THE TRANSITION FROM POPULATION III TO POPULATION II STAR FORMATION IN THE EARLY UNIVERSE

A Thesis in
Astronomy & Astrophysics

by
Britton Devon Smith

© 2007 Britton Devon Smith

Submitted in Partial Fulfillment of the Requirements for the Degree of
Doctor of Philosophy

December 2007
The thesis of Britton Devon Smith was read and approved* by the following:

Steinn Sigurdsson  
Associate Professor of Astronomy & Astrophysics  
Thesis Adviser  
Chair of Committee

Niel Brandt  
Professor of Astronomy & Astrophysics

Jane Charlton  
Professor of Astronomy & Astrophysics

Deirdre Shoemaker  
Assistant Professor of Physics

Richard Wade  
Associate Professor of Astronomy & Astrophysics

Lawrence Ramsey  
Professor of Astronomy & Astrophysics  
Head of the Department of Astronomy & Astrophysics

*Signatures on file in the Graduate School.
Abstract

The first stars in the universe formed in a unique environment that was free of heavy elements. The lack of efficient radiative cooling in primordial gas meant that the collapse of the first star-forming cloud-cores proceeded very slowly and without fragmenting into multiple objects. This resulted in the first stars being very massive (30 $M_\odot \leq M \leq 300$ $M_\odot$), isolated objects. When these stars died, in violent supernovae, they produced the very first heavy elements, or metals, and dispersed them into the surrounding gas. The addition of these metals changed forever the way stars formed by allowing the gas to cool much more efficiently as it collapsed. It is thought that when the chemical abundance in the next generation star-forming environments reached a critical level, the process of star-formation began producing stars that resemble those observed in the local universe, with characteristic masses of $\sim 1$ $M_\odot$, instead of the behemoths of the early universe.

Simulating this transition in star-formation mode requires the inclusion of the complex chemistry and radiative cooling of heavy elements, which has traditionally been too computationally expensive to be done properly in three-dimensional simulations. In this dissertation, I introduce a new method for treating the radiative cooling from metals in large-scale, three-dimensional hydrodynamic simulations that is fast, accurate, and complete in its coverage of the first 30 elements. I use this cooling method to examine the ability of metals to induce fragmentation in collapsing gas-clouds through lowering of the cooling time-scales and the creation of thermal instabilities. Comparing the cooling and dynamical time-scales within collapsing gas, I calculate that the critical metallicity, $Z_{cr}$, required for fragmentation into multiple, low-mass objects is $\sim 10^{-4.2}$ $Z_\odot$, where $Z_\odot$ denotes the metallicity of the sun. Thermal instabilities are also present in gas-clouds with metallicities, $Z \geq 10^{-4}$ $Z_\odot$.

I use the methodology introduced here to perform a series of adaptive mesh refinement hydrodynamic simulations of pre-enriched primordial star-formation with varying metallicities. For metallicities below $Z_{cr}$, only massive, singular objects form, nearly identical to the metal-free case. For metallicities well above $Z_{cr}$, efficient cooling rapidly lowers the gas temperature to the temperature of the cosmic microwave background (CMB), which is significantly higher in the distant past. The gas is physically unable to radiatively cool below the CMB temperature, and thus, becomes very thermally stable. For moderately high metallicities, $Z \geq 10^{-3.5}$ $Z_\odot$, this occurs early in the evolution of the gas-cloud, when the central density is still relatively low. The resulting cloud-cores show little or no fragmentation, and have mass-scales of a few hundred $M_\odot$. On the other hand, if the metallicity is only slightly above $Z_{cr}$, the cloud slowly cools without ever reaching the CMB temperature. In this case, the minimum cloud temperature is achieved at much higher densities than in the high-metallicity case, resulting in mass-scales of just a few $M_\odot$. This implies that not 2, but 3 star-formation modes were present in the early universe: primordial (high-mass), metallicity-regulated (low-mass), and CMB-regulated (moderate-mass). As the universe evolves to the current epoch, the CMB-regulated mode will slowly transition into the metallicity-regulated mode, as
the CMB temperature gradually decreases. This suggests that the metallicity-regulated mode, which is fully dominant today, may not become so until the CMB temperature drops below the observed temperatures of molecular clouds, \( \sim 10 \) K, which does not occur until redshift, \( z \sim 2 \).
# Table of Contents

List of Tables ......................................................................... vii

List of Figures ....................................................................... viii

Acknowledgments ................................................................... x

Chapter 1. Introduction .......................................................... 1
  1.1 The First Stars ............................................................... 1
    1.1.1 First Insights into the First Stars ......................... 1
    1.1.2 What We Know Now ............................................ 2
  1.2 Moving from the First to the Second Stars .................... 7
  1.3 Numerical Methods ....................................................... 9
    1.3.1 Hydrodynamics with Enzo ................................. 9
    1.3.2 Radiative Processes with Cloudy ....................... 11

Chapter 2. Metal Cooling in Simulations of Cosmic Structure Formation .............................................. 16
  2.1 Introduction ............................................................... 16
  2.2 Numerical Method ....................................................... 17
    2.2.1 Calculation of Metal Cooling Rates .................... 17
    2.2.2 Implementation in Hydrodynamic Simulations .......... 18
  2.3 Metals in Low-Temperature Gases ............................... 21
    2.3.1 Dominant Coolants ......................................... 21
    2.3.2 Dust Grains .................................................... 22
    2.3.3 Thermal Instability and Fragmentation ................ 23
    2.3.4 Effects of the Cosmic Microwave Background ....... 24
  2.4 Discussion ............................................................... 25
  2.5 Future Development ................................................... 26

Chapter 3. Simulations I ........................................................ 44
  3.1 Introduction ............................................................... 44
  3.2 Simulation Setup ....................................................... 45
  3.3 Results ................................................................. 46
  3.4 Discussion ............................................................... 48

Chapter 4. Simulations II ....................................................... 54
  4.1 Introduction ............................................................... 54
  4.2 Simulation Setup ....................................................... 56
  4.3 Results ................................................................. 57
  4.4 Discussion ............................................................... 59
### List of Tables

<table>
<thead>
<tr>
<th>Table</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.1</td>
<td>Solar Abundances in Cloudy</td>
<td>27</td>
</tr>
<tr>
<td>3.1</td>
<td>Final States</td>
<td>50</td>
</tr>
<tr>
<td>4.1</td>
<td>Final States</td>
<td>63</td>
</tr>
</tbody>
</table>
# List of Figures

<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.1</td>
<td>First Star Simulation Slices 1</td>
<td>13</td>
</tr>
<tr>
<td>1.2</td>
<td>First Star Simulation Slices 2</td>
<td>14</td>
</tr>
<tr>
<td>1.3</td>
<td>First Star Simulation Radial Profiles</td>
<td>15</td>
</tr>
<tr>
<td>2.1</td>
<td>Cooling Functions without H₂</td>
<td>28</td>
</tr>
<tr>
<td>2.2</td>
<td>Low-Temperature Cooling Functions</td>
<td>29</td>
</tr>
<tr>
<td>2.3</td>
<td>Cooling Components at $n_H = 10^2$ cm⁻³: C and O</td>
<td>30</td>
</tr>
<tr>
<td>2.4</td>
<td>Cooling Components at $n_H = 10^2$ cm⁻³: Fe, S, and Si</td>
<td>31</td>
</tr>
<tr>
<td>2.5</td>
<td>Cooling Components at $n_H = 10^3$ cm⁻³: C and O</td>
<td>32</td>
</tr>
<tr>
<td>2.6</td>
<td>Cooling Components at $n_H = 10^3$ cm⁻³: Fe, S, and Si</td>
<td>33</td>
</tr>
<tr>
<td>2.7</td>
<td>Cooling Components at $n_H = 10^4$ cm⁻³: C and O</td>
<td>34</td>
</tr>
<tr>
<td>2.8</td>
<td>Cooling Components at $n_H = 10^4$ cm⁻³: Fe, S, and Si</td>
<td>35</td>
</tr>
<tr>
<td>2.9</td>
<td>Cooling Components at $n_H = 10^5$ cm⁻³: C and O</td>
<td>36</td>
</tr>
<tr>
<td>2.10</td>
<td>Cooling Components at $n_H = 10^5$ cm⁻³: Fe, S, and Si</td>
<td>37</td>
</tr>
<tr>
<td>2.11</td>
<td>Dominant Coolants at $n_H = 10^9$ cm⁻³</td>
<td>38</td>
</tr>
<tr>
<td>2.12</td>
<td>Cooling from Dust Grains</td>
<td>39</td>
</tr>
<tr>
<td>2.13</td>
<td>The Fragmentation Criterion at Various Metallicities</td>
<td>40</td>
</tr>
<tr>
<td>2.14</td>
<td>Thermal Instabilities at Various Metallicities</td>
<td>41</td>
</tr>
<tr>
<td>2.15</td>
<td>Double Instabilities at Various Metallicities</td>
<td>42</td>
</tr>
<tr>
<td>2.16</td>
<td>Double Instabilities at Various Metallicities with CMB</td>
<td>43</td>
</tr>
<tr>
<td>3.1</td>
<td>Density Slices</td>
<td>51</td>
</tr>
<tr>
<td>3.2</td>
<td>Radial Profiles</td>
<td>52</td>
</tr>
<tr>
<td>3.3</td>
<td>Clump Masses</td>
<td>53</td>
</tr>
<tr>
<td>4.1</td>
<td>Cooling Functions at Low Temperature</td>
<td>64</td>
</tr>
<tr>
<td>4.2</td>
<td>$Z_{cr}$ at 200 K</td>
<td>65</td>
</tr>
<tr>
<td>4.3</td>
<td>Density Slices - $Z = 0$</td>
<td>66</td>
</tr>
<tr>
<td>4.4</td>
<td>Density Slices - $Z = 10^{-6} Z_\odot$</td>
<td>67</td>
</tr>
<tr>
<td>4.5</td>
<td>Density Slices - $Z = 10^{-5} Z_\odot$</td>
<td>68</td>
</tr>
<tr>
<td>4.6</td>
<td>Density Slices - $Z = 10^{-4} Z_\odot$</td>
<td>69</td>
</tr>
<tr>
<td>4.7</td>
<td>Density Slices - $Z = 10^{-3.5} Z_\odot$</td>
<td>70</td>
</tr>
<tr>
<td>4.8</td>
<td>Density Slices - $Z = 10^{-3} Z_\odot$</td>
<td>71</td>
</tr>
<tr>
<td>4.9</td>
<td>Density/Mass Profiles</td>
<td>72</td>
</tr>
<tr>
<td>4.10</td>
<td>Temperature/Velocity Profiles</td>
<td>73</td>
</tr>
<tr>
<td>4.11</td>
<td>Accretion Rates</td>
<td>74</td>
</tr>
<tr>
<td>4.12</td>
<td>Density-Temperature Evolution</td>
<td>75</td>
</tr>
<tr>
<td>4.13</td>
<td>Density Slices at $n \sim 10^2$ cm⁻³ (1)</td>
<td>76</td>
</tr>
<tr>
<td>4.14</td>
<td>Density Slices at $n \sim 10^2$ cm⁻³ (2)</td>
<td>77</td>
</tr>
<tr>
<td>4.15</td>
<td>Density Slices at $n \sim 10^5$ cm⁻³ (1)</td>
<td>78</td>
</tr>
<tr>
<td>4.16</td>
<td>Density Slices at $n \sim 10^5$ cm⁻³ (2)</td>
<td>79</td>
</tr>
<tr>
<td>4.17</td>
<td>Density Slices for $Z = 10^{-3.5} Z_\odot$ at $n \sim 10^3$, $10^4$, and $10^5$ cm⁻³</td>
<td>80</td>
</tr>
<tr>
<td>Chapter 4.18</td>
<td>Density Slices for $Z = 10^{-3} Z_\odot$ at $n \sim 10^2, 10^3, \text{and} 10^4 \text{cm}^{-3}$</td>
<td>81</td>
</tr>
<tr>
<td>Chapter 4.19</td>
<td>Density Slices - $Z = 10^{-3} Z_\odot$ w/o CMB</td>
<td>82</td>
</tr>
<tr>
<td>Chapter 4.20</td>
<td>Mass-scale vs. Metallicity</td>
<td>83</td>
</tr>
<tr>
<td>Chapter 4.21</td>
<td>Cooling with $3 \times C$ and O</td>
<td>84</td>
</tr>
<tr>
<td>Chapter 4.22</td>
<td>Cooling with $10 \times C$ and O</td>
<td>85</td>
</tr>
<tr>
<td>Chapter 4.23</td>
<td>Cooling with $100 \times C$ and O</td>
<td>86</td>
</tr>
<tr>
<td>Chapter 4.24</td>
<td>Mass-scale vs. Metallicity with $3 \times C$ and O</td>
<td>87</td>
</tr>
<tr>
<td>Chapter 4.25</td>
<td>Mass-scale vs. Metallicity with $10 \times C$ and O</td>
<td>88</td>
</tr>
<tr>
<td>Chapter 4.26</td>
<td>Mass-scale vs. Metallicity with $100 \times C$ and O</td>
<td>89</td>
</tr>
</tbody>
</table>

| Chapter 5.1 | Thermal Instabilities for Nonsolar Abundance Patterns | 95 |
Acknowledgments

I am deeply indebted to my advisor, Steinn Sigurdsson, for providing me with invaluable guidance and encouragement that extended far past scientific development. I also thank my thesis committee, Niel Brandt, Jane Charlton, Deirdre Shoemaker, and Richard Wade for their participation. Special thanks to Jane Charlton for comments on the manuscript, and to Richard Wade for detailed comments and interesting coffee-time discussions.

