envelope enrichment. The positive correlation between stellar mass and metallicity was also observed with the Valenti & Fischer (2005) data, conducted by Gonzalez (2006) (see their Fig. 1).

To take advantage of the various elements within the Hypatia Catalog, we have also plotted stellar mass with respect to different abundance ratios, namely $[\text{Si/Fe}]$ (pink), $[\text{Ni/Fe}]$ (orange), and $[\text{Na/Fe}]$ (gray) in Fig. 4.19. We have chosen these elements because they are a part of the $\alpha$-group, iron-peak group, and odd-Z elements, respectively, and therefore representative of each nucleosynthetic process. Similar to Fig. 4.18, we have excluded the stars for which $B-V < 0.46$ and $[\text{X/Fe}] < -1.0$. The error for both sets of stars (full Hypatia Catalog and the exoplanet hosts) is equivalent to the oscillation seen in the respective lines. Unlike the plot for $[\text{Fe/H}]$ with stellar mass, there is no clear distinction between the SWPs and the disk stars, not even for $[\text{Ni/Fe}]$. As was mentioned in §4.1.4, a KS-test for the $[\text{Ni/Fe}]$ abundances found that the two stellar populations were not
significantly different. According to the discussion in Murray & Chaboyer (2002), an enhancement in $\alpha$-process elements, possibly also the iron-group, would signify the accretion of a giant planet. On the other hand, enrichment in only iron-like elements, and not $\alpha$-process elements, could be due to asteroids and terrestrial planets. While we do note enrichment in three iron-peak or beyond elements, $[\text{Fe/H}]$, $[\text{Mn/Fe}]$, and $[\text{Cu/Fe}]$, this result is not consistent for other iron-group elements such as $[\text{V/Fe}]$ or $[\text{Ni/Fe}]$. Therefore, we hesitate before making any conclusions.

From Fig. 4.14 (right), and to a lesser extent Figs. 4.15-4.17 (right), there does not appear to be a strong, consistent correlation between the
planet’s SMA and host’s metallicity. Therefore, to better clarify our results, we plotted the metallicity with respect to SMA, per Rice & Armitage (2005), shown in Fig. 4.20. To the left, we have plotted [Fe/H] with SMA for the exoplanet host stars, where the vertical dashed lines show the various SMA distances. While Fig. 4.20 (left) mimics their Fig. 6, we have the benefit of including all of the exoplanets discovered since Rice & Armitage (2005). The interesting feature of our figure is that it very strongly resembles the shape given in their Fig. 1, where they show an “idealized model” of the effect of orbital migration and core formation on exoplanets. Exoplanets within a region of the gas disk that exhibits metallicity above a critical value will attain runaway accretion, while those below the critical metallicity could form close-orbit super-Earths. By assuming that metallicity increases linearly with SMA, they argued that stellar metallicity was the controlling factor for planetary formation, orbit, and timescale. Given trend seen in Fig. 4.20, our results concur.

On the right of Fig. 4.20, we show [Si/Fe] (pink circles), [Ni/Fe] (orange triangles), and [Na/Fe] (×’s) with respect to SMA. Unlike the [Fe/H] counterplot, there does not appear to be upside-down triangle feature, predicted by Rice & Armitage (2005), despite the inclusion of the iron-peak element ratio [Ni/Fe]. The three elements plotted on the right do not mimic the trend seen similarly for [Fe/H], just like Fig. 4.19.

There are overall trends seen in [Fe/H] with respect to the physical parameters of both exoplanets and their host stars. While these trends are tentatively seen in [Mn/Fe] and [Cu/Fe], they are not duplicated when analyzing the abundance ratios for the majority of the elements. There is very strong evidence that stellar metallicity affects the presence of planets, as
Figure 4.20: [Fe/H] with respect to SMA for all SWPs on the left. To the right, a similar plot but for [Si/Fe] (pink circles), [Ni/Fe] (orange triangles), and [Na/Fe] (×’s). These figures were created to compare with the work done by Rice & Armitage (2005), their Figs. 1 and 6, respectively.
well as their possible migration, but the degree of that relationship is unclear given the lack of trends in other elements. The strengths and weaknesses for the presented trends have been argued by many authors in the literature, but none have had the extensive abundance data that we present, which must be taken into account when reaching a conclusion. We have found evidence that supports both stellar composition theories, but not in a fully conclusive way. Additional element measurements for SWPs with reduced errorbars, which could be achieved by studies conducted using systematically similar techniques, are needed in order to better understand the chemical effect on stars by their exoplanets. Therefore, we leave it to further analysis before we are able to assert self-enrichment or primordial enrichment as the explanation for compositional anomalies seen in exoplanet host stars.

4.4 Planetary Formation Implications

Since high metallicity may affect the formation and evolution of terrestrial exoplanets, especially given the potential for short-period giants to produce instabilities in the orbits, we wanted to understand our data with respect to the current planetary formation theories. One theory suggests that planetesimals in the protoplanetary disk collided to form a core of $\sim 10-15 \, M_{\oplus}$, at which point solar nebula gas would then be rapidly accreted onto the core to form a giant planet (Pollack et al., 1996). The second theory postulates that the solar nebula gas was broken up into over-dense regions of dust and gas via gravitational instability, at which point they would collapse to form giant planets (Boss, 1997).

The core accretion model has potential issues, since the time it may take to form a $10 \, M_{\oplus}$ core is on the order of $10^6$ years, which is longer than
the lifetime of a solar-type protostellar disk (Pollack et al., 1996). However, these issues may be resolved with the inclusion of migration and disk evolution into the models (e.g. Alibert et al., 2004). While the gravitational disk instability theory forms giant planets on shorter timescales, it is not dependent on the metallicity of the host-star. It predicts that stars with metallicities lower by a factor of 10, compared to the standard disk model, should also harbor planets (Boss, 2002). The core accretion model, on the other hand, is inherently dependent on the metallicity of the host-star and protostellar disk, since the higher the metallicity, the higher the grain content of the disk, and the easier it is to amalgamate large cores before the nebula gas dissipates (Ida & Lin, 2004).

Since the main observational trend when examining SWPs is that the number of known exoplanets increases with metallicity, it is imperative that this result be replicated in a model. Ida & Lin (2004), for example, assuming that the stellar hosts were primordially enriched and using the core accretion model, were able to reproduce the metallicity trend seen in exoplanet host stars. They also simulated the core masses within the gas giants of the Solar System. While the mass of protoplanetary disks, planetary dependence on stellar mass, gas-to-dust ratio with respect to metallicity, and the timescale of disk reduction for various metallicities is not precisely observed and understood (Udry & Santos, 2007), these are very promising results given the two assumed theories were primordial enrichment and core accretion.

Some studies have proposed that orbiting planets preferentially deplete the solar nebula of refractory elements during core accretion, leaving the host-star’s photosphere diminished with respect to those elements (e.g. Meléndez et al., 2009; Ramírez et al., 2009; Chambers, 2010). Meléndez et al.
have also analyzed the Sun with respect to solar analog twins and found that the Sun is unusual (although not unique) with respect to similar neighborhood stars. According to their study, the Sun is enriched in the lighter elements by an average 0.04 dex, save aluminum, and shows average-to-low abundances for the heavier elements (see their Fig. 2).

However, observations typically measure elements with respect to iron and the Sun, \([X/Fe]\), see §1. Therefore, for volatile elements within an iron-enriched SWP that have not been potentially accreted by the exoplanet, we might expect to see near-solar \([X/Fe]\) volatile abundances. If the stellar host was stripped of it’s refractory elements by an exoplanet, we would expect to see low, sub-solar \([X/Fe]\) abundances for the refractory elements.