Thanks to Tom Abel for introducing me to computational astrophysics, to Greg Bryan for extremely helpful discussions and for creating the Enzo code, and to Mike Norman for providing me with the resources I needed to finish this work. Thanks to Brian O’Shea and Matthew Turk for helpful discussions, and endless help with Enzo, and to Jason Tumlinson for even more helpful discussions.

Special thanks to my family, for giving me everything I have needed to make it this far, and for always making me feel good about myself. Finally, thanks most of all to Ana de Prada Pérez for everything else. Te quiero mucho como la trucha al trucho.

This work was supported by the Department of Astronomy & Astrophysics at The Pennsylvania State University, and by Hubble Space Telescope Theory Grant HST-AR-10978.01. Portions of this thesis have been published or submitted for publication (Smith & Sigurdsson 2007; Smith et al. 2007).
Chapter 1

Introduction

1.1 The First Stars

1.1.1 First Insights into the First Stars

One of the major successes of the Big Bang model was the prediction of the chemical composition of the early universe. A scenario in which elements were produced in a nonequilibrium period of high temperature and density, quickly curtailed by the expansion and cooling of the universe was laid out in Alpher et al. (1948), the famous $\alpha \beta \gamma$ paper, and in Alpher & Herman (1950). Due to the short period in which temperatures were hot enough for fusion, only a few minutes, and the absence of stable nuclei with atomic weights of 5 and 8, only H and He, along with scarce amounts of D and Li were present at the end of Big Bang Nucleosynthesis, as was predicted accurately in some of the earliest calculations of this nature, e.g., (Peebles 1966; Wagoner et al. 1967).

The consequences of this were realized by Saslaw & Zipoy (1967), who first theorized that radiative cooling from H$_2$ would play a crucial role in the formation of the first structures out of gas that was void of heavy elements. Soon after, Peebles & Dicke (1968) paired the concept of H$_2$ cooling in primordial gas with the cosmological Jeans length (Gamow 1948; Peebles 1965) to calculate that the first bound structures in the universe were of the scale of $\sim 10^5 \, M_\odot$. Noting that this is roughly the mass of globular clusters, they wrongly predicted that thermal instabilities brought on by H$_2$ cooling would lead to fragmentation of the cloud into solar-mass-sized objects, creating these globular clusters. They realized, however, that this could not explain why globular clusters were universally observed to be enriched with, at least, some finite amount of metals. Interestingly, just prior to this, Doroshkevich et al. (1967) arrived at a similar value for the mass of the first bound objects, yet concluded that no fragmentation would occur, resulting in the formation of a single, gigantic star. More studies soon after this investigated the cooling and formation of H$_2$ in the context of the formation the first structures (Matsuda et al. 1969; Takeda et al. 1969; Hirasawa 1969).

More than 20 years earlier, Baade (1944) observed that stellar populations fell into two distinct groups, type I and type II, now referred to as Population I and Population II. Population I stars have metallicities that are roughly solar and feature many O and B stars, while Population II, found mainly in globular clusters, are deficient in metals by, at least, a factor of ten from the sun, with no bright, early type stars. In 1957, Burbidge, Burbidge, Fowler, and Hoyle published a comprehensive report on the various physical processes responsible for the synthesis of all elements observed in the universe (Burbidge et al. 1957). The formation of many of these elements involved the triple-$\alpha$ process, something that requires extremely high temperatures sustained for longer than the period of Big Bang Nucleosynthesis. Schwarzschild & Spitzer (1953) proposed
that a now-extinct generation of massive stars was required to provide the level of metal-enrichment observed in Population I stars. In the conclusion of their work, Schwarzschild and Spitzer also noted that the idea of metallicity evolving with time could only fit into the framework of a universe that had an actual beginning. van den Bergh (1962) and Schmidt (1963) later noted that G and K stars with iron abundances less than about 10% of the solar value were far more scarce than expected within the solar neighborhood. This became known as the “G-dwarf problem.” After many years of fruitless searching for stars with no heavy elements, e.g. (Bond 1970), it was determined most likely that no purely, metal-free stars could have formed with main sequence lifetimes longer than the age of the universe \((M \lesssim 0.8 \, M_\odot)\). The classification system of Baade (1944) was extended by Bond (1981) to include the predicted, yet undiscovered, population of nearly zero-metallicity stars, referred to for the first time as Population III. While the original definition of Population III from Bond (1981) applies to stars with \([\text{Fe}/\text{H}] < -3\), from here the term Population III will only refer to stars with exactly zero metallicity, as it is currently used.

### 1.1.2 What We Know Now

The importance of \(\text{H}_2\) has been understood since the days of Saslaw & Zipoy (1967) and Peebles & Dicke (1968). Much of the advancement of our knowledge of the first stars since then has come from continually improved physical treatment of the chemistry of primordial gas, but in particular, \(\text{H}_2\) (Hutchins 1976; Lepp & Shull 1984; Mac Low & Shull 1986; Dalgarno & Lepp 1987; Abel et al. 1997; Galli & Palla 1998; Stancil et al. 1998; Lepp et al. 2002). In the current epoch, \(\text{H}_2\) forms mainly via association on the surfaces of dust-grains (Gould & Salpeter 1963). In the early universe, where no dust yet exists, \(\text{H}_2\) forms mainly through two sets of reactions: the \(\text{H}^-\) channel,

\[
\begin{align*}
\text{H} + \text{e}^- & \rightarrow \text{H}^- + \gamma, \\
\text{H}^- + \text{H} & \rightarrow \text{H}_2 + \text{e}^-,
\end{align*}
\]

and the \(\text{H}_2^+\) channel,

\[
\begin{align*}
\text{H} + \text{H}^+ & \rightarrow \text{H}_2^+ + \gamma, \\
\text{H}_2^+ + \text{H} & \rightarrow \text{H}_2 + \text{H}^+.
\end{align*}
\]

Very recently, it has been argued by Hirata & Padmanabhan (2006) that an \(\text{HeH}^+\) channel:

\[
\begin{align*}
\text{He} + \text{H}^+ & \rightarrow \text{HeH}^+ + \gamma, \\
\text{HeH}^+ + \text{H} & \rightarrow \text{H}_2^+ + \text{He},
\end{align*}
\]

can out-compete the \(\text{H}_2^+\) channel. Before the formation of luminous objects, all of these channels rely on a small amount of \(\text{H}\) ions and free electrons remaining after recombination, due to the expansion of the universe. Stancil et al. (1998) calculated the level of fractional ionization after recombination to be \(~2 \times 10^{-4}\). At much higher densities \((n \gtrsim 10^9 \, \text{cm}^{-3})\), \(\text{H}_2\) forms very quickly via 3-body reactions (Palla et al. 1983):

\[
\text{H} + \text{H} + \text{H} \rightarrow \text{H}_2 + \text{H},
\]
and

\[ H + H + H_2 \rightarrow H_2 + H_2. \]  

(1.5)

The major importance of \( H_2 \) comes from the fact that it is the only coolant in primordial gas for temperatures less than \( 10^4 \) K. For \( T \gtrsim 10^4 \) K, primordial gas cools very efficiently through collisional excitations of H and He, Bremsstrahlung, and inverse-Compton. Without \( H_2 \), the cooling rate essentially drops to zero below \( 10^4 \) K. As a perfectly symmetric molecule, \( H_2 \) lacks a permanent dipole moment, and is actually a relatively inefficient radiator, cooling through rotational and vibrational transitions. The lowest-lying transition is the \( 2\rightarrow0 \) rotational transition, with an energy equivalent temperature, \( T = \frac{h \nu}{k} \), of 512 K, where \( h \) is Planck’s constant, \( \nu \) is the transition frequency, and \( k \) is Boltzmann’s constant. The \( 1\rightarrow0 \) transition is forbidden in \( H_2 \). In low density gas, emission from an \( H_2 \) molecule occurs immediately following a collisional excitation. Hence, the cooling from \( H_2 \) is proportional to \( n^2 \). As the number density rises to \( n \sim 10^{24} \) cm\(^{-3} \), however, the \( H_2 \) energy levels begin to be populated according to local thermodynamic equilibrium (LTE). At this point, the cooling rate only scales as \( n \). As will be shown later, the cooling behavior of \( H_2 \) has a profound influence on the nature of metal-free stars.

Long before any baryons were able to have an impact on the evolution of the universe, however, the formation and growth of structure was completely dominated by the dynamics of cold dark matter (CDM), which we now know comprises roughly 85% of the total matter and 24% of the total energy density (Spergel et al. 2003, 2007). In CDM theory, dark matter acts like a collisionless fluid which interacts with itself and normal matter only through gravity. Shortly after the Big Bang, the dark-matter density is almost constant, with only small deviations resulting from quantum mechanical fluctuations magnified by a brief period of exponential growth of the universe, known as inflation. The concept of inflation, first introduced by Guth (1981), explains why the temperature of the cosmic microwave background (CMB) is observed to be so similar in regions of the universe that are not causally connected and eliminates the need for fine-tuning of the cosmological parameters in order to produce a flat universe. The over-density,

\[ \delta \equiv \frac{\rho - \bar{\rho}}{\bar{\rho}}, \]  

(1.6)

where \( \bar{\rho} \) is the mean matter density, for a tiny dark-matter perturbation grows as the scale factor,

\[ a \equiv \frac{1}{1 + z}, \]  

(1.7)

where \( z \) is the redshift, for as long as \( \delta \ll 1 \). Very early on, baryons are coupled to the radiation, prohibiting the growth of any baryonic structure. Only after they have decoupled from the radiation, at \( z_{\text{dec}} \sim 1000 \), are the baryons free to settle into dark-matter potential wells. Even though the density continues to increase, through steady accretion and mergers, the size of the perturbation initially increases, due to the expansion of the universe. Eventually, however, the density becomes great enough to overcome Hubble expansion, and the dark-matter halo begins to collapse. Even without baryons, asymmetries in the structure of the halo prevent it from collapsing to a point.
Instead, the halo undergoes a process known as violent relaxation (Lynden-Bell 1967), ending up in a state of virial equilibrium. The baryons, powerless to control their own destiny, are heated via shocks during violent relaxation to the virial temperature of the halo, given by

\[ T_{\text{vir}} = \frac{GM\mu m_H}{2kR_{\text{vir}}}, \]

(1.8)

where \( G \) is the gravitational constant, \( M \) is the mass of the halo, \( \mu \) is the mean molecular weight, \( k \) is Boltzmann's constant, and \( R_{\text{vir}} \), the virial radius, is defined as the radius at which the mean density exceeds the critical density at that redshift by \( \sim 18\pi^2 \) (Peebles 1980; Bryan & Norman 1998).

After virialization, the next phase of evolution is now determined by the baryons. In order for a gas cloud to collapse, it must be able to efficiently rid itself of its excess thermal energy (Silk 1977; Rees & Ostriker 1977). As discussed earlier, the rate of cooling in primordial gas is dependent on the amount of \( \text{H}_2 \) that is able to form. Using analytical approximations for the growth of spherically symmetric dark-matter halos (Press & Schechter 1974) and the formation and cooling rate of \( \text{H}_2 \) (Hollenbach & McKee 1979; Lepp & Shull 1983), Tegmark et al. (1997) found that halos in which the \( \text{H}_2 \) fraction is able to reach a critical value of \( \sim 5 \times 10^{-4} \) are able cool efficiently enough to collapse. Halos where the \( \text{H}_2 \) fraction does not reach this critical value remain supported by gas pressure and do not collapse. Similar results have been achieved using full numerical simulations to model the evolution of cosmic structure (Abel et al. 1998; Fuller & Couchman 2000; Yoshida et al. 2003). Knowing the requirements for a dark-matter halo to host a collapsing gas-cloud, one can make a reasonable statement about when the first stars are able to form. Since the field of initial density fluctuations is Gaussian, however, it is impossible to say when the very first star formed, because it is impossible to know what the largest deviation was from the mean density (Glover 2005). Instead, a compromise is made between choosing a level of deviation from the mean density that is high enough to result in a relatively early collapse of the halo, yet not so high that the probability of its occurrence is exceedingly small. This has led to the selection of the 3\( \sigma \) peak, which reaches the critical \( \text{H}_2 \) fraction at \( z \sim 20 \), when its virial temperature is \( \sim 1000 \) K (Tegmark et al. 1997). One study to locate the truly first star, performed by Gao et al. (2005), identified the most massive halo in a simulation of large-scale structure and followed its evolution backward in time to the formation of the first parent halo. Following the criteria of previous works, they concluded that a primordial star could have formed inside this halo as early as \( z = 49 \).

Star-formation is one of the most challenging processes to simulate numerically, as it demands extreme dynamic range, defined roughly as the ratio of a simulation box-size to the smallest resolved length-scale. In 2000, Martin Rees claimed that numerical simulations were now able to include the baryonic physics required to accurately study the formation of the first structures (Rees 2000). In fact, some of the greatest advancements in the study of the formation of the first stars came around this time, with the adaptive mesh refinement simulations of Abel et al. (2000, 2002), and the smoothed particle hydrodynamics simulations of Bromm et al. (1999, 2002), both performed in three dimensions. The first simulations by each group were able to follow the evolution of the collapsing gas-cloud to densities of \( n \geq 10^4 \) cm\(^{-3} \). The implementation of 3-body
formation of $H_2$ in Abel et al. (2002) allowed them to reach densities of $n > 10^{12} \text{ cm}^{-3}$. To follow the later stages of evolution, Bromm et al. (2002) added the use of sink particles to their simulations. Both simulations begin at $z = 100$, centering on a 3-4$\sigma$ peak in the density field. Figures 1.1–1.3 show the results of a first star simulation run with same code as Abel et al. (2002), to be used as a control run in a future study. The star-forming halo sits at the intersection of dense filaments (Figure 1.1 left). The gas in the halo has been shock-heated up to the virial temperature, $T \sim 1000$ K (Figure 1.1 bottom-center), stimulating the formation of $H_2$ to a fraction, $f_{H_2} \gtrsim 10^{-4}$ (Figure 1.1 bottom-right). Near the center of the halo, the $H_2$ fraction quickly rises to $\sim 10^{-3}$ (Figures 1.2 top-right and 1.3D). As previously discussed, the lowest lying transition of $H_2$ has an energy equivalent temperature of 512 K. In practice, collisions between $H_2$ molecules and $H$ atoms in the high-energy tail of the thermal distribution allows the gas to cool to a minimum temperature of $\sim 200$ K (Figures 1.2 top-center and 1.3B). When the central density reaches $\sim 10^4$ cm$^{-3}$, the $H_2$ populations become thermalized, resulting in a decrease in cooling efficiency and an increase in temperature. The temperature floor at 200 K and $n \sim 10^5$ cm$^{-3}$ marks the end of free-fall collapse and fragmentation for the gas-cloud (Larson 2005). The resulting mass-scale, given by the Jeans mass, at this temperature, $T$, and density, $\rho$, is $\sim 1000 \, M_\odot$, where the Jeans mass is expressed as

$$M_J = \left( \frac{5kT}{G\mu m_H} \right)^{3/2} \left( \frac{3}{4\pi \rho} \right)^{1/2}.$$ (1.9)

The cooling time has now risen above the dynamical time, and the central core is in a quasi-hydrostatic state, slowly increasing in density. Once the core has reached densities of $n \sim 10^9$ cm$^{-3}$, $H_2$ formation via 3-body processes (Equations 1.4 and 1.5) quickly raise the $H_2$ fraction to near unity. The drastic increase in $H_2$ fraction increases the cooling rate, lowering the temperature slightly. The simulation of Abel et al. (2002) ends with a single, fully molecular core of a few $M_\odot$ (Figure 1.2 bottom-right). At the endpoint of the simulations, the central core is accreting very rapidly, and both Abel et al. (2002) and Bromm et al. (2002) conclude that the first star will be very massive ($M > 100 \, M_\odot$) and essentially isolated. Abel et al. (2002) found that only one prestellar core forms, while Bromm et al. (2002) claimed that a few cores can form if the halo has a slightly higher spin parameter than the halo simulated by Abel et al. (2002). The spin parameter is expressed as

$$\lambda = \frac{L E^{1/2}}{GM^{3/2}},$$ (1.10)

where $L$ is the angular momentum, $E$ is the energy, and $M$ is the mass. N-body simulations by Barnes & Efstatthiou (1987) found that the average halo spin parameter to be, $\lambda \simeq 0.05$. Similar massive prestellar clumps were also found in the two-dimensional simulations of Nakamura & Umemura (2001) when starting from filaments with initial densities of $n \leq 10^5$ cm$^{-3}$. Surprisingly, though, Nakamura & Umemura (2001) found that filaments with higher initial densities would continue to fragment to very high densities, producing low-mass clumps. It is unlikely, however, that such initial conditions are actually realistic. Very recently, a new generation of three-dimensional simulations by Yoshida et al. (2006) were able to follow the formation of the first star to densities
of $n \sim 10^{16}$ cm$^{-3}$, where cooling via collisionally-induced emission (CIE) of H$_2$ becomes important. CIE occurs when H$_2$ molecules collide with either an H or He atom or another H$_2$ molecule, temporarily creating a 'supermolecule' with a nonzero dipole moment (Lenzuni et al. 1991). Despite the sudden increase in cooling rate, Yoshida et al. (2006) found that, much like the case of increased cooling from 3-body H$_2$ formation, the thermal instability resulting from the onset of CIE it too weak to trigger renewed fragmentation, which agrees with the one-dimensional simulations of Ripamonti & Abel (2004). The main conclusion from these simulations is that the collapsing gas-cloud does not fragment, unless there is considerable rotation, and that the resulting star is, most likely, very massive.

Other works have investigated the role of other coolants available in primordial gas. Deuterium, D, can be an efficient coolant when paired with an H atom to make HD. Its asymmetry makes it a much more efficient radiator than H$_2$. HD can also cool to lower temperatures, since the $1 \rightarrow 0$ rotational transition, with an effective temperature of $\sim$160 K, is allowed. HD cooling was included in the simulations of Bromm et al. (2002) and Yoshida et al. (2006). Both of these works conclude that the evolution of the protostar is largely unaffected by the inclusion of HD, owing mainly to the low ratio of HD to H$_2$ ($\lesssim 10^{-3}$) throughout most of the collapse. Li has not been included in simulations of primordial star-formation, but was studied extensively in the context of the chemistry of the early universe by Galli & Palla (1998). The vast majority of LiH is in the form of LiH$^+$, whose total abundance peaks at $\sim$10$^{-17}$, making Li essentially negligible.

Despite their successes, however, numerical simulations have only been able to come within roughly 10 orders of magnitude of actual stellar densities. In essence, they have not yet even formed what is considered to be a protostar. Numerical simulations have entered the realm where considerations of optical depth must be made, making the task at hand significantly more difficult. While it appears most likely, from the current knowledge, that only a single star will form out of the dense clump, the final mass of the star when it moves onto the main sequence is constrained only within a couple orders of magnitude. At the heart of the problem is understanding the complex and opposing processes of protostellar accretion and feedback. The accretion onto a primordial protostar was studied with one-dimensional simulations by Omukai & Nishi (1998) and Ripamonti et al. (2002). Tan & McKee (2004) used analytical approximations to study accretion through an accretion disk. While slightly different, they all arrived at accretion rates that can be approximated by power-laws in time, with a power-law index between -0.34 and -0.27, normalized to $\sim$0.1 $M_\odot$ yr$^{-1}$. Bromm & Loeb (2004) employed sink particles created at high densities in three-dimensional simulations. Their results were similar to the previous works described above for the first $10^3$ years, but found that the power-law index steepens to -0.6 after that. Very recently, O'Shea & Norman (2007) performed a series of three-dimensional, primordial star-formation simulations with host halos forming at different redshifts. Their results showed that the maximum rate of accretion onto the protostar varied by 2 order of magnitude between stars forming at $z = 33$ and $z = 20$. While they were not able to follow the evolution any further than previous works, their work suggested that the first stars had a wide range of masses. Currently, the general consensus from first-star formation theory is that the first stars
had masses, $30 M_\odot \leq M \leq 300 M_\odot$. A direct calculation of the masses of the first stars will require three-dimensional hydrodynamics coupled with full radiative transfer, something that is still some years away.

1.2 Moving from the First to the Second Stars

The original stellar initial mass function (IMF) proposed by Salpeter (1955),

$$\frac{dN}{dM} \propto M^{-2.35},$$

where $dN/dM$ is the number of stars with masses between $M$ and $M + dM$, has been supported by observations for $M \geq 1 M_\odot$ (Larson 2005). Below $1 M_\odot$, the IMF appears to flatten and then decline below $0.1 M_\odot$ (Scalo 1998). More generally, the star-formation process at work in the local universe seems to have a favored mass-scale, just below $1 M_\odot$. Despite our lack of knowledge of the exact nature of the first stars, it is well accepted that they were completely unlike the stars that occupy the universe at the present day. The question then arises: how did we get from there (the first stars) to here?

Currently, the only observational evidence for the existence of the first stars is the metals they left behind. Heger & Woosley (2002) calculated that metal-free stars in the mass range, $140 M_\odot \leq M \leq 260 M_\odot$, ended their lives in pair-instability supernovae that could create up to $\sim 100 M_\odot$ of metals and disperse them into the intergalactic medium (IGM) (Madau et al. 2001). Detections of CIV and OVI in the IGM have revealed the universe to be enriched to metallicities, $Z \leq 10^{-3} Z_\odot$, past redshifts, $z \sim 2.5$ (Cowie & Songaila 1998; Ellison et al. 2000; Schaye et al. 2003; Pettini et al. 2003; Aracil et al. 2004). Qian & Wasserburg (2002) and Qian et al. (2002) claimed that the pattern of heavy elements observed in the IGM is consistent with pair-instability supernovae from the first stars, although Tumlinson et al. (2004) have argued against this idea in favor of metal-production from core-collapse supernovae of slightly lower mass, metal-free stars. Nevertheless, it appears that large amounts of metals were produced very early in the history of the universe.

When these metals were injected into the gas that would form the next generation of stars, they increased the efficiency with which that gas could cool by increasing the number of available atomic and molecular transitions. Schneider et al. (2004) claimed that dust could also be produced in the first supernovae, which would raise the cooling rate in star-forming gas through continuum infrared emission and enhanced $H_2$ formation on grain surfaces. Examples of the effect of metals on the cooling rate of gas are shown in Figures 2.1 and 2.2. The collapse of metal-enriched gas was studied in depth, by Omukai (2000); Schneider et al. (2003, 2004); Omukai et al. (2005), using one-zone models with analytical approximations for the density evolution, coupled with very complex chemical networks that include the H, D, He, C, O, and in the latter two cases, dust-grains. For very low metallicities, the additional cooling provided by the metals is not enough to prevent the temperature from increasing when the gas-cloud reaches the temperature floor of $\sim 200$ K at $n \sim 10^4$ cm$^{-3}$ (Figure 1.1). In such cases, star-formation proceeds in the same manner as the first stars. At some critical metallicity, $Z_{cr}$, the cooling rate is high enough that the gas continues to cool below the metal-free temperature floor,
thus, extending the period of free-fall collapse and fragmentation to higher densities and lower temperatures. This critical metallicity is believed to be the point at which the universal mode of star-formation shifts from the high-mass, singular mode of metal-free, Population III stars, to the low-mass, multiply producing mode of Population II and I stars (Bromm & Loeb 2003b). The value of $Z_{cr}$ has been calculated by finding the metallicity, $Z$, at which the cooling time,

$$t_{cool} = \frac{3kT}{2n_H \Lambda(n_H, T, Z)}, \quad (1.12)$$

where $\Lambda$ is the cooling rate, is equal to the dynamical time,

$$t_{dyn} = \sqrt{\frac{3\pi}{16G\rho}}, \quad (1.13)$$

at $n = 10^4$ cm$^{-3}$ and $T = 200$ K. At low temperatures, ($T \leq 1000$ K), the majority of the cooling from metals comes from fine-structure emission of C and O. Bromm & Loeb (2003b) performed the above calculation for individual C and O abundances, finding $[C/H]_{crit} \approx -3.5$ and $[O/H]_{crit} \approx -3.05$, where $[X/H] \equiv \log_{10}(n_X/n_H) - \log_{10}(n_X/n_{H})_\odot$. In their calculation, Bromm & Loeb (2003b) assumed the presence of an ultra-violet, ionizing background, from existing Population III stars, with photon energies, $E_{ph} < 13.6$ eV, that would dissociate all $H_2$ and atomic C, since C$^+$ has an ionization energy of 11.26 eV. O$^+$, by contrast, has an ionization energy of 13.62 eV. Thus, the cooling in Bromm & Loeb (2003b) comes from C$^+$ and O$^+$. A more sophisticated calculation was carried out by Santoro & Shull (2006), who included cooling from $H_2$, C$^+$, O$^+$, Si$^+$, and Fe$^+$. Noting that the cooling rate at a given temperature is not constant with changing density, Santoro & Shull (2006) performed their calculations for number densities up to $10^8$ cm$^{-3}$. When considering all of the coolants listed above, Santoro & Shull (2006) found the critical metallicity to be $10^{-3.78} Z_\odot$ at the density and temperature used by Bromm & Loeb (2003b). They also found, though, that the metal cooling reached peak efficiency at $n \sim 10^6$ cm$^{-3}$, at which point $Z_{cr}$ drops to $10^{-4.05} Z_\odot$.