We do find some differences between the volatile and the refractory elements found within SWPs and the full Hypatia Catalog, but those differentiations are not consistent and are within error of the abundance measurements. We also admit that we do not have the abundance accuracy of Meléndez et al. (2009), \(\sim 0.01\) dex accuracy. Their analysis showed a promising discrepancy between the abundances for stars with and without planets in their sample of 21 host and non-host stars.

We have shown the strong dependency of planetary occurrence on stellar metallicity with our data. Not only are SWPs consistently enriched in iron, but multiple-planet systems exhibit higher abundances in all three representative elements. This lends more evidence to the core accretion model of planetary formation. However, we cannot conclusively confirm the extent of the accretion, due to the lack of enrichment in other elements. We found that, on average, the bio-essential elements decrease with increasing \([Fe/H]\) abundance. The lower-mass stars \(< 0.1 \text{M}_J\) exhibit higher average
bio-essential element abundances and lower \([Fe/H]\) ratios. While we are not able to conclusively predict the presence of one or more exoplanets given the depletion in certain stellar abundances, the accumulation of abundance determinations for stars in the solar neighborhood point us in the right direction. We anticipate that additional large, standardized analyses of SWPs with respect to multiple elements, similar to Meléndez et al. (2009) and the work shown here, will greatly help to understand the mechanism by which planets are formed.
APPLICATION TO POTENTIALLY HABITABLE STELLAR SYSTEMS

As was briefly discussed in §4, there are several ways in which the structure, atmosphere, and overall habitability of an orbiting exoplanet might be limited by the characteristics of the host star. The mass of the host star determines, for example, the lifetime of the stellar system and the extent of the habitable zone, both of which are dependent on temperature (Kasting et al., 1993; Kane & Gelino, 2012). The surface abundances of the host-star are also likely related to the chemical abundances available within an exoplanet (Bond et al., 2010; Delgado Mena et al., 2010; Petigura & Marcy, 2011). Turnbull & Tarter (2003a) used the Hipparcos Catalogue along with data on age, variability, metallicity, Galactic kinematics, multiplicity and known giant planets to compile the Catalog of Potentially Habitable Stellar Systems (or HabCat). Their catalog includes stars whose physical characteristics are consistent with the existence of terrestrial planets in a stable habitable zone throughout the last 3 billion years. Evolved stars and massive stars whose main sequence lifetimes are less than 3 billion years were ruled out; this resulted in large set of low-mass, main sequence stars of late F, G, K, and M-types. Stars with measured variability greater than five times that of the Sun were excluded; chromospheric variability and X-ray emissions were used to take out very young stars. Double- or multiple-star systems were removed if their separations or orbital data indicated that planet orbits would not be stable within the habitable zone. Stellar metallicity, a potential indicator for the presence of planets (Reid, 2002), was
used to cut stars with \([\text{Fe/H}] < -0.4\). However, the lower \([\text{Fe/H}]\) limit below which no planets can be formed is still not fully understood (Sozzetti et al., 2009; Santos et al., 2011). After applying these habitability criteria to the Hipparcos Catalogue, the resulting HabCat contains 17,129 stars.

The habitability of a planet is based upon both the physical and chemical environment of that planet. By using HabCat in conjunction with the Hypatia Catalog, we have tried to place reasonable limits on the physical properties of the stellar systems we are analyzing that are conducive to terrestrial biogeochemistry. However, we caution that stellar abundances do not necessarily reflect the abundances in the planets (Santos et al., 2001; Reid, 2002; Santos et al., 2004; Sousa et al., 2011; Bond et al., 2010; Delgado Mena et al., 2010; Petigura & Marcy, 2011), as was also discussed in §4. By matching our Hypatia Catalog to HabCat, we are able to analyze the abundances in 1224 potentially habitable stars, see Fig. 5.1.

We define bio-essential elements as: C, N, O, Mg, Si, S, and Fe, which are required for the biogeochemistry on Earth (Pace, 2001) and are discussed in §3.2 and §3.3. Other elements that are known to be important in biogeochemistry such as Na, P, K, Mo, and Se, are difficult to measure in stellar atmospheres (see Fig. 5.1), and while discussed in this chapter, are not included in this bio-essential element application. We also consider suitable abundance ranges for the bio-essential elements that are favorable to our biogeochemistry. Drawing upon the work done by Gonzalez (1998b); Santos et al. (2000); Gonzalez et al. (2001); Bodaghee et al. (2003); Beirão et al. (2005); Fischer & Valenti (2005); Bond et al. (2006), who found that stars hosting exoplanets tend to be chemically enriched compared to non-host-stars, we only analyze those stars whose element abundance is
[X/Fe] > −0.4, per the discussion given in Turnbull & Tarter (2003a). It is beyond the scope of this chapter to place upper-bounds on the abundances ranges.

5.1 Abundance Maps

We have created abundance maps of the sky that may aid in finding possible regions that are enhanced with bio-essential elements. Fig. 5.2 shows the number of stars along a line-of-sight in a Mollweide projection of the sky, where Right Ascension (RA) is along the horizontal varying from 0-24\textdegree\, and Declination (Dec) is on the vertical from [-90°, 90°]. The bin size is scaled to equal a telescope beam of 3°, like that of the Allen Telescope Array or the Large Synoptic Survey Telescope. While the RA/Dec bins are rectangular by definition, they appear as polygons in the contour map of Fig. 5.2. The Ecliptic plane has been overlaid in red for guidance, however, since all stars in Hypatia have radial distances less than 150 pc, they are within the Galactic disk.
Figure 5.1: Number of stars in both the Hypatia Catalog and HabCat with measured abundances for 44 different element species.
Figure 5.2: A Mollweide projection of the positions of stars in Hypatia in RA (horizontal from 0-24 h) and Dec (vertical from [-90°, 90°]), where stars that lie in the same bin, or beam area equal to 3°, are grouped together. Overlayed on this map is the position of the Ecliptic plane for orientation. The stars in Hypatia are relatively uniform in RA and Dec since they all have a radial distance less than 150 pc and are, therefore, in the Galactic disk.
Figs. 5.3-5.8 show the total abundances for the bio-essential elements, summed along the lines of sight in a Mollweide projection and similar to Fig. 5.2, where the colorbar indicates the average total abundance per star within a bin. For example, near (3.00°, -4.78°) in Fig. 5.3, the yellow highlighted area indicates carbon enrichment in that region of the sky. For each bio-essential element, there is at least one “hotspot”, or individual bin/beam along a line of sight that has a preponderance of that element. In some cases, a particular region of the sky is “hot” because one star has an exceptionally high abundance. However, for the majority of the time, a beam is “hot” because a number of stars with moderate abundances are located within that area. In those instances of multiplicity, the total abundance within a beam is determined as a sum of the abundances from the stars within that beam, such that:

$$[X/Fe]_{\text{beam}} = \log[10^{(X/Fe)_{\text{star1}}} + 10^{(X/Fe)_{\text{star2}}} + ...].$$