All of these calculations, however, are unable to provide any conclusive evidence that $Z_{cr}$ marks the transition from Population III to Population II and I star-formation modes. While they can say that the classical fragmentation criterion, $t_{cool} < t_{dyn}$ (Field 1965), is satisfied for some level of chemical enrichment, they cannot confirm whether fragmentation actually occurs. One-zone models, such as those described above, are inherently incapable of this brand of insight, as well. However, Omukai et al. (2005) were able to make some statistical predictions of fragmentation in star-forming clouds by considering the evolution of the elongation of protostellar cores, $\varepsilon \equiv (b - a)/a$, where $a$ and $b$ are the short and long axes of a core. Cores begin with some value of $\varepsilon$, assigned randomly according some distribution function. The growth of $\varepsilon$ is governed by the thermal evolution of the gas during collapse. Simplified significantly, the elongation increases when the cloud cools and decreases when it heats up. When $\varepsilon$ reaches 1, the core fragments into 2 cores, whose elongations are then assigned randomly as before, and the process continues. Their results predicted the formation of high-mass ($M \sim 1000 M_\odot$) clumps for zero metallicity, as expected. They found low-mass ($M \leq 1 M_\odot$) clumps
for $Z = 10^{-5} \ Z_\odot$ and $Z \geq 10^{-3} \ Z_\odot$, but only moderate-mass ($M \sim 10 \ M_\odot$) clumps for $Z = 10^{-4} \ Z_\odot$, due to a sudden temperature increase from chemical heating from 3-body $\text{H}_2$ formation that quickly lowers the elongation. These predictions are only statistical, however, and do not capture the three-dimensional hydrodynamic complexities of actual cloud fragmentation. The first and only three-dimensional, hydrodynamic simulation to study the effect of metal-enrichment on star-forming gas was performed by Bromm et al. (2001). They performed simulations of pre-enriched primordial star formation at metallicities, $Z = 10^{-4} \ Z_\odot$ and $10^{-3} \ Z_\odot$, excluding $\text{H}_2$ cooling. The cloud with $Z = 10^{-4} \ Z_\odot$ is unable to cool and becomes pressure supported at $n \sim 10^3 \ \text{cm}^{-3}$ and temperatures of a few thousand K, and is unable to collapse. On the other hand, the gas in the higher metallicity case cools rapidly to the CMB temperature, and then settles into a disk in which multiple clumps form. Unfortunately, their simulations only had a mass-resolution of $100 \ M_\odot$, which prevented them from following the collapse past densities of $\sim 10^6 \ \text{cm}^{-3}$. Thus, they were unable to know for certain whether low-mass stars could actually form.

To date, many issues regarding the formation of the first low-mass stars are unresolved. How, and during what phases of protostellar evolution does fragmentation occur? When in the history of the universe does the transition from Population III to Population II take place? Does reaching the critical metallicity result in an instantaneous shift from the first-star IMF to a Salpeter IMF, or is there a unique transitional IMF? Also, it is unknown whether star-formation in regions of high pressure and high radiation, such as massive clusters and galactic nuclei, proceeds in the same manner as in less extreme environments. The answers to these questions will require both a definitive calculation of the masses of the first stars, as well as numerical methods that incorporate the complex physics of heavy elements into three-dimensional, hydrodynamic simulations capable of following the collapse of star-forming gas to at least solar-mass scales.

### 1.3 Numerical Methods

Incorporating radiative transfer into hydrodynamic simulations is one of the greatest challenges to computational astrophysics. In theory, a full solution to the radiative transfer equation is straightforward, but it requires integration over position, angle, and frequency, and is well beyond present computation power, and will be so for quite some time. However, many astrophysical situations can be properly modeled with the assumption that the gas is perfectly optically thin. In this case, only the rate of radiative cooling is important, since emitted photons can be considered to escape the medium without further interaction. Even this, however, is a difficult problem, requiring the treatment of a plethora of atomic and molecular processes and chemical reactions. In the research presented here, we have chosen to treat the physics on macroscopic scales (hydrodynamic) separately from the physics on microscopic scales (radiative processes).

#### 1.3.1 Hydrodynamics with Enzo

The problem of star-formation in a cosmological context creates a unique challenge to numerical simulations. Simulating the evolution of cosmic structure requires the use
of large computational volumes, while the star-formation process is one that deals with ever-decreasing scales of space and time. The dynamic range required would make such a calculation impossible on a grid with fixed resolution. We circumvent this obstacle by using a simulation code capable of solving the equations of fluid dynamics on a set of nested grids with varying resolution that can be created and destroyed as needed during the run of the simulation. This technique, originated by Berger & Colella (1989) and known as adaptive mesh refinement, is the basis for the Enzo code, originally written by Greg Bryan, and continually updated by numerous collaborators (Bryan et al. 1995; Bryan & Norman 1997a,b; Norman & Bryan 1999; O'Shea et al. 2004). The operation of Enzo is thoroughly detailed in O'Shea (2005), but a brief description of the main components follows. To follow the evolution of gas in a cosmological setting, Enzo solves the Euler equations of hydrodynamics in an expanding universe (Bryan et al. 1995), defined as

\[
\frac{\partial \rho_b}{\partial t} + \frac{1}{a} \vec{v}_b \cdot \nabla \rho_b = - \frac{1}{a} \rho_b \nabla \cdot \vec{v}_b, \tag{1.14}
\]

\[
\frac{\partial \vec{v}_b}{\partial t} + \frac{1}{a} (\vec{v}_b \cdot \nabla) \vec{v}_b = - \frac{\dot{a}}{a} \vec{v}_b - \frac{1}{a \rho_b} \nabla p - \frac{1}{a} \nabla \phi, \tag{1.15}
\]

\[
\frac{\partial E}{\partial t} + \frac{1}{a} \vec{v}_b \cdot \nabla E = - \frac{\dot{a}}{a} \left(3 \frac{p}{\rho_b} + \vec{v}_b^2 \right) - \frac{1}{a \rho_b} \nabla \cdot (p \vec{v}_b) - \frac{1}{a} \vec{v}_b \cdot \nabla \phi, \tag{1.16}
\]

where \( \vec{v}_b \) is the proper baryon velocity, \( p \) is the proper gas pressure, \( E \) is the energy per unit mass, and \( a \) is the expansion factor (Equation 1.7). The comoving baryon density, \( \rho_b \), and gravitational potential, \( \phi \), in the above equations are related to their proper counterparts by the expansion factor in the following manner:

\[
\rho_b = \frac{1}{a^3} \rho_{b,\text{proper}}. \tag{1.17}
\]

\[
\phi = \Phi + \frac{1}{2} a \ddot{a} x^2. \tag{1.18}
\]

When radiative heating and cooling are included, the term, \((\Gamma - \Lambda)\), is added to the right-hand side of Equation 1.16, where \( \Gamma \) and \( \Lambda \) are the heating and cooling rates. Equations 1.14–1.16 are closed with:

the equation of state,

\[
E = \frac{p}{(\gamma - 1) \rho_b} + \frac{1}{2} \vec{v}_b^2; \tag{1.19}
\]

the Poisson equation,

\[
\nabla^2 \phi = \frac{4 \pi G}{a} (\rho_b + \rho_{dm} - \rho_0), \tag{1.20}
\]

and the expansion of the universe,

\[
\frac{\ddot{a}}{a} = - \frac{4 \pi G}{3a^3} \left( \rho_0 + \frac{3 \rho_0}{c^2} \right) + \frac{\Lambda}{3}, \tag{1.21}
\]

where \( \rho_{dm} \) is the dark-matter density and \( \rho_0 \) is the background density. In Equation 1.21, \( \Lambda \) is the cosmological constant, not the cooling rate. The dark matter is treated as discrete set of collisionless particles with an N-body scheme. The movement of the
particles is described by Newton’s equations of motion:

$$\frac{d\mathbf{x}_{dm}}{dt} = \frac{1}{a} \mathbf{v}_{dm},$$

(1.22)

$$\frac{d\mathbf{v}_{dm}}{dt} = \frac{1}{a} \mathbf{a} - \frac{1}{a} \nabla \phi.$$  

(1.23)

Equations 1.14–1.16 are integrated using a version of the piecewise parabolic method (PPM) of Colella & Woodward (1984), adapted for cosmological simulations, which is second-order accurate in time and space, and conserves mass, momentum, and energy. The gravitational potential in Equation 1.20 is solved by sampling the dark-matter particles onto a grid with the baryon density and performing a fast fourier transform over the grid. The primary chemical network in Enzo follows the nonequilibrium chemistry and cooling of 9 species of H and He: H, H+, H−, H2, H2+, He, He+, He++, and e− (Abel et al. 1997; Anninos et al. 1997), with the addition of 3-body H2 formation. The inclusion of the radiative cooling from elements heavier than He in Enzo is described in Chapter 2. For each grid in the computation box, the gravity (Equation 1.20) is solved first, followed by the expansion of the universe (Equation 1.21 and the expansion terms in Equations 1.14–1.16), then the ρ, v, and E terms in Equations 1.14–1.16, then the positions and velocities of the dark-matter particles, and finally, the energy term is updated with the calculation of the cooling rate. After all of the physical quantities are updated, each grid cell is evaluated to see if a new grid should be constructed with finer spatial resolution. Refinement can be set to occur for critical overdensities of gas and dark matter, large gradients in density, energy, or pressure, and if the cooling time is shorter than the integration timestep. If any cells within a grid are flagged for refinement, a new child grid with, typically, twice the spatial resolution is constructed that minimally covers the flagged cells. The steps described above, including refinement evaluation, are performed in the same manner for the new child grid. Refinement can occur indefinitely within the physical limits of the machine. In a simulation of star-formation, where spatial and time-scales are progressively smaller, a maximum level of refinement is chosen before-hand, ending the simulation when it is reached.

1.3.2 Radiative Processes with Cloudy

Cloudy is a one-dimensional photoionization code, written by Gary Ferland and associates (Ferland et al. 1998). Its primary purpose is to compute the transmitted spectrum through a gas-cloud of known density, or density behavior, and chemical composition, that is irradiated by a source of known spectral intensity and shape. This is accomplished by breaking the cloud up into layers, or zones, over which the physical conditions within the cloud change very little. Radiation transport in Cloudy is treated by escape probability formalism, e.g., (Rybicki 1984; Hubeny 2001). The major strength of this code is that it does not assume a mean opacity for the radiation transport. Instead, the opacity is rigorously calculated over an energy range, $1.36 \times 10^{-7}$ eV (λ ≈ 910 cm) ≤ hν ≤ 102 MeV. Included in the opacity calculation are the following processes: electron scattering, photoelectric absorption for all elements up to atomic number 30 (Zn) and their ionic species including H−, molecular and dust-grain absorption, inverse
Bremsstrahlung, damping wings of strong lines, and e\(^-\)-e\(^+\) pair-production (Ferland 2006). Collisional excitation, de-excitation, ionization, and recombination are also included in the radiation transport calculation. Cloudy can handle virtually any spectral shape within the energy range listed above. The code is valid within the temperature range, 10 K \(\leq T \leq 10^9\) K, for number densities of \(10^{-8} \text{ cm}^{-3} \leq n \leq 10^{13} \text{ cm}^{-3}\).

As described further in Chapter 2, we use Cloudy in a somewhat unconventional manner. We are not interested in the transmission of radiation through a medium, but we are interested in the process by which Cloudy calculates the thermal state of that medium. Cloudy calculates an LTE solution for the cloud by matching the heating and cooling rates, which are functions of the numerous radiative and collisional processes in the code’s expansive arsenal. At low temperatures, the cooling is dominated by fine-structure transitions, and vibration and rotation transitions of molecules. Above \(10^4\) K, the cooling is dominated by bound-bound transitions and recombination of the atomic species. At even higher temperatures, Bremsstrahlung radiation is the main coolant. At low densities, inverse-Compton scattering off the CMB is also important. If dust-grains are present, they contribute to the cooling through infrared continuum emission. Since the code allows us to specify the temperature of the gas, we are able to extract non-LTE heating and cooling rates for any set of physical conditions we choose. These rates can then be stored and used within our numerical simulations. Our use of Cloudy is detailed further in §2.2.1.
Fig. 1.1 Logarithmic slices in number density (left), temperature (center), and H$_2$ fraction (right) of a simulation of first star formation, to be used as a control run in a future study. The slices have widths of $\sim 17$ kpc (top) and $\sim 860$ pc (bottom) proper. The terms, left, center, right, top, and bottom, refer to the figure after being rotated clockwise by 90 degrees. The cosmological parameters used in this simulation are: $\Omega_m = 0.3$, $\Omega_b = 0.04$, $\Omega_{\Lambda} = 0.7$, and $H_0 = 70$ km s$^{-1}$ Mpc$^{-1}$. Initial conditions are courtesy of Brian O’Shea.
Fig. 1.2 Logarithmic slices in number density (left), temperature (center), and H$_2$ fraction (right) of a simulation of first star formation. The slices have widths of $\sim 8.6$ pc (top) and $\sim 1776$ AU (bottom) proper. The terms, left, center, right, top, and bottom, refer to the figure after being rotated clockwise by 90 degrees. Initial conditions are courtesy of Brian O’Shea.
Fig. 1.3 Radial profiles for the first star simulation. A: Number density vs. radius. B: Temperature vs. enclosed gas mass. C: Mass vs. radius. D: H$_2$ fraction vs. enclosed gas mass. The initial output, denoted by the dashed line in each panel, is at $z = 24.5635$. The periods of time separating the subsequent outputs are $\sim 4.5 \times 10^6$, $4.7 \times 10^5$, $3.2 \times 10^5$, $9.5 \times 10^4$, $3.2 \times 10^4$, $1.1 \times 10^4$, 3900, 1500, 700, 300, 200, 100, and 69 years.
Chapter 2

Metal Cooling in Simulations of Cosmic Structure Formation

2.1 Introduction

The first luminous objects in the universe formed from primordial gas, comprised solely of H and He, with only trace amounts of D and Li. The relatively simple chemistry of metal-free gas, combined with tightly constrained cosmological parameters (Spergel et al. 2007), has allowed the formation of the first stars to be simulated with extremely high precision, from the hierarchical growth of their host dark matter halos through to the point where the dense proto-stellar cores becomes optically thick (Abel et al. 2002; Bromm et al. 2002; Bromm & Loeb 2004; Yoshida et al. 2006; O'Shea & Norman 2007; Gao et al. 2007). With the deaths of these stars came the creation of the first heavy elements. Core-collapse and pair-instability supernovae created metals in copious amounts (Heger & Woosley 2002) and ejected them into the IGM (Madau et al. 2001).

The presence of metals alters the dynamics of collapsing gas-clouds by increasing the number of available atomic and molecular transitions, allowing the gas to lose its internal energy more quickly than in case of no metals (Omukai 2000; Bromm et al. 2001; Bromm & Loeb 2003b). The introduction of metals adds a new level of complexity to the problem of simulating the formation and evolution of cosmic structure. Abel et al. (1997) identified a minimal set of 21 chemical reactions necessary for accurately following the non-equilibrium evolution of a gas consisting solely of species of H and He, including H$_2$. Galli & Palla (1998) showed that 33 total reactions were required when including D and Li species to the gas. Omukai (2000) performed one of the first numerical studies of collapsing gas-clouds to consider the contribution of metals. Their chemical network of H, He, C, and O included 50 atomic and molecular species and 478 reactions. While theirs was not a minimal model, the above examples illustrate the great expense associated with the expansion of chemical networks to include additional elements. Other works have studied the effect of metals on star-forming gas using similar methodologies to that of Omukai (2000), e.g., Schneider et al. (2002, 2003, 2006); Omukai et al. (2005). The complexity of the chemical networks used in these studies limited their treatment of gas evolution to one-zone, semi-analytical models. In the earliest work to incorporate metal cooling into three-dimensional hydrodynamic simulations to study metal-enriched star formation, Bromm et al. (2001) used a small set of the most dominant atomic transitions of C, N, O, Fe, Si, and S, as described by Ricotti et al. (1997). Their method also ignored the cooling from H$_2$, which was justified within their study by the assumption of a very large photo-dissociating UV background, but is otherwise an extremely important coolant in low-metallicity environments. For high temperature gases, Sutherland & Dopita (1993) computed metal cooling functions that included 14 heavy elements over a
range of metallicities, with solar abundance patterns. These cooling functions are useful for simulating the IGM and other hot, ionized environments, but a minimum temperature of $10^4$ K makes them inapplicable to studies of the cold, neutral gas associated with star-formation. These cooling functions assume collisional equilibrium of the species and as such cannot capture the important role of UV and X-ray radiation.

We introduce a new method for including the cooling from heavy elements in large-scale hydrodynamic simulations that is valid over a wide range of physical conditions, covers a great number of elemental species, and is fast enough to be used in large-scale numerical simulations. We have utilized the established photoionization software, Cloudy (Ferland et al. 1998) to construct large grids of metal cooling data. We have developed a method to include both the cooling from heavy elements and the non-equilibrium cooling from $\text{H}_2$ in hydrodynamic simulations. This method has been used successfully in the numerical simulations of star formation performed by Smith & Sigurdsson (2007). In §2.2, we describe our method for creating the metal cooling data, including a new code to expedite the process. We, then, present three implementations of the cooling method in the AMR, hydrodynamic/N-body code, Enzo (Bryan & Norman 1997a; O'Shea et al. 2004). In §2.3, we focus on the application of metals to low-temperature environments, identifying the dominant cooling mechanisms, and studying the possibility of fragmentation and thermal instability in metal-enriched gas. Finally, we end with a discussion in §2.4 of the role played by the heavy elements in the formation of structure in the early universe.

2.2 Numerical Method

2.2.1 Calculation of Metal Cooling Rates

At the current time, it is still too computationally expensive and memory intensive to follow the non-equilibrium chemistry for a large set of heavy elements in a three-dimensional hydrodynamic simulation. The exact mass of the first massive stars is not known (Abel et al. 2002; Tan & McKee 2004; Yoshida et al. 2006). Also unknown are the exact yields of early supernovae (Heger & Woosley 2002; Maeder et al. 2005; Nomoto et al. 2006; Rockefeller et al. 2006). Similarly, in many astrophysical systems one might want to model computationally the exact metal distributions. Consequently, it is not clear a priori what level of sophistication of cooling model is needed to adequately capture the hydro and thermodynamic evolution of the gas under consideration. Note that uncertain grain physics also increases the potentially important parameter space. In our approach, we assume ionization equilibrium, which allows us to calculate, in advance, the cooling rate for a parcel of gas with a given density and temperature, with incident radiation of known spectral shape and intensity. For this problem, we find the photoionization code, Cloudy (Ferland et al. 1998), especially apt. Cloudy is conventionally used to model the transmitted spectrum from a cloud of gas with a given chemical composition, being irradiated by a specified source. The code must calculate an equilibrium solution by balancing the incident heating with the radiative cooling from a full compliment of atomic and molecular transitions, as well as continuum emission from dust. The chemical network of Cloudy covers all atomic species from H to Zn, as
well as a multitude of molecular species. Each elemental abundance can be specified individually, giving us the ability to model the cooling from a gas with any composition. Table 2.1 lists the solar abundances of the first 30 elements, relative to H, adopted by Cloudy (Table 9 of Ferland (2006)). The sources for the abundances listed in Table 2.1 are, for C and O, Allende Prieto et al. (2001, 2002); N, Ne, Mg, and Fe, Holweger (2001); and all the rest, Grevesse & Sauval (1998). Since Cloudy permits the use of virtually any input spectrum, we are able to create cooling data that is suitable for any radiation environment. Instead of allowing the code to cycle through temperatures until converging on a thermodynamic equilibrium solution, we use the constant temperature command to fix the temperature externally, allowing us to utilize Cloudy’s sophisticated machinery to calculate cooling rates out of thermal equilibrium. In this manner, we create a grid of heating and cooling values as a function of temperature, gas density, chemical composition, and incident spectrum.

To automate the process of data production and organization, we have created a code, called ROCO (Recursively Organized Cloudy Output.) ROCO uses a recursive algorithm to process user-specified loop parameters, making it possible to create data-grids of any dimension. Commands that are to be issued to Cloudy are given to the ROCO code in either one of two formats - loop commands with a set of parameters through which the code will iterate, and constant commands that are to be issued with the same value during each iteration over the loop commands. Since most uses of Cloudy involve the creation of large grids of models constructed by looping over a set of input parameters, the capabilities of ROCO give it the potential to be useful to a broader community of Cloudy users than just those who would use it to create the cooling tables discussed here. To this end, ROCO is structured in such a way that the post-Cloudy data analysis routines can be easily interchanged to suit the needs of different users. The code features an extra running mode that simply runs Cloudy over the specified parameter-space with no further processing of the data, as well as a template designed to help users create new running modes suited to their specific needs. ROCO also has the ability to run multiple instances of Cloudy simultaneously, greatly reducing runtime. The parallel feature works well on individual machines with multiple processors, as well as Beowulf clusters using the MPI (Message Passing Interface) framework. A copy of the ROCO code will be made available upon request to the authors.

In Figure 2.1, we display the resulting cooling function for gas with \( n_H = 1 \text{ cm}^{-3} \) at metallicities, from \( Z = 0 \) (metal-free) to \( 10 Z_\odot \), over the temperature range, \( 50 \leq T \leq 10^8 \text{ K} \). For these cooling rates, we use the coronal equilibrium command in Cloudy to simulate an environment free of radiation, where all ionization is collisional. We also neglect the cooling from H\(_2\), so as to better illustrate the cooling contribution from metals at temperatures less than \( 10^4 \text{ K} \). We accomplish this by issuing the Cloudy command, no H\(_2\) molecule.

### 2.2.2 Implementation in Hydrodynamic Simulations

We implement our metal cooling method in the Eulerian adaptive mesh refinement hydrodynamic/N-body code, Enzo (Bryan & Norman 1997a; O’Shea et al. 2004). When a simulation is initialized, Enzo reads in the Cloudy/ROCO data-grid, storing the
heating and cooling values as functions of temperature, H number density, and any other parameters, such as spectral intensity, depending on the nature of the simulation. The heating, $\Gamma$, and cooling, $\Lambda$, are stored with code units corresponding to [ergs s$^{-1}$ cm$^3$]. During the simulation, Enzo stores the mass density and internal energy for each grid cell in the box. At each hydrodynamic time-step, the radiative cooling solver cools the gas by lowering the internal energy via a simple Euler update,

$$u_{i,j,k}^{n+1} = u_{i,j,k}^n + \dot{u}_{i,j,k}^n \times \delta t,$$

where $u_{i,j,k}^{n+1}$ denotes the internal energy of the grid cell with (x,y,z) coordinates, (i,j,k), at the (n+1)'th time-step, $\dot{u}$ is the cooling rate in code units corresponding to [ergs s$^{-1}$], and $\delta t$ is the adopted time-step, which is discussed further below. The internal energy and mass density for each grid cell are converted to temperature and number density and the heating and cooling values are calculated by linearly interpolating over the Cloudy/ROCO data-grid. The change in internal energy from the Cloudy/ROCO cooling rates is expressed as

$$\dot{u}_{C/R} = (\Gamma - \Lambda)n_H,$$

where $n_H$ is the H number density. The time-step, $\delta t$, in Equation 2.1, adopts the minimum of the following three values: (1) half of the hydrodynamic time-step, (2) 10% of the cooling time, $(u/\dot{u})$, or (3) the time remaining to have integrated over one full hydrodynamic time-step. For every hydrodynamic time-step, the code subcycles through Equation 2.1, selecting from the three time-steps listed above, until one full hydrodynamic time-step has been completed. This method of subcycling prevents the gas from over-cooling by continuously adjusting the cooling rate as the temperature changes. In the future, we will consider updating Equation 2.1 to a more sophisticated integration scheme.