(5.1)
Table 5.1: Top 5 Bio-essential Element Hotspots for a 3° beam

<table>
<thead>
<tr>
<th>Abundance (X/Fe)</th>
<th>Stars in Hotspot</th>
<th>HIP</th>
<th>[X/Fe]</th>
<th>[pc]</th>
</tr>
</thead>
<tbody>
<tr>
<td>[C/Fe]</td>
<td>(4.20, 0.96)</td>
<td>10723 [0.16]</td>
<td>10818 [0.06] (38.8), 9911 [-0.11] (37.0)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(3.00, -4.78)</td>
<td>14241 [0.69]</td>
<td>(35.0)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(17.40, -2.86)</td>
<td>85042 [0.04]</td>
<td>85090 [0.13] (98.2), 84374 [0.04] (54.8)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(22.20, 54.67)</td>
<td>108689 [-0.02]</td>
<td>108921 [0.78] (69.0)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(22.60, -48.52)</td>
<td>110843 [-0.01]</td>
<td>112117 [0.10] (23.6), 112414 [0.62] (38.0)</td>
<td></td>
</tr>
<tr>
<td>[N/Fe]</td>
<td>(0.00, 4.78)</td>
<td>3765 [0.98]</td>
<td>(7.5)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(13.00, 4.78)</td>
<td>63354 [0.58]</td>
<td>(53.4)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(21.40, -28.88)</td>
<td>65352 [0.33]</td>
<td>(15.5), 65355 [0.32] (16.1)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(16.60, -2.86)</td>
<td>81691 [0.68]</td>
<td>(29.6)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(20.60, -4.78)</td>
<td>100783 [0.36]</td>
<td>(98.3), 101136 [0.25] (55.2)</td>
<td></td>
</tr>
<tr>
<td>[O/Fe]</td>
<td>(4.60, -67.75)</td>
<td>20677 [0.20]</td>
<td>(42.8), 21731 [0.06] (37.2), 21889 [-0.02] (55.7)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(20.20, -67.75)</td>
<td>98959 [-0.01]</td>
<td>(17.7), 99240 [0.03] (61.1), 100396 [-0.01] (52.3), 98621 [0.04] (37.7), 98764 [0.07] (36.3)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(20.60, -4.78)</td>
<td>100783 [0.03]</td>
<td>(98.3), 101136 [0.04] (55.2), 102203 [0.01] (30.7)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(22.60, -48.52)</td>
<td>110843 [-0.04]</td>
<td>(35.4), 112117 [-0.02] (23.6), 112414 [0.19] (38.0)</td>
<td></td>
</tr>
<tr>
<td>[Mg/Fe]</td>
<td>(1.00, 4.78)</td>
<td>3765 [0.43]</td>
<td>(7.5)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(20.60, -4.78)</td>
<td>100783 [0.07]</td>
<td>(98.3), 101136 [0.09] (55.2)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(22.60, -48.52)</td>
<td>110843 [-0.00]</td>
<td>(35.4), 112117 [0.04] (23.6), 112414 [0.18] (38.0)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(23.00, -4.78)</td>
<td>113357 [-0.01]</td>
<td>(15.6), 114034 [0.06] (74.4)</td>
<td></td>
</tr>
<tr>
<td>[Si/Fe]</td>
<td>(2.20, 0.96)</td>
<td>10723 [0.06]</td>
<td>(24.4), 10818 [0.02] (38.8), 9911 [-0.01] (37.0)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(4.60, -67.75)</td>
<td>20677 [0.16]</td>
<td>(42.8), 21731 [0.02] (37.2), 21889 [0.09] (55.7)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(20.20, -67.75)</td>
<td>98959 [0.07]</td>
<td>(17.7), 99240 [0.06] (61.1), 100396 [0.03] (52.3), 98621 [0.02] (37.7), 98764 [0.04] (36.3)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(22.60, -48.52)</td>
<td>110843 [0.00]</td>
<td>(35.4), 112117 [0.04] (23.6), 112414 [0.18] (38.0)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(23.00, -4.78)</td>
<td>113357 [-0.01]</td>
<td>(15.6), 114034 [0.14] (74.4)</td>
<td></td>
</tr>
<tr>
<td>[S/Fe]</td>
<td>(1.00, 4.78)</td>
<td>3765 [0.43]</td>
<td>(7.5)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(20.60, -4.78)</td>
<td>100783 [0.07]</td>
<td>(98.3), 101136 [0.09] (55.2)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(22.20, 24.61)</td>
<td>109176 [0.07]</td>
<td>(43.3), 109931 [0.06] (71.5)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(23.00, 20.48)</td>
<td>113357 [-0.01]</td>
<td>(15.6), 114034 [0.14] (74.4)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(23.40, 54.67)</td>
<td>114924 [0.02]</td>
<td>(20.5), 115761 [0.15] (95.1)</td>
<td></td>
</tr>
</tbody>
</table>

The average abundance per star per beam is then calculated by dividing [X/Fe]_{beam} by the number of stars within the beam. Table 5.1 delineates the five beams for each bio-essential element that contain the highest total abundance, where each beam has its central coordinate position in RA and Dec, the HIP name of the stars within it, their respective, re-normalized abundance in brackets, and their radial distance from the Sun in parsecs within parentheses. In the case of carbon, the “hot” region near (3.00h, -4.78°) is due to one particularly carbon-rich star, HIP 14241.

Fig. 5.9 graphically illustrates the “hotspots” from the bio-essential elements listed in Table 5.1. While the hotspots for each element do not necessarily align, many of them are in similar regions of the sky. For example, many of the hotspots are clustered within 5° of the celestial equator, along the RA = 22h line, and also near lower declination. This bias may due to the angle of the Earth with respect to the equatorial coordinate system.
Figure 5.4: RA/Dec maps similar to Fig. 5.2 for the bio-essential element N/Fe. The brightest hotspots are listed in Table 5.1, along with the stars in that beam, their abundance, and coordinates.

Only a handful of the hotspots are from one star in a beam; and in the case of [N/Fe], this is due to the low number of stars for which that element was observed (see Fig. 5.1). We find that near the coordinates (20.6$^h$, -4.8$^\circ$) and (22.6$^h$, -48.5$^\circ$), there are a number of overlapping bio-essential hotspots due to the presence of multiple stars with moderate- to high-abundances. While there are no causal, astrophysical reasons to expect any preferred directions within our solar neighborhood, that does not mean that these regions are not physical. The presence of these “windows” could be random and still remain favorable RA and Dec directions for targeted or beamed searches.

5.2 Regional Merit within Hypatia

Habitability depends on many physical and chemical properties, both of the host-star and the exoplanet. Turnbull & Tarter (2003b) developed a metric by which the stars within their catalog could be prioritized based on
Figure 5.5: RA/Dec maps similar to Fig. 5.2 for the bio-essential element O/Fe. The brightest hotspots are listed in Table 5.1, along with the stars in that beam, their abundance, and coordinates.

the B-V color spectrum of the host-star \((M_{\text{spec}})\) and the radial distance from the Sun \((M_{\text{dist}})\), where closer, solar-like stars are preferable. They quantified this concept of “spectral-distance merit” using \(M_{\text{HabCat}} = M_{\text{spec}} + M_{\text{dist}}\).

They defined

\[
M_{\text{spec}} = e^{-[(M_V-4.78)^2/2\sigma_{M_V}]} \times e^{-[(B-V)-0.65)^2/2\sigma_{B-V}]}
\]  

(5.2)

and

\[
M_{\text{dist}} = \frac{(15 \text{ pc})^2}{(\text{distance, pc})^2},
\]

(5.3)

where the absolute magnitude \((M_V)\) and color, respectively, are offset by \(\sigma_{M_V} = 5\) and \(\sigma_{B-V} = 0.25\), such that both Gaussians in Eq. 5.2 are centered on the Sun and correspond to a merit of 1.0. They plotted the total physical merit for all stars in HabCat in their Fig. 8.

Similarly, we have determined the merit function for stars in Hypatia, with the addition of another term, \(M_{\text{chem}}\), which takes into account the
Figure 5.6: RA/Dec maps similar to Fig. 5.2 for the bio-essential element Mg/Fe. The brightest hotspots are listed in Table 5.1, along with the stars in that beam, their abundance, and coordinates.

presence of bio-essential elements and augments the total physical and chemical merit of a star. We have experimented with two ways of determining $M_{chem}$. The first is defined with respect to the total number of bio-essential elements, $N$, a star has had measured for it, where $M_{num} = \frac{N}{6} \times 0.25$. In the ideal case, a star has had all six bio-essential elements measured, which contributes $M_{chem} = M_{num} = 0.25$, so as to scale with the other terms in the merit equation. This new definition of merit is plotted in Fig. 5.10, where the plot on the left mimics that from Turnbull & Tarter (2003b). The plot on the right shows $N$ only with respect to RA and Dec and illuminates a number of hotspot regions with stars that have multiple bio-essential elements measured, which may be worth targeting in telescopic surveys.

We have also investigated how $M_{chem}$ would be affected if we defined it with respect to the sum of the actual abundances of the bio-essential
Figure 5.7: RA/Dec maps similar to Fig. 5.2 for the bio-essential element Si/Fe. The brightest hotspots are listed in Table 5.1, along with the stars in that beam, their abundance, and coordinates.

elements per star, $T$. We define $M_{abund}$ with respect to the total sum of all bio-essential element abundances in a star, $T$, averaged over the number of possible bio-essential elements that could be measured, such that $M_{abund} = T/6$. Since $[X/Fe]$ is already normalized to solar (Lodders et al., 2009), this equation implies that any abundance greater than solar has a positive impact on habitability, and therefore merit, which may not necessarily be the case (Sousa et al., 2008; Sousa et al., 2011; Ghezzi et al., 2010). Fig. 5.11 shows the merit function for Hypatia stars with the inclusion of $M_{abund}$ on the left, similar to that in Turnbull & Tarter (2003b). The plot on the right shows $T$ with respect to RA and Dec, similar to Fig. 5.2, where the highest regions of merit are shown in red.

For both definitions of $M_{chem}$, many hotspots are located near the equator, of note are those found at $(20.6^h, -4.8^\circ)$ and $(22.6^h, -48.5^\circ)$. These are the same as the hotspots shown in Fig. 5.9, due to bio-essential
abundance measurements from multiple stars within the beam. The two regions appear to be preferential directions on the sky for potential host-stars of habitable exoplanets, what may be called “Habitability Windows.” The windows at (20.6°, -4.8°) and (22.6°, -48.5°) may not be due to astrophysical phenomena, such as an injection from a nearby supernovae or the presence of a dense molecular cloud, however, that doesn’t negate the physical existence of these regions. The inclusion of additional catalogs and data for the bio-essential elements will help to explore and define these regions of potential habitability.

5.3 Current 3D Abundance Positions and Kinematics

The abundance maps that we created to find possible regions of enhanced bio-essential elements represent the stars and their abundances as they currently appear. Fig. 5.12 illustrates those positions in 3D, centered on
Figure 5.9: A RA/Dec map depicting the brightest 5 hotspots for all 6 bio-essential elements, as denoted by the legend on the right. The brightest hotspots are listed in Table 5.1, along with the stars in that beam, their abundance, and coordinates.

the Sun, and with respect to the present [Ni/Fe] abundances. Each star’s abundance is smoothed over a sphere with radius equal to the distance to its nearest neighbor, the average being $\sim 7.16$ pc. The directionality of the North and South Galactic Poles and the Galactic center and anti-center are denoted for orientation, as well as the color-bar scale and opacity Gaussians. We chose to analyze the [Ni/Fe] abundances in nearby stars for similar reasons as given in §4.3, namely that nickel is representative of the iron-peak group with similar nucleosynthetic origins as iron (see also §3.7). The [Ni/Fe] abundance gradients between stars on the surface of the solar neighborhood “cube”, with $\sim 200$ pc to a side, are shown by the close proximity change from red to blue. Similar to the abundance variations seen in Figs. 5.3 and 5.11, while there does not appear to be directional preferences for [Ni/Fe] enrichment, that does not nullify the existence of enhanced regions. The [Ni/Fe] abundances can vary by 0.6dex within very close proximity.
Figure 5.10: The merit function from Turnbull & Tarter (2003b) with an added term to take into account the number of bio-essential elements measured per star (left). To the right is the respective Mollweide RA/Dec plot showing only the additional term, $N$, and numerous hotspots.
Figure 5.11: Merit function from Turnbull & Tarter (2003b) with an added term to take into account the sum of the bio-essential abundances measured per star (left), and the respective Mollweide RA/Dec plot showing only that additional term, $T$, and only a handful of hotspots (right).
Figure 5.12: 3D abundance map showing the smoothed \([\text{Ni}/\text{Fe}]\) distribution in the Galactic plane, where the smoothing-length is the distance to the nearest neighboring star. The Sun is located at the center of the cube, measuring 200 pc on each side, with the ecliptic plane and celestial equator overlayed, as well as the directionality of the North/South Galactic Poles, Galactic center, and anti-center, and the \([\text{Ni}/\text{Fe}]\) color bar is to the left. The distribution of \([\text{Ni}/\text{Fe}]\) in the solar neighborhood is varied but well mixed, as can be seen by the high and low abundance regions in close proximity to each other.

The present location of enriched regions and “Habitability Windows” are time dependent, due to the velocity of the Hypatia-HabCat stars, or stars found in both catalogs. In this chapter we used the calculations performed by Turnbull & Tarter (2003a) for galactic radial velocity. The coordinates, proper motions, and parallax measurements were all taken from the Hipparcos Catalogue, while the radial velocities came from Barbier-Brossat & Figon (2000). The galactic velocities were determined with respect to the Sun, since calculations with respect to the local standard of rest did not significantly change the velocities. We show the magnitude of velocity versus \([\text{Fe}/\text{H}]\) for Hypatia-HabCat stars in Fig. 5.13 (left). Compared to the full list
of HabCat stars (their Fig. 5), we note that none of the stars shown here achieve a velocity above 100 km/s in any direction. However, while the Hypatia-HabCat stars are not as scattered in velocity-space, they are still moving relatively quickly, with an average total velocity of 36 km/s. If we assume that a typical molecular cloud is 150 pc, or roughly the radius of the solar neighborhood, a star moving at 36 km/s would take $\sim 5.4 \times 10^6$ years to cross the diameter. This is a relatively short timescale compared to the age of F/G/K/M-type stars. More than likely, stars currently observed in the solar neighborhood were not all formed from the same molecular cloud, but are traveling near the Sun in random directions.

A Toomre diagram in Fig. 5.13 (right) depicts orbital velocity (V) versus the magnitude of velocities perpendicular to Galactic rotation, specifically the radial and vertical directions. A majority of the Hypatia stars are grouped near the zero-point orbital velocity, meaning these stars have similar peculiar velocities and predominantly stay within the same circular orbit around the center of the Milky Way. Thus, while stars in the solar neighborhood are moving relatively quickly on the timescale for chemical and stellar evolution, it is likely that the mixing is localized.
Figure 5.13: Galactic velocity (U,V,W) for those stars in Hypatia showing the total velocity by [Fe/H] (left). Total velocities are, in general, much smaller than HabCat velocities but large enough to ensure mixing. The Toomre plot (right) is similar to Fig. 1 in Neves et al. (2009) and shows the tight local orbits for the majority of Hypatia stars.
Chapter 6

CONCLUSION

We have assembled spectroscopic abundance data from 49 literature sources for 46 elements across 2836 stars within 150 pc of the Sun to build the Hypatia Catalog. This is the largest, most complete catalog of spectroscopic abundance data for stars in the solar neighborhood to date, of which we are aware (see Fig. 2.1).