We implement three distinct versions of the method described above. In the first and simplest version, the cooling is calculated solely from the Cloudy/ROCO data, as in Equation 2.2. The total change in internal energy is

$$\dot{u}_{tot} = \dot{u}_{C/R}.$$

When converting the internal energy to temperature, it is necessary to know the value of the mean molecular weight, $\mu$. In this implementation, we assume $\mu$ to be a constant with the value 1.22. For high temperatures, $T \gtrsim 10^4$ K, this method is sufficient for providing accurate gas cooling within hydrodynamic simulations. This implementation is not suitable, however, when $T \lesssim 10^4$ K and the formation of $H_2$ becomes important. Disregarding formation on grain surfaces and three-body formation, $H_2$ primarily forms through the following channels:

the $H^-$ channel,

$$H + e^- \rightarrow H^- + \gamma,$$

$$H^- + H \rightarrow H_2 + e^-,$$
and the \( \text{H}_2^+ \) channel,

\begin{align*}
\text{H} + \text{H}^+ & \rightarrow \text{H}_2^+ + \gamma, \\
\text{H}_2^+ + \text{H} & \rightarrow \text{H}_2^+ + \text{H}^+.
\end{align*}

(2.5)

When a significant electron fraction exists, these reactions proceed to form \( \text{H}_2 \) very quickly, with the \( \text{H}^- \) channel typically dominating, except in the very high redshift universe \((z > 100)\), where \( \text{H}^- \) is readily destroyed by the CMB (Abel et al. 1997; Bromm et al. 2002). Recently, Hirata & Padmanabhan (2006) have suggested that formation of \( \text{H}_2^+ \) via

\begin{align*}
\text{He} + \text{H}^+ & \rightarrow \text{HeH}^+ + \gamma, \\
\text{HeH}^+ + \text{H} & \rightarrow \text{H}_2^+ + \text{He},
\end{align*}

(2.6)

is responsible for more \( \text{H}_2 \) than the \( \text{H}_2^+ \) channel in Equation 2.5. If, however, the ionization fraction is low, \( \text{H}_2 \) forms very slowly, with equilibrium timescales that can exceed the current age of the universe. The consequence is that \( \text{H}_2 \) formation is so sensitive to the thermal history of the gas that \( \text{H}_2 \) fractions cannot be known without explicitly following the non-equilibrium chemistry during the simulation. We find this to be the case when using Cloudy to compute the cooling rate from \( \text{H}_2 \). In searching for ionization equilibrium, Cloudy integrates over timescales that are unphysically long, leading to an overcalculation of the \( \text{H}_2 \) fraction, producing cooling rates that are too high. We solve this problem in our second implementation by removing the \( \text{H}_2 \) molecule from Cloudy’s chemical network with the \texttt{no H2 molecule} command. We, then, use the established H/He network in Enzo (Anninos et al. 1997; Abel et al. 1997), to follow the abundance of \( \text{H}_2 \), and calculate its associated cooling using the equations of Galli & Palla (1998).

We also include the option to use the \( \text{H}_2 \) cooling rates of Lepp & Shull (1983), which are somewhat outdated, but provide a means of comparison to older simulations. We also include the cooling, or heating, from electrons scattering off the CMB as

\[
\Lambda_{\text{Comp}} = 5.4 \times 10^{-36} (1 + z)^4 n_e (T - T_{\text{CMB}}),
\]

(2.7)

where \( T_{\text{CMB}} = 2.7 (1 + z) \) K (Bromm et al. 2002). We prevent the metals from cooling the gas below the CMB temperature by subtracting the metal cooling rate at \( T = T_{\text{CMB}} \), as in Bromm et al. (2001). The total rate of energy loss applied to the simulation gas in the second implementation is

\[
\dot{u}_{\text{tot}} = \dot{u}_{\text{H}_2} + \dot{u}_{\text{Comp}} + \dot{u}_{C/R},
\]

(2.8)

where \( \dot{u}_{C/R} \) is the cooling rate taken from the Cloudy/ROCO data in the manner described above, with the \( \text{H}_2 \) molecule removed from the calculation. In this implementation, as well as the next one, we calculate the value of \( \mu \) directly from the H/He species fractions, neglecting any addition to the mean molecular weight from the metals. In low-metallicity gases, this approach is reasonable, as the increase in \( \mu \) from the metals only reaches \( \sim 10^{-4} \) for \( Z = 10^{-2} Z_\odot \). Since the Cloudy/ROCO data-grids also store the values of \( \mu \) for each point, this can be added to the value calculated without the heavy elements when the metallicity is very high. It is important to note that we do not
actually pay a price for the lack of H number conservation, since the regions of temperature space where atomic and molecular hydrogen cooling each dominate are mutually exclusive. In other words, even though there are extra hydrogen atoms present for \( T \lesssim 10^4 \) K because of our removal of the \( \text{H}_2 \) molecule in Cloudy, they add nothing to the cooling in this temperature regime.

In the third version, we use the same H/He network of Anninos et al. (1997); Abel et al. (1997) to provide the cooling from atomic H and He, as well as \( \text{H}_2 \). The \( \text{H}_2 \) cooling rates are the same as those used in our second version of the method. Here, the Cloudy/ROCO data-grid contributes only the cooling from the metals. The data-grid is constructed by subtracting a data-grid made with only H and He from one made with the full compliment of elements. In this final method, the total rate of change in internal energy is

\[
\dot{u}_{\text{tot}} = \dot{u}_{\text{H,He}} + \dot{u}_{\text{H}_2} + \dot{u}_{\text{Comp}} + \dot{u}_{\text{C}/\text{R}},
\]

where \( \dot{u}_{\text{H,He}} \) includes the cooling from all atomic species of H and He (Black 1981; Cen 1992). In Figure 2.2, we display low-temperature cooling functions for gases with varying density and metallicity, constructed with the third implementation of the metal cooling method. To produce the data for Figure 2.2, we set up an unphysical, two-dimensional grid in Enzo that varies smoothly over density and temperature. We iterate the reaction network for a time equivalent to that between \( z = 99 \) and 20 (\( \sim 160 \) Myr), with hydrodynamics disabled, then compute the cooling with the third implementation of our metal cooling method, using the \( \text{H}_2 \) cooling rates of Galli & Palla (1998). Since the first stars are predicted to form at the centers of \( \sim 10^6 \) \( M_\odot \) dark matter halos at \( Z \sim 20 \) (Tegmark et al. 1997), integrating the rate equations over this time interval places each of the species in the relative abundances in which they would be found during the epoch of first-star formation. Hence, Figure 2.2 provides a direct comparison of the cooling rate of the gas that formed the first and successive generations of stars.

2.3 Metals in Low-Temperature Gases

2.3.1 Dominant Coolants

Much attention has been given recently to the role of the first heavy elements in transitioning from the singular, high-mass mode of star formation of the first stars to the mode producing stars with a Salpeter initial mass function (IMF). Analytical studies by Bromm & Loeb (2003b) and Santoro & Shull (2006) have focused on the contributions of individual elements toward triggering fragmentation in star-forming clouds. Bromm & Loeb (2003b) suggest C and O to be the dominant coolants in low-metallicity gas, in the presence of an \( \text{H}_2 \) dissociating UV background created by the first stars (Bromm & Loeb 2003a). By calculating the cooling rate necessary to equate the cooling time to the free-fall time at \( n = 10^4 \) \( \text{cm}^{-3} \) and \( T = 200 \) K, the point where \( \text{H}_2 \) cooling becomes inefficient (Abel et al. 2002; Bromm et al. 2002), Bromm & Loeb (2003b) predict individual critical abundances of C and O to be \([C/\text{H}]_{\text{crit}} \simeq -3.5\) and \([O/\text{H}]_{\text{crit}} \simeq -3.05\), where \([A/\text{H}] = \log_{10} (N_A/N_H) - \log_{10} (N_A/N_H)_{\odot}\). Santoro & Shull (2006) consider the cooling from Fe and Si, in addition to C and O, and take into account the density dependence of metal cooling. In doing so, they find that the critical abundance of each element varies with
density, reaching a minimum at a critical density that is different in each case. They also note that different elements dominate different density and temperature regimes.

In Figs. 2.3–2.10, we plot the individual cooling contributions for number densities, \( n_H = 10^2 \) to \( 10^5 \) cm\(^{-3} \). In each case, we create a set of cooling data with the full compliment of elemental species, from H through Zn, with a metallicity of \( 10^{-1} Z_\odot \), neglecting \( \text{H}_2 \). We plot only the coolants whose contributions reach, at least, \( 10^{-3} \) of the total cooling within the temperature range, \( 50 \text{ K} \leq T \leq 5000 \text{ K} \). Since the cooling data were made assuming no incident ionizing radiation, as described in §2.2.1, we observe the dominant C transitions to be from C \( \text{i} \), instead of C \( \text{ii} \), as in Bromm & Loeb (2003b) and Santoro & Shull (2006). The most important coolants in the range plotted are C \( \text{i} \) and O \( \text{i} \). The 369.7 \( \mu \text{m} \) and 609.2 \( \mu \text{m} \) [C \( \text{i} \)] transitions are the strongest for low densities \( (n \leq 10^{-3}) \) and low temperatures \( (T \leq 200 \text{K}) \), as seen in Fig. 2.3. For higher temperatures and densities, [O \( \text{i} \)] emission at 63.2 \( \mu \text{m} \) dominates the cooling (Figs. 2.3, 2.5, 2.7, 2.9). The contribution from CO peaks at \( T = 250 \text{ K} \), but its relative strength is highest at the lowest temperatures \( (T \leq 50 \text{ K}) \). The relative contribution from Si peaks at \( n_H = 10^4 \) cm\(^{-3} \), for \( T \leq 100 \text{ K} \), through emission from [Si \( \text{i} \)] at 129.6 \( \mu \text{m} \). Fe cooling is relatively unimportant up to \( n_H = 10^5 \) cm\(^{-3} \), but is completely dominant for \( T \geq 200 \text{ K} \) by \( n_H = 10^6 \) cm\(^{-3} \), with O \( \text{i} \) strongest below that temperature (Fig. 2.11). In addition to the elements covered by Santoro & Shull (2006), we note that cooling from neutral S reaches roughly the 10% level at \( n_H = 10^3 \) cm\(^{-3} \). The [S \( \text{I} \)] 25.2 \( \mu \text{m} \) transition reaches 40% of the total cooling at \( n_H = 10^7 \) cm\(^{-3} \) and \( T \sim 1000 \text{ K} \). The only other coolant that contributes at the level of at least \( 10^{-3} \) of the total cooling is the 60.6 \( \mu \text{m} \) transition of [P \( \text{II} \)] at \( n_H = 10^5 \) cm\(^{-3} \). The number of coolants that reach \( 10^{-3} \) of the total grows quickly with density. We observe 21 distinct emitters at that level at \( n_H = 10^9 \) cm\(^{-3} \), and 33 by \( 10^9 \) cm\(^{-3} \). If we lower the threshold to \( 10^{-6} \), there are a total of 91 coolants at \( n_H = 10^9 \) cm\(^{-3} \), illustrating the strength of Cloudy and our cooling method.