We encountered a number of issues by trying to amalgamate such large and diverse data sets, which we attempted to ameliorate in the most unbiased manner. We undertook to minimize the spread, or the variation in abundance measurements for the same star and element reported by different literature sources (see Fig. 2.2), by retaining stars whose spread in \([\text{Fe/H}]\) is less than 1.0 dex and renormalizing all the stars in Hypatia to the Lodders et al. (2009) solar abundance scale. We find this last measure only slightly reduces the spread and indicates the underlying cause lies in the observed spectra, techniques, or models implemented by the various literature sources.

We found abundance trends that are consistent with previously discovered Galactic mean trends. The large number of stars in Hypatia allows us to observationally quantify the extent of the scatter, or the width about the mean abundance trend, for each element (Figs. 3.2-3.28, and also see Tinsley, 1980; Malinie et al., 1993; van den Hoek & de Jong, 1997; Kobayashi & Nakasato, 2011). The magnitude of the scatter, for most elements, is larger than the magnitude of the spread of each star, suggesting the scatter is physical and not driven by uncertainties in the abundance
determinations. We found no systematic correlations of the abundances with position, distance, or velocity, supporting the notion stars in the solar neighborhood are well-mixed.

We studied the abundances within the Hypatia Catalog for 204 known exoplanet host stars. We found that planetary occurrence increases with stellar [Fe/H], a trend observed in a number of literature sources (see §3.1). However, the number of SWPs did not noticeably change as a function of other element abundances, including those elements with similar nucleosynthetic origins as iron. We also analyzed nine element abundances (six that were bio-essential and three that were representative of nucleosynthetic origins) for correlations in stellar color, velocity, mass, effective temperature, and surface gravity, as well as planet mass, orbital period, eccentricity, and multiple/single-planet systems. Our data shows that smaller stellar and planet masses are enriched in the bio-essential elements, excluding Neptune-mass planets. Stars with large, super-Jupiter planets exhibit near-solar abundances in the three “representative” elements. Because we analyzed the abundances for a variety of elements within a statistically significant sample of SWPs, we were able to contribute new information to both the self- and primordial-enrichment theories on the compositional anomalies within exoplanet hosts. We are hopeful that the investigation of elements other than iron, specifically the refractory elements, will aid in the understanding of stellar host compositions. In a similar vein, while the abundances presented here seem to offer support to the core accretion model of planetary formation, the results are not conclusive and requires more analysis.
We also explored an application of the Hypatia Catalog with respect to stars already designated as potential hosts to habitable exoplanets, as per Catalog of Potentially Habitable Stellar Systems put together by Turnbull & Tarter (2003a). By assuming the star-planet abundance correlation, an enhancement in the stellar atmosphere of bio-essential elements may have an effect on the planet’s composition, structure, and atmosphere. We were able to locate a number of specific “hotspots” on the sky with respect to the bio-essential elements (Figs. 5.2-5.12). The overlap of these hotspots have ultimately demonstrated the presence of two “habitability windows” which exhibit increased observational merit, located at (20°, -4°) and (22.6°, -48.5°). In comparison, Fig. 6.1 shows a map of the positions for the known exoplanets within the Hypatia Catalog. Most likely due to the significantly lower number of known exoplanets, we do not see a correlation between the habitability windows and the observed exoplanets. The majority of large-scale full-sky surveys take many months or years to observe and later confirm the presence of exoplanets. We anticipate that our maps may aid in more specific, ground-based searches for new terrestrial exoplanets. In addition, as future missions confirm the presence of additional exoplanets, our maps and estimations of potential hotspots will continue to improve.

After examining the abundances in known and potential exoplanet hosts, we have found that there is a large variation in both stellar and planetary properties in our solar neighborhood. While the majority of the stellar abundances are similar to those observed in our Sun, the same cannot be said for the planetary systems. Only a small percentage of the confirmed exoplanets have Earth-like masses and only fraction of those could possibly be found within the habitable zone (Kane & Gelino, 2012).
Figure 6.1: Similar to Fig. 5.2, a Mollweide projection of the known exoplanet host stars in the Hypatia Catalog. Since the number of exoplanet hosts is significantly less than the number of Hypatia stars in HabCat, we do not see any correlation between the known exoplanets and the hotspots shown in Fig. 5.9.
The Hypatia Catalog is a large, flexible collection of stellar abundances for stars in the solar neighborhood. There are a multitude of questions and applications that can be addressed as a result of having the physical and chemical characteristics compiled for \( \sim 2800 \) nearby stars. For example, studies can be undertaken that examine the trends seen in specific stellar types, thick versus thin disk stars, slow velocity stars, and many other possibilities. As new abundance determinations are published, they can be easily integrated into the Hypatia Catalog, keeping it current as instruments and data reduction techniques are improved. A collection of physical and chemical information for nearby stars, such as Hypatia, can greatly help to understand overarching abundance trends. This, with the use of chemical evolution models, may help explain nearby astrophysical events that have impacted nearby stars, our region of the Galaxy, and our chemical evolution.

“The pursuit of knowledge is hopeless and eternal. Hooray!”

\(~\sim\) Professor Hubert J. Farnsworth
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APPENDIX A

AREA & VOLUME FRACTIONS WITHIN A GRID CELL
We have developed an ionization routine to compare the ionizing flux from a source star with the recombination rate of the surrounding medium. This was written for a chemical evolution simulation in a grid-based (as opposed to particle-based) environment. By computing the area/volume fraction crossed by the ionization front in a cell, we quantify the effect that the star has on the temperature of that cell. The temperature then determines the hydrodynamic expansion of the stellar Strömgren sphere. In order to calculate the ionization fraction in each cell, we ported and implemented a “hybrid characteristics” ray-tracing algorithm originally written by Rijkhorst et al. (2006). We then replaced the prescriptions for local column density with a computation for the recombination rate for each cell, according to

\[
R = \alpha_H \eta_p \eta_e = 2.59 \times 10^{-13} \left( \frac{10^4}{T(K)^{0.85}} \right) \eta_p \eta_e \quad (\text{cm}^{-3} \text{ s}^{-1}). \tag{A.1}
\]

Here, \( R \) is the number of recombinations per unit time in a unit volume, \( \alpha_H \) is the hydrogen recombination rate, \( T(K) \) is temperature in Kelvin, and \( \eta_p \) and \( \eta_e \) are the electron and proton number densities, respectively, proportional to their collisional rates per unit volume. Similar to column density, the recombination rate was integrated from the source to the center of each cell. We have also determined the degree of ionization within a grid cell due to radiation from a nearby star, to take into account partially ionized interstellar medium (ISM) across the ionizing front.

A.1 Ray Tracing

Ray tracing is a simulated method that follows the path of light and radiation to determine the interaction between it and other virtual objects.
It is common to implement ray tracing algorithms in order to replicate radiative transfer within astronomical simulations. For grid-based codes, this is arguably the most correct treatment for radiative transfer if both diffusion and scattering are ignored. Due to the physical scales, adaptive-mesh refinement (AMR), and parallel processing usually employed within chemical evolution simulations, we require a ray tracing mechanism that is both accurate and computationally fast.

There are two traditional methods that are utilized in ray tracing calculations: “long”- and “short” characteristics. Long characteristic algorithms calculate the direct contribution from the source to the target grid cell between every simulation time step, which slows the computational time through redundancy. Short characteristic routines compute the contribution to a target by first determining the contributions to all of the cells between the target and the source, then summing their total contribution. This method is inherently serial. Therefore, we have chosen to work with the “hybrid characteristic” ray tracing method developed by Rijkhorst et al. (2006). They have taken advantage of both techniques in order to make the code accurate on a local scale and efficiently parallel.

The algorithm by Rijkhorst et al. (2006) was originally released in FLASH2. FLASH is a multidimensional, Lagrangian hydrodynamics code (Fryxell et al., 2000) that solves the Riemann problem on a Cartesian grid using a directionally-split piecewise-parabolic method (PPM) solver (Colella & Glaz, 1985; Colella & Woodward, 1984; Fryxell et al., 1991). The code is both scalable and modular, and utilizes AMR. It is capable of running across multiple processors, using non-permanent guard cells that border each cell.
and maintain updated data to be communicated across block faces and processors.

Since the release of FLASH2, there have been numerous developments in the structure and environment within FLASH, published now as FLASH3. With those changes include several improvements, for example, direct variable indexing via ‘solnData’ and a unique global identification of each cell using both the corner coordinate and level of refinement via ‘cornerID.’ These modifications altered the way in which information is communicated to the parent block and the child grid cells. Much time was spent meticulously porting the algorithm by Rijkhorst et al. (2006) from FLASH2 to FLASH3, to ensure that data communication was accurate within the FLASH3 structure. All simulations were performed with FLASH v3.1. The FLASH3 port has been successfully tested with respect to the original code. The hybrid characteristics technique has also been updated to eliminate source placement issues, which were limited to only cell corners in FLASH2. The code is now able to place the source star anywhere on the grid, without detriment to the underlying physics.

The calculations done by Rijkhorst et al. (2006) are presented for column density across multiple cells, blocks, and processors, without the inclusion of physics in the routine. When the authors originally published their paper, they used the DORIC code (Frank & Mellema, 1994) to determine ionization, heating, and cooling rates. We have replaced those column density routines in order to determine the total and partial ionization within a grid cell due to a source star.
A.2 Geometry of a Ray within a Grid Cell

The recombination rate, per Eq. A.1, of each cell is determined at the center of that cell. However, in order to properly determine the degree to which a cell is ionized, we calculate \( R \) at the side nearest and furthest from the source. We first determine the far side rate by adding the integrated recombination, summed to the cell center, to the amount accumulated from the center to the far corner, respectively:

\[
R_{\text{far}} = \int_{s}^{c} R + \alpha H \eta_p \eta_e \left[ \sqrt{(x_s - x_c)^2 - (y_s - y_c)^2} \right] - \sqrt{((x_s - x_c) - dx/2)^2 - ((y_s - y_c) - dy/2)^2}. \tag{A.2}
\]

The subscript “s” denotes the coordinate of the source, “c” refers to the cell center, and \( dx \) is the length of the cell on a side, such that a cell is a perfect square where \( dx = dy \).

The near side calculations could not be done in the same manner as the far-side due to the manner in which the recombination rate is summed across the cells. For example, the recombination rate on each block face is calculated using long characteristics, to ensure as many processes as possible were used in parallel (Rijkhorst et al., 2006). Once that information is made available, the local recombination rate on a block is done via short characteristics across each cell. Because of this feature, simply subtracting the recombination accrued from the cell center back towards the source results in mathematical inconsistencies. To determine the near side, we took advantage of symmetry inherent to the grid: the recombination rate calculated on the far side of the nearest- or next-nearest-neighbor closest to the source is equivalent to the recombination rate on the near-side of the cell.
Thus, the near side recombination rate is the smallest neighbor’s far side calculation.

Figure A.1: A cartoon illustrating the various parameters used when describing the recombination rate and flux on both the near and far sides of the cell. These variables determine if a cell is neutral, partially- or fully-ionized.

In order to synthesize an ionization front, we determine whether each cell is neutral, partially- or fully-ionized by looking at the volume traversed by the front in each cell. The volume fraction is calculated by finding the distance within the cell where the flux from the source star is equal to the integrated recombination rate, or $dl$. The ionizing flux goes as $F(d) = Q/(4\pi d^2)$, where $Q$ is the number of photons per second, used here as a spectral type O8 star (Osterbrock, 1989), and $d$ is the distance from the source to the cell. The ray enters the cell at an angle, $\alpha$, where $0 < \alpha < \pi/4$ to avoid asymptotes, and bisects the cell, see Fig. A.1. The ionization front is assumed to be far from the source and therefore, orthogonal to the ray. The locations of $R_{far}$ and $R_{near}$ are also designated.

To determine the ionization front, we cannot compare the flux at the center of the cell to the recombination rates on the side of a cell; the distance
discrepancy is too large. Therefore, we find the flux at the ionization front:

\[
F(dl) = \frac{F(d) d^2}{(d - a + dl)^2} = \frac{F(d)}{(1 + \frac{d}{d-a})^2} \approx F(d) \left(1 - \frac{2(dl - a)}{d}\right),
\]

(A.3)

using a Taylor approximation in the limit where \(d \gg a\) as well as \(dl\). The variable \(a\) is defined as the distance from the near side to the center of the cell, \(a = (R_{far} - R_{near})/(2\alpha_H \eta_p \eta_e)\), as shown in Fig. A.1. The flux at the near and far sides are then found when \(dl = 0\) and \(dl = 2a\), respectively:

\[
F(0) = F_{near} = F(d) \left(1 + \frac{2a}{d}\right) \quad \text{and} \quad F(2a) = F_{far} = F(d) \left(1 - \frac{2a}{d}\right).
\]

(A.4)

If the flux is greater than the recombination rate at the corner furthest from the source, that cell is fully ionized with a temperature of 10,000 K. Similarly, if the flux is less than the recombination rate on the near side, than the temperature remains that of the ambient medium, or 100 K, since it is not ionized.

A.3 Partial Area Fraction (2D)

A partially ionized cell has flux greater than recombination on the near side but less than recombination on the far side. To determine the fraction of area the ionization front traverses within a grid cell, we first utilize Eq. (A.3) to quantitatively define \(dl\) as:

\[
dl = \frac{[F(dl) - R_{near}]}{(\alpha_H \eta_p \eta_e)}.
\]

(A.5)

We then substitute Eq. (A.3) into Eq. (A.5) and solve for \(dl\):

\[
dl = \frac{d [F(d) - R_{near}] + 2a F(d)}{d \alpha_H \eta_p \eta_e} \left[1 + \frac{2 F(d)}{d \alpha_H \eta_p \eta_e}\right],
\]

(A.6)
or the distance the plane travels within a cell before it stops. The plane may
traverse the cell in one of three geometric ways, shown in Fig. A.2, which we
use to calculate the area fraction and subsequent temperature change.

We first define the distances of the ionization front along the
coordinate axes: \( x = dl / \cos \alpha \) and \( y = dl / \sin \alpha \). When \( x < dx \) and \( y < dx \),
the front intersects two adjacent sides of the cell closest to the source (Fig.
A.2a), so the area fraction is

\[
\Delta A_a = \frac{1}{2 dx^2} \left[ \frac{1}{2} \frac{dl}{\cos \alpha} \frac{dl}{\sin \alpha} \right] = \frac{xy}{2 dx^2}.
\] (A.7)

When \( \alpha \) is shallow such that the front cuts across two opposing faces of the
cell (Fig. A.2b), or \( x < dx \) and \( y > dx \), then the bounded triangle goes
beyond the bounds of the cell. Note, because \( \alpha < \pi/4 \), it is always the case
that \( y \geq x \). We calculate the area fraction by subtracting off the outlying
smaller, similar triangle:

\[
\Delta A_b = \frac{1}{2 dx^2} \left[ xy - (y - dx)^2 \tan \alpha \right]
\] (A.8)

When the front intersects two adjacent sides furthest from the source (Fig.
A.2c), or when \( x \) and \( y > dx \), then we find the ionized region by calculating
the area of the triangle not subtended by the bisecting plane (shown as the
shaded region in Fig. A.2c) and subtract it from the total area of the cell:

\[
\Delta A_c = \frac{1}{2 dx^2} \left[ xy - (y - dx)^2 \tan \alpha - \frac{(x - dx)^2}{\tan \alpha} \right].
\] (A.9)