### 2.3.2 Dust Grains

Recently, studies have suggested that dust cooling at high densities can trigger fragmentation for metallicities as low as \( 10^{-6} Z_\odot \) (Omukai et al. 2005; Schneider et al. 2006; Tsuribe & Omukai 2006; Clark et al. 2007). Schneider et al. (2004) have claimed that between 15 and 30% of the mass of the progenitor of a pair-instability supernova is converted in dust. However, observations of the Crab nebula (Green et al. 2004) and the Cassiopeia A supernova remnant (Krause et al. 2004) have returned little or no signs of dust, suggesting that type II supernova may not actually be large dust producers. Given the controversy surrounding the existence of dust grains in the formation environments of second-generation stars, we do not include the cooling from dust in the analysis, but leave it for a separate work. To provide an example of the effect of dust on the cooling rate, we run a simple model including dust in Cloudy. We use a model designed to simulate the dust within the ISM, using the Cloudy command, grains ISM. The dust physics used in Cloudy is described in detail by van Hoof et al. (2004). The ISM dust model in Cloudy consists of both graphite and silicates with sizes ranging from \( 5 \times 10^{-3} \mu \text{m} \) to 0.25 \( \mu \text{m} \) and a power-law size-distribution with a power-law index of -3.5. For solar metallicity, the total grain abundances per H are \( 10^{-9.811} \), for graphite and \( 10^{-9.748} \), for
for silicates. In Fig. 2.12, we plot the cooling rate from metals at $n_H = 10^9 \text{ cm}^{-3}$, with and without dust grains, for metallicities, $Z = 10^{-6} \ Z_\odot$, $10^{-4} \ Z_\odot$, and $10^{-2} \ Z_\odot$. Since it is inappropriate to think of the dust and gas-phase metal abundances as independent, we directly scale the dust abundances with the gas-phase metal abundances. For number densities lower than $10^9 \text{ cm}^{-3}$, the additional cooling from dust is almost negligible. At higher densities, dust becomes even more important. If dust is, in fact, produced in the supernovae of the first stars, it is likely to be as important as previous studies have claimed.

2.3.3 Thermal Instability and Fragmentation

In order to study the ability of a collapsing gas-cloud to fragment, we first identify the regions of density and temperature where the classical fragmentation criterion, $t_{\text{cool}} < t_{\text{dyn}}$ (Field 1965), is met, with the dynamical time expressed as

$$t_{\text{dyn}} = \sqrt{\frac{3\pi}{16G\rho}}$$

(2.10)

For simplicity, we limit this analysis to solar abundance patterns. We create a Cloudy/ROCO data-grid with the following parameters: $50 \text{ K} \leq T \leq 1000 \text{ K}$ with $\delta \log(T) \simeq 0.012$ (100 points), $1 \text{ cm}^{-3} \leq n_H \leq 10^{12} \text{ cm}^{-3}$ with $\delta \log(n_H) = 0.1$, and $10^{-6} \ Z_\odot \leq Z \leq 10^{-2} \ Z_\odot$ with $\delta \log(Z) = 1$. We, then, follow the same procedure used to produce Fig. 2.2, as described in §2.2.2. In this section, we omit the decrease in the cooling rate caused by Compton heating on the CMB. In Fig. 2.13, we plot the log of the ratio of the dynamical time to the cooling time for each of the metallicities in the data-grid and for the metal-free case. A cloud is able to fragment when $\log_{10}(t_{\text{dyn}}/t_{\text{cool}}) > 0$. As expected, there is no density at which metal-free gas can fragment for $T < 200 \text{ K}$. As the metallicity increases, the value of $\log_{10}(t_{\text{dyn}}/t_{\text{cool}})$ slowly increases, first in the low-temperature regime, where $H_2$ cooling is inefficient, so even a small amount of metals has an effect. For gas with $n_H = 10^4 \text{ cm}^{-3}$ at $T = 200 \text{ K}$, the fragmentation criterion is nearly met by $Z = 10^{-5} \ Z_\odot$ and well satisfied one order of magnitude higher in metallicity. Once the metallicity reaches $10^{-2} \ Z_\odot$, the entire parameter-space is fragmentable. At high densities, however, fragmentation will be curtailed as the cloud becomes optically thick to its own radiation (Low & Lynden-Bell 1976; Rees 1976). As was also reported by Santoro & Shull (2006), the efficiency of the metal cooling peaks at $n_H \sim 10^6 \text{ cm}^{-3}$, significantly lowering the critical metallicity required for fragmentation.

The addition of metals to a gas also has the potential to trigger thermal instabilities during cloud-collapse. As in Abel et al. (2002) (Field 1965), we define a parcel of gas losing energy at a rate, $L$, to be thermally unstable if

$$\rho \left(\frac{\partial L}{\partial \rho}\right)_{\text{T}} - T \left(\frac{\partial L}{\partial T}\right)_{\rho} + L(\rho, T) > 0,$$

(2.11)

where $L$ is expressed in terms of the cooling rate, $\Lambda$, as

$$L(\rho, T) = \rho \Lambda(\rho, T).$$

(2.12)
The cooling rate, $\Lambda$, can be locally approximated by a power-law in both temperature and density as

$$\Lambda(\rho, T) \propto \left( \frac{T}{T_0} \right)^\alpha \left( \frac{\rho}{\rho_0} \right)^\beta.$$  \hfill (2.13)

The partial derivatives of Eqn. 2.11 become

$$\left( \frac{\partial \Lambda}{\partial \rho} \right)_T = (\beta + 1)\Lambda(\rho, T)$$  \hfill (2.14)

and

$$\left( \frac{\partial \Lambda}{\partial T} \right)_\rho = \frac{\rho \Lambda(\rho, T)}{T}.$$  \hfill (2.15)

The thermal instability criterion simplifies to

$$\alpha - \beta < 2.$$  \hfill (2.16)

In Fig. 2.14 we plot the value of the instability parameter, $(\alpha - \beta)$, for the same cooling data used for Fig. 2.13. For metal-free gas (Fig. 2.14, top-left), the instability parameter is greater than 3 over nearly the entire parameter space, and always greater than 4 at high densities. Abel et al. (2002) and Yoshida et al. (2006) both arrive at the same conclusion using this analysis for metal-free gas, with the added assumption that the cooling function is independent of density. As the metallicity increases, a region of thermal instability forms at low density and temperature. When the metallicity reaches $10^{-4} Z_\odot$ (Fig. 2.14, middle-right), a second unstable region exists for $10^3 \text{ cm}^{-3} \lesssim n_H \lesssim 10^6 \text{ cm}^{-3}$, at a temperature of a few hundred K. The second unstable region coincides with the increase in cooling efficiency to its maximum value, illustrated in Fig. 2.13.

Fragmentation is more likely to occur when the gas is both thermally unstable, and can cool faster than the dynamical time. We indicate the regions where both the fragmentation and thermal instability criteria are met in white in Fig. 2.15. No doubly unstable realm exists for metallicities, $Z \lesssim 10^{-5} Z_\odot$.

### 2.3.4 Effects of the Cosmic Microwave Background

The CMB creates a temperature floor, below which gas cannot cool radiatively. We study the influence of the CMB on the evolution of star-forming gas by applying a CMB floor at $z = 20$ in the manner described in §2.2.2 to the cooling data-grid used in §2.3.3. The CMB affects the cooling properties of the gas in two ways. The first is by increasing the cooling time at temperatures near the CMB temperature to greater than the dynamical time so that the fragmentation criterion is no longer satisfied. The second is by steepening the slope of the cooling rate as a function of temperature near $T_{CMB}$. This increases the value of $\alpha$, from Equation 2.16, making the gas thermally stable. In Fig. 2.16, we illustrate the influence of the CMB on the doubly unstable regions, shown previously. The unstable region that existed in the low-density, low-temperature regime is completely eliminated. There remains, however, a small area of instability for metallicities as low as $10^{-4} Z_\odot$. 

2.4 Discussion

We have introduced a new method for including the radiative cooling from metals in large, three-dimensional hydrodynamic simulations. In addition to its implementation in the AMR code, Enzo, this method has also been used by Bogdanović et al. (2006) in numerical simulations with the smoothed particle hydrodynamics (SPH) code, Gadget (Springel et al. 2001; Springel 2005). Our technique takes advantage of the extremely complex chemical reaction network of the preexisting radiative transfer code, Cloudy, which includes a full elemental coverage from H to Zn, along with a variety of molecular species and dust. With the singular assumption of ionization equilibrium for the heavy elements, we are able to precalculate cooling rates for gases with any chemical abundance in all manners of radiation environments over a temperature range of 50 to $10^8$ K. With cooling rates computed in advance, we eliminate the barrier that has classically prevented large chemical models from being incorporated into three-dimensional numerical simulations. Because our cooling scheme is valid over such a large range of density and temperature, and features so many coolants, it can be applied to a huge variety of astrophysical problems, such as the evolution of the ISM and IGM, normal star formation, planetary nebulae, accretion disks, and protoplanetary disks.

One advantage of the large chemical network of Cloudy is that we are able to determine the dominant coolants from a complete sample of atomic species up to an atomic number of 30. Fine-structure transitions of C and O are the greatest contributors to the cooling up to number densities of about $10^6$ cm$^{-3}$, where Fe cooling becomes significant and C is marginalized. The importance of these three elements, along with Si, in triggering the formation of the first low-mass stars has been studied in great detail by Santoro & Shull (2006). The cooling models we have constructed using solar abundance patterns reveal S cooling to be important for $10^3$ cm$^{-3} \leq n_H \leq 10^9$ cm$^{-3}$. S is produced only slightly less than Si in type II (Woosley & Weaver 1995) and pair-instability supernovae (Heger & Woosley 2002), and should be taken into account when considering the metals responsible for the transition from Population III to Population II star formation. The ability to specify individual abundances in our cooling method makes it straightforward to simulate the evolution of gas with non-solar abundance patterns.

In addition to elevating the cooling rate of a gas to satisfy the classical fragmentation criterion, metals also increase the potential for fragmentation by creating thermal instabilities. We have identified regions in temperature and density in which both the classical fragmentation and thermal instability criteria are met to be the physical conditions most likely to see fragmentation occur. We observe these doubly unstable regions to exist for metallicities as low as $10^{-4} Z_{\odot}$. If fragmentation cannot occur outside these regions, then the fate of a star-forming gas-cloud will be determined by the path taken through density-temperature space as it collapses. If we consider the doubly unstable regions in Fig. 2.15, appropriate for star-formation in current epoch, there will almost certainly be a period of double instability when $Z \geq 10^{-3} Z_{\odot}$. Interestingly, the density-temperature tracks shown in Fig. 1 of Omukai et al. (2005) indicate that gas with $Z = 10^{-4} Z_{\odot}$ will pass right through the stable region that separates two instabilities. Omukai et al. (2005) also find that star formation at that metallicity only produces high-mass fragments. At high redshift, the CMB significantly reduces the size of the
doubly unstable regions. Thermal instabilities, though, are extremely sensitive to the slope of the cooling rate as a function of density and temperature. Every element has distinct cooling properties, and will, therefore, produce different thermal instabilities. As such, the key to uncovering the nature of the first Population II stars will be in the determination of the mass function of their precursors.

2.5 Future Development

In papers to follow, we will extend our study to gases with non-solar abundance patterns. We will explore thermal and double instabilities created by individual elements, as well as abundance patterns produced in Population III supernovae. Future studies will also investigate the effects of background radiation on the evolution of star-forming gas. The final word, however, will only come from three-dimensional, numerical simulations. The simulations by Smith & Sigurdsson (2007), employing the methods described here with solar abundance patterns, have confirmed that fragmentation occurs for metallicities, $Z \geq 10^{-3} Z_\odot$. We intend to pair all future predictions made from analysis of thermal instabilities with full numerical simulations.

Although dust physics has been implemented in Cloudy, we currently treat only metals in the gas-phase. In the future, we will study the effects of dust cooling in more detail. We will also couple the dust chemistry to the H/He chemical network in Enzo, so as to properly model the formation of H$_2$ on grain surfaces. A great strength of this method is the use of the ever-expanding chemical network of Cloudy. As more physical processes are incorporated into the Cloudy software, the utility of this method will increase as well. One major constraint of this work, however, is that its validity is confined to the optically thin limit. The approximations made here break down at opacities of order unity. For higher opacities, our method provides a core module for flux-limited diffusion schemes. Complex geometries introduce problems of self-heating and shadowing, which will require full, three-dimensional radiative transfer.
Table 2.1. Solar Abundances in Cloudy

<table>
<thead>
<tr>
<th>Z</th>
<th>Symbol</th>
<th>Element</th>
<th>log_{10}(n/n(H))</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>H</td>
<td>Hydrogen</td>
<td>0.00</td>
</tr>
<tr>
<td>2</td>
<td>He</td>
<td>Helium</td>
<td>-1.00</td>
</tr>
<tr>
<td>3</td>
<td>Li</td>
<td>Lithium</td>
<td>-8.69</td>
</tr>
<tr>
<td>4</td>
<td>Be</td>
<td>Beryllium</td>
<td>-10.58</td>
</tr>
<tr>
<td>5</td>
<td>B</td>
<td>Boron</td>
<td>-9.21</td>
</tr>
<tr>
<td>6</td>
<td>C</td>
<td>Carbon</td>
<td>-3.61</td>
</tr>
<tr>
<td>7</td>
<td>N</td>
<td>Nitrogen</td>
<td>-4.07</td>
</tr>
<tr>
<td>8</td>
<td>O</td>
<td>Oxygen</td>
<td>-3.31</td>
</tr>
<tr>
<td>9</td>
<td>F</td>
<td>Fluorine</td>
<td>-7.52</td>
</tr>
<tr>
<td>10</td>
<td>Ne</td>
<td>Neon</td>
<td>-4.00</td>
</tr>
<tr>
<td>11</td>
<td>Na</td>
<td>Sodium</td>
<td>-5.67</td>
</tr>
<tr>
<td>12</td>
<td>Mg</td>
<td>Magnesium</td>
<td>-4.46</td>
</tr>
<tr>
<td>13</td>
<td>Al</td>
<td>Aluminium</td>
<td>-5.53</td>
</tr>
<tr>
<td>14</td>
<td>Si</td>
<td>Silicon</td>
<td>-4.46</td>
</tr>
<tr>
<td>15</td>
<td>P</td>
<td>Phosphorus</td>
<td>-6.50</td>
</tr>
<tr>
<td>16</td>
<td>S</td>
<td>Sulphur</td>
<td>-4.74</td>
</tr>
<tr>
<td>17</td>
<td>Cl</td>
<td>Chlorine</td>
<td>-6.72</td>
</tr>
<tr>
<td>18</td>
<td>Ar</td>
<td>Argon</td>
<td>-5.60</td>
</tr>
<tr>
<td>19</td>
<td>K</td>
<td>Potassium</td>
<td>-6.88</td>
</tr>
<tr>
<td>20</td>
<td>Ca</td>
<td>Calcium</td>
<td>-5.64</td>
</tr>
<tr>
<td>21</td>
<td>Sc</td>
<td>Scandium</td>
<td>-8.83</td>
</tr>
<tr>
<td>22</td>
<td>Ti</td>
<td>Titanium</td>
<td>-6.98</td>
</tr>
<tr>
<td>23</td>
<td>V</td>
<td>Vanadium</td>
<td>-8.00</td>
</tr>
<tr>
<td>24</td>
<td>Cr</td>
<td>Chromium</td>
<td>-6.33</td>
</tr>
<tr>
<td>25</td>
<td>Mn</td>
<td>Manganese</td>
<td>-6.54</td>
</tr>
<tr>
<td>26</td>
<td>Fe</td>
<td>Iron</td>
<td>-4.55</td>
</tr>
<tr>
<td>27</td>
<td>Co</td>
<td>Cobalt</td>
<td>-7.08</td>
</tr>
<tr>
<td>28</td>
<td>Ni</td>
<td>Nickel</td>
<td>-5.75</td>
</tr>
<tr>
<td>29</td>
<td>Cu</td>
<td>Copper</td>
<td>-7.79</td>
</tr>
<tr>
<td>30</td>
<td>Zn</td>
<td>Zinc</td>
<td>-7.40</td>
</tr>
</tbody>
</table>
Fig. 2.1 Cooling functions, excluding cooling from H$_2$, for gases with $n_H = 1$ cm$^{-3}$ and metallicities, $Z = 0$ (solid), $10^{-3}$ $Z_{\odot}$ (dot), $10^{-2}$ $Z_{\odot}$ (dash), $10^{-1}$ $Z_{\odot}$ (dot-dash), 1 $Z_{\odot}$ (dot-dot-dash), and 10 $Z_{\odot}$ (dot-dash-dash).
Fig. 2.2 Cooling functions, including H$_2$ cooling, for gases with $n_H = 1$ cm$^{-3}$ (top-left), $n_H = 10^3$ cm$^{-3}$ (top-right), $n_H = 10^6$ cm$^{-3}$ (bottom-left), and $n_H = 10^9$ cm$^{-3}$ (bottom-right). Metallicities are $Z = 0$ (solid), $10^{-6}$ Z$_\odot$ (dot), $10^{-5}$ Z$_\odot$ (dash), $10^{-4}$ Z$_\odot$ (long dash), $10^{-3}$ Z$_\odot$ (dot-dash), and $10^{-2}$ Z$_\odot$ (dot-long dash).
Fig. 2.3 Cooling contributions from C and O species that reach at least $10^{-3}$ of the total cooling for gas with $n_H = 10^2$ cm$^{-3}$ and $Z = 10^{-1} Z_\odot$. The total cooling (solid, black) includes all species contained within the Cloudy chemical network. Components shown are CO (dot), [O i] 145.5 $\mu$m (dot-dot-dash), [O i] 63.2 $\mu$m (dash-dash-dot), [C i] 369.7 $\mu$m (dash), [C i] 609.2 $\mu$m (long dash), C i 985 nm (dash-dot), and [C ii] 157.6 $\mu$m (long dash-dot). The solid, grey line indicates the sum of all the components plotted.
Fig. 2.4 All other coolants not plotted in Fig. 2.3 that reach at least $10^{-3}$ of the total cooling for gas with $n_H = 10^2 \text{ cm}^{-3}$ and $Z = 10^{-1} Z_\odot$. The total cooling (solid, black) includes all species contained within the Cloudy chemical network. Components shown are [Fe ii] (dot), [S i] 25.2 $\mu$m (dash), [S i] 56.3 $\mu$m (long dash), [Si i] 129.6 $\mu$m (dash-dot), [Si i] 68.4 $\mu$m (long dash-dot), and [Si ii] 34.8 $\mu$m (dash-dash-dot). The solid, grey line indicates the sum of all the components plotted.
Fig. 2.5 Cooling contributions from C and O species that reach at least $10^{-3}$ of the total cooling for gas with $n_H = 10^3$ cm$^{-3}$ and $Z = 10^{-1} Z_{\odot}$. The total cooling (solid, black) includes all species contained within the Cloudy chemical network. Components shown are CO (dot), [O i] 145.5 μm (dot-dot-dash), [O i] 63.2 μm (dash-dash-dot), [C i] 369.7 μm (dash), [C i] 609.2 μm (long dash), C i 985 nm (dash-dot), and [C ii] 157.6 μm (long dash-dot). The solid, grey line indicates the sum of all the components plotted.
Fig. 2.6 All other coolants not plotted in Fig. 2.5 that reach at least $10^{-3}$ of the total cooling for gas with $n_H = 10^3$ cm$^{-3}$ and $Z = 10^{-1}$ $Z_{\odot}$. The total cooling (solid, black) includes all species contained within the Cloudy chemical network. Components shown are [Fe II] (dot), [S I] 25.2 μm (dash), [S I] 56.3 μm (long dash), [Si I] 129.6 μm (dash-dot), [Si I] 68.4 μm (long dash-dot), and [Si II] 34.8 μm (dash-dash-dot). The solid, grey line indicates the sum of all the components plotted.
Fig. 2.7 Cooling contributions from C and O species that reach at least $10^{-3}$ of the total cooling for gas with $n_H = 10^4$ cm$^{-3}$ and $Z = 10^{-1} Z_\odot$. The total cooling (solid, black) includes all species contained within the Cloudy chemical network. Components shown are CO (dot), [O i] 145.5 μm (dot-dot-dash), [O i] 63.2 μm (dash-dash-dot), [C i] 369.7 μm (dash), [C i] 609.2 μm (long dash), C i 985 nm (dash-dot), and [C ii] 157.6 μm (long dash-dot). The solid, grey line indicates the sum of all the components plotted.
Fig. 2.8 All other coolants not plotted in Fig. 2.7 that reach at least $10^{-3}$ of the total cooling for gas with $n_H = 10^4$ cm$^{-3}$ and $Z = 10^{-1} Z_\odot$. The total cooling (solid, black) includes all species contained within the Cloudy chemical network. Components shown are [Fe II] (dot), [S I] 25.2 μm (dash), [S I] 56.3 μm (long dash), [Si I] 129.6 μm (dash-dot), [Si I] 68.4 μm (long dash-dot), and [Si II] 34.8 μm (dash-dash-dot). The solid, grey line indicates the sum of all the components plotted.
Fig. 2.9 Cooling contributions from C and O species that reach at least $10^{-3}$ of the total cooling for gas with $n_H = 10^5$ cm$^{-3}$ and $Z = 10^{-1} Z_\odot$. The total cooling (solid, black) includes all species contained within the Cloudy chemical network. Components shown are CO (dot), [O i] 145.5 µm (dot-dot-dash), [O i] 63.2 µm (dash-dash-dot), [C i] 369.7 µm (dash), [C i] 609.2 µm (long dash), C i 985 nm (dash-dot), and [C ii] 157.6 µm (long dash-dot). The higher dotted line represents CO emission from $^{12}$O$^{16}$, while the lower dotted line shows emission from $^{13}$O$^{16}$. The solid, grey line indicates the sum of all the components plotted.
Fig. 2.10 All other coolants not plotted in Fig. 2.9 that reach at least $10^{-3}$ of the total cooling for gas with $n_H = 10^5$ cm$^{-3}$ and $Z = 10^{-1} Z_\odot$. The total cooling (solid, black) includes all species contained within the Cloudy chemical network. Components shown are [Fe II] (dot), [S I] 25.2 $\mu$m (dash), [S I] 56.3 $\mu$m (long dash), [Si I] 129.6 $\mu$m (dash-dot), [Si I] 68.4 $\mu$m (long dash-dot), [Si II] 34.8 $\mu$m (dash-dash-dot), and [P II] 60.6 $\mu$m (dot-dot-dot-dot). The solid, grey line indicates the sum of all the components plotted.
Fig. 2.11 Subset of the most dominant coolants at \( n_H = 10^9 \text{ cm}^{-3} \) and \( Z = 10^{-1} Z_\odot \). The total cooling (solid) includes all species contained within the Cloudy chemical network. Components shown are [Fe II] (dot), [O I] 63.2 \( \mu \text{m} \) (dash), [S I] 25.2 \( \mu \text{m} \) (long dash), and CO (dash-dot).
Fig. 2.12 Total cooling rate from metals for gas at $n_H = 10^9$ cm$^{-3}$, with metallicities $Z = 10^{-2} Z_\odot$ (solid), $10^{-4} Z_\odot$ (dashed), and $10^{-6} Z_\odot$ (dash-dot). The black lines indicate the total cooling from gas-phase metals only. The grey lines show the cooling with gas-phase metals and dust grains, created with the ISM dust grain model in Cloudy, using the command, `grains ISM`. The ISM dust model in Cloudy consists of both graphite and silicates with sizes ranging from $5 \times 10^{-3}$ μm to 0.25 μm and a power-law size-distribution with a power-law index of -3.5. For solar metallicity, the total grain abundances per H are $10^{-9.811}$ for graphite and $10^{-9.748}$ for silicates. In each case shown, the dust grain abundances have been scaled to the gas-phase abundances.
Fig. 2.13 Contours of $\log_{10}(t_{\text{dyn}}/t_{\text{cool}})$ over number density and temperature for gases with metallicities, $Z = 0$ (top-left), $10^{-6} \ Z_\odot$ (top-right), $10^{-5} \ Z_\odot$ (middle-left), $10^{-4} \ Z_\odot$ (middle-right), $10^{-3} \ Z_\odot$ (bottom-left), and $10^{-2} \ Z_\odot$ (bottom-right). H$_2$ cooling is included.
Fig. 2.14 Contours of the instability parameter, $(\alpha - \beta)$ over number density and temperature. The medium is unstable for values less than 2. The metallicities are $Z = 0$ (top-left), $10^{-6} Z_\odot$ (top-right), $10^{-5} Z_\odot$ (middle-left), $10^{-4} Z_\odot$ (middle-right), $10^{-3} Z_\odot$ (bottom-left), and $10^{-2} Z_\odot$ (bottom-right). At $Z = 10^{-4} Z_\odot$, two separate thermally unstable regions exist. These two regions merge by $10^{-3} Z_\odot$. 
Fig. 2.15 The white patches indicate regimes of density and temperature where \( \log_{10}(t_{\text{dyn}}/t_{\text{cool}}) > 0 \) and \((\alpha - \beta) < 2\) for metallicities, \( Z = 10^{-4} \ Z_\odot \) (top), \( 10^{-3} \ Z_\odot \) (middle), and \( 10^{-2} \ Z_\odot \) (bottom). As in Fig. 2.14, there are two individual doubly unstable regions at \( Z = 10^{-4} \ Z_\odot \) that have merged by \( 10^{-3} \ Z_\odot \).
Fig. 2.16 Doubly unstable regions for the same metallicities as in Fig. 2.15, but with a CMB temperature floor at $z = 20$ included.
Chapter 3

Simulations I

3.1 Introduction