The temperature of a cell increases with respect to the fractional area, \( \Delta A \),
when the ionization front only covers a fraction of the cell. Within the
FLASH regime, this was done either manually, via:

\[
T = (10^4 - 100)[\Delta A + 100(1 - \Delta A)],
\] (A.10)
or according to the hydrodynamic sweeps that update the cells, whichever is larger, in order to ensure a fluid expansion.

\[ \frac{dl}{\cos(\alpha)} \]
\[ \frac{dl}{\sin(\alpha)} \]
\[ dx \]

\[ \frac{dl}{\cos(\alpha)} \]
\[ \frac{dl}{\sin(\alpha)} \]
\[ dx \]

\[ \frac{dl}{\cos(\alpha)} \]
\[ \frac{dl}{\sin(\alpha)} \]
\[ dx \]

\[ \frac{dl}{\cos(\alpha)} < dx \]
\[ \frac{dl}{\sin(\alpha)} > dx \]

\[ \frac{dl}{\cos(\alpha)} > dx \]
\[ \frac{dl}{\sin(\alpha)} < dx \]

\[ \frac{dl}{\cos(\alpha)} < dx \]
\[ \frac{dl}{\sin(\alpha)} > dx \]

Figure A.2: The ionization front can bisect a cell in one of three ways. To determine the volume fraction traveled by the front, we look at the geometry when a) \( \frac{dl}{\cos \alpha}, \frac{dl}{\sin \alpha} < dx \), b) \( \frac{dl}{\cos \alpha}, \frac{dl}{\sin \alpha} > dx \), or c) \( \frac{dl}{\cos \alpha} < dx \) and \( \frac{dl}{\sin \alpha} > dx \).

FLASH utilizes optional guard cells on the boundary of each cell. These allow for copacetic hydrodynamic communication between cells as well as neighboring blocks. We carefully placed our variable calculations within the FLASH3 structure to ensure they initialized properly at the beginning of the simulation run. For example, before calculating the recombination rates at the near and far sides of the cell, we first calculate the integrated recombination rates at the center of each cell and then allow for a hydrodynamic sweep. After two separate hydrodynamic sweeps we then determine in what way a cell is ionized, if it is ionized, and how the temperature is affected. Fortunately, we are able to take advantage of the two hydrodynamic sweeps in each FLASH time step. The individual and integrated recombination rates are performed at the top of the first time step, the near and far rates are determined at the bottom. At the top of the second time step, all of the temperature calculations are performed, and at
the bottom, the near and far recombination rates were updated again. After this second time step, the quantities are updated during both hydrodynamic sweeps within each time step.

Figure A.3: The temperature of the Strömgren sphere in a spatial plane for the 2D simulation, where \( \eta_H = 100 \, \text{cm}^{-3} \), \( Q = 10^{49.23} \), \( T_{\text{env}} = 100 \, \text{K} \), \( T = 10^4 \, \text{K} \), and the size of the simulation area is 9.72 pc on a side. The uniform, AMR grid is overlayed.

For our simulations, we assumed that the gas was composed of, by mass, 24\% helium and trace heavy metals, while the rest was hydrogen. On a square grid, with \( 3.0 \times 10^{19} \, \text{cm} \approx 9.72 \, \text{pc} \) on a side, we placed a star at the exact center with \( Q = 10^{49.23} \), as is typical for an O8 star (Osterbrock, 1989). The ISM density was \( \eta_H = 100 \, \text{cm}^{-3} \), with an ambient temperature of \( T_{\text{env}} = 100 \, \text{K} \). Once the star is “turned on”, the recombination time is

\[
t_{\text{rec}} = [\alpha_H \eta_H]^{-1} = 1.22 \times 10^3 \, \text{yr},
\]

where \( \alpha_H \) is similarly defined as in Eq. A.1, with a Strömgren radius of 3.15 pc. It is assumed that the flux from the star only ionizes hydrogen, and the temperature changes from 100 K outside the
Strömgren sphere to 10,000 K inside. An example of a temperature output for our 2D simulation is given in Fig. A.3.

A.4 Partial Volume Fraction (3D)

The intersection between a box and a plane is a geometric computation with numerous applications in computer graphics (Ratscheck & Rokne, 2000), solid modeling (Rezk-Salama et al., 2005), and, in the present context, determining the extent of partial ionization on a 3D Cartesian grid in FLASH. Most of the ray-box algorithms we could find provided a binary answer to the question of whether a given ray, normal to the plane, was inside a specified box or not. A few algorithms even computed the vertices of the intersection plane. We detail two methods to compute the volume of the intersection between a cube and a plane. The first method is founded on adding and subtracting triangular pyramids, while the second method is based on computing the volume of an arbitrary polyhedron given the vertices of each bounding face. We show both methods give volume fractions that have a maximum relative difference of $10^{-7}$. The pyramid method was implemented in FLASH since it has a smaller operational count than the general polyhedron method.

Determining the volume fraction in 3D is not as simple as the 2D case, since the ionization front is no longer a bisecting line, but a bisecting plane. Fortunately, Eq. (A.2) easily expands to include the z-direction and Eqs. (A.3)-(A.6) remain the same. We define the angle in the x-z plane, $\beta$, allowing $\alpha$ to remain solely in the x-y plane, as in the 2D case.
A.4.1 Triangular Pyramid Method

The triangular pyramid method constructs 9 explicit formulae for the volume of the polyhedron generated by the intersection a plane with a cube. The intersecting plane is defined by the length of the normal ray, $dl$, and the spherical angles $0 \leq \alpha \leq 2\pi$ and $\pi/2 \leq \beta \leq -\pi/2$ (similar to spherical coordinates). The maximum length of the normal ray in this coordinate system is $dl_{\text{max}}/dx = [\cos(\alpha) + \sin(\alpha)] \cdot \cos(\beta) + \sin(\beta)$, which ensures that the plane intersects the cube. Reflection symmetry about $dl_{\text{max}}/2$ allows the same 9 formulae to be reused.

We assume the grid cube is perfect, such that the edges have length $dx = dy = dz$. We first define the distances along the coordinate axes of the intersecting plane:

$$x = \frac{dl}{\cos(\beta) \cos(\alpha)}, \quad y = \frac{dl}{\cos(\beta) \sin(\alpha)}, \quad \text{and} \quad z = \frac{dl}{\sin(\beta)}, \quad (A.11)$$

where $dl \leq 0.5 \ d l_{\text{max}}$. We take the limit of $\alpha$ and $\beta$ values near 0 and $\pi/2$ so the denominators do not go to zero. The simplest pyramid has $x < dx$, $y < dx$, and $z < dx$, with a volume fraction of

$$\Delta V_{ia} = \frac{xyz}{6 \ dx^3}. \quad (A.12)$$

This case is shown in Figure A.4 (left) as the green pyramid. The overlying blue pyramid in Figure A.4 (left) has $x < dx$, $y < dx$, and $z > dx$, such that the pyramid extends beyond the top of the cube, requiring the smaller sub-pyramid be subtracted to calculate the proper volume fraction

$$\Delta V_{ib} = \frac{1}{6 \ dx^3} \left( xyz - \frac{xyz}{z^2} \right)^3. \quad (A.13)$$

The figure on the right in Figure A.4 shows the cases when $x < dx$ and
y > dx. The green pyramid, again, has z < dx and volume

$$\Delta V_{2a} = \frac{1}{6 dx^3} \left( x y z - \frac{x z (y - dx)^3}{y^2} \right),$$

(A.14)

while the blue pyramid on the right has z > dx and volume

$$\Delta V_{2b} = \frac{1}{6 dx^3} \left( x y z - \frac{x z (y - dx)^3}{y^2} - \frac{xy (z - dx)^3}{z^2} \right).$$

(A.15)

The red pyramid Figure A.4 (right) also has z > dx but with the bisecting plane at such an angle that the extraneous z-axis pyramid overlaps with the additional y-axis pyramid (shown as opaque). This results in a region that is subtracted twice. In this case the volume fraction is

$$\Delta V_{2c} = \frac{1}{6 dx^3} \left[ x y z - \frac{x z (y - dx)^3}{y^2} - \frac{xy (z - dx)^3}{z^2} + \frac{x}{z} \left( \frac{y(z - dx)}{z} - dx \right) \left( \frac{z(y - dx)}{y} - dx \right)^2 \right].$$

(A.16)

All of the volume fractions calculated at this point have had x < dx.

For the remaining four cases of volumes where dl < dl_{max}/2, shown in Figure A.5, x > dx and y > dx. The green pyramid on the left has z < dx and volume fraction

$$\Delta V_{3a} = \frac{1}{6 dx^3} \left( x y z - \frac{x z (y - dx)^3}{y^2} - \frac{yz(x - dx)^3}{x^2} \right),$$

(A.17)

while the blue pyramid on the left has z > dx and volume fraction

$$\Delta V_{3b} = \frac{1}{6 dx^3} \left( x y z - \frac{x z (y - dx)^3}{y^2} - \frac{yz(x - dx)^3}{x^2} - \frac{xy (z - dx)^3}{z^2} \right).$$

(A.18)

The red pyramid on the right in Figure A.5 has z < dx, but the extraneous pyramids from both x > dx and y > dx are large enough to overlap (shown
Figure A.4: The cube on the left illustrates the pyramids where $x < dx$ and $y < dx$, while the cube on the right shows the pyramids where $x < dx$ and $y > dx$. In both cases the green pyramid corresponds to $z < dx$ and the blue pyramid to $z > dx$. The red pyramid on the right also has $z > dx$ but with a large enough to cover the extra $y > dx$ pyramid.

as opaque). Eliminating this double subtraction gives a volume fraction

$$
\Delta V_{3c} = \frac{1}{6 \, dx^3} \left[ xyz - \frac{xz (y - dx)^3}{y^2} - \frac{yz (x - dx)^3}{x^2} + \frac{z}{x} \left( \frac{y(x - dx)}{x} - dx \right) \left( \frac{(y - dx)}{y} - dx \right)^2 \right],
$$

(A.19)

The yellow pyramid on the right has $z > dx$ and a similar double subtraction that must be corrected, giving a volume fraction of

$$
\Delta V_{3d} = \frac{1}{6 \, dx^3} \left[ xyz - \frac{xz (y - dx)^3}{y^2} - \frac{yz (x - dx)^3}{x^2} - \frac{xz (z - dx)^3}{z^2} + \frac{z}{x} \left( \frac{y(x - dx)}{x} - dx \right) \left( \frac{x(y - dx)}{y} - dx \right)^2 - \frac{xy (z - dx)^3}{z^2} \right],
$$

(A.20)

When $dl > d_{max}/2$, we use the reflective symmetry about $d_{max}/2$ to
Figure A.5: Pyramids cases when $x > dx$ and $y > dx$. The green pyramid on the left has $z < dx$, while the blue pyramid on the left has $z > dx$. The red ($z < dx$) and yellow ($z > dx$) pyramids on the right have corrections pyramids that overlap (orange pyramid), which gives rise to a double subtraction that must be eliminated.
compute the volume fraction. That is, we define

\[ x' = \frac{dl_{\text{max}} - dl}{\cos(\beta) \cos(\alpha)}, \quad y' = \frac{dl_{\text{max}} - dl}{\cos(\beta) \sin(\alpha)}, \quad \text{and} \quad z' = \frac{dl_{\text{max}} - dl}{\sin(\beta)} \quad (A.21) \]

and substitute them into Eqs. A.12 - A.20 for \( x, y \) and \( z \), respectively, to compute the volume fraction on the “empty” or “backside” of the cube. We then subtract this “empty” volume from the total volume. For example, Eq. (A.12) becomes

\[ \Delta V_{4a} = dx^3 - \left( \frac{x'y'z'}{6 dx^3} \right). \quad (A.22) \]

The 3D simulation uses the same parameters as that of the 2D, extended into the third dimension and placed on a grid with side length 4.0 \( \times 10^{19} \) cm \( \approx 12.96 \) pc. A 2D-slice in the x-y plane of the temperature is given in Fig. A.6.

Figure A.6: A two dimensional slice of the 3D simulation in the x-y plane for the temperature of the Strömgren sphere, where \( \eta_H = 100 \) cm\(^{-3} \), \( Q = 10^{49.23} \), \( T_{\text{env}} = 100 \) K, \( T = 10^4 \) K, and the size of the simulation area is 12.96 pc on a side. The uniform, AMR grid is overlayed.
A.4.2 General Polyhedra Method

The intersection between a cube and a plane results in an inscribed, irregular polygon with one of five basic shapes that have 3 to 6 intersection points, as illustrated in Figure A.7. The resulting irregular polyhedron is composed of 4 to 7 faces, 6 to 14 edges, 4 to 9 vertices, and satisfies the Euler identity $N_{\text{faces}} - N_{\text{edges}} + N_{\text{vertices}} = 2$. Our approach extends the method of Rezk-Salama et al. (2005) by simultaneously constructing the faces, edges, vertices, and volume of the irregular polyhedron.

Due to this technique only being implemented as a comparison against which to test the triangular pyramid method, we do not provide the details here.

Figure A.7: The 5 irregular polygons resulting from the intersection of a cube and a plane, where one case has with 3 intersecting points, yielding an irregular polyhedron with 4 faces, 6 edges, and 4 vertices. There are two cases with 4 intersecting points — yielding an irregular polyhedron with either 5 faces, 9 edges and 6 vertices or with 6 faces, 12 edges, and 8 vertices. There is one case with 5 intersecting points, for an irregular polyhedron with 6 faces, 12 edges, and 8 vertices, and one case with 6 intersecting points, for an irregular polyhedron with 7 faces, 14 edges, and 9 vertices.
A.4.3 Comparison of the Two Methods

The top row of Figure A.8 shows the volume fraction calculated by the triangular pyramid method in the $\alpha$-$\beta$ plane for $dl/dx = 0.9$ (left) and $dl/dx = 1.3$ (right). For a fixed $\beta$, the volume fraction reaches a maximum at $\alpha = \tan^{-1}(1/1) = 45^\circ$, or when the ray travels along the diagonal of the x-y plane. For a fixed $\alpha$, the volume fraction reaches a maximum at $\beta = \tan^{-1}(1/\sqrt{2}) \approx 35.26^\circ$, or when the length, width, and height projections are all equal to $dx$. White regions correspond to angles where the plane does not intersect the cube because the specified length of the normal vector $dl/dx$ is larger than maximum length $dl_{max}/dx$.

The bottom row of Figure A.8 shows the relative difference of the volume fractions calculated by the pyramid method and the polyhedron method. The maximum error across the entire $\alpha$-$\beta$ plane for $dl/dx = 0.9$ and $dl/dx = 1.3$ is about $10^{-7}$. Often the relative difference is much smaller.

Both methods give robust and accurate volume fractions, but the pyramid method was implemented in FLASH because it has a smaller operational count than the polyhedron method.
Figure A.8: Volume fractions as given by the pyramid method (where $dh = dl$) for $dl/dx=0.9$ (top left) and $dl/dx=1.3$ (top right). Also shown is the relative difference in the volume fractions calculated by the pyramid and polyhedron method for $dl/dx=0.9$ (bottom left) and $dl/dx=1.3$ (bottom right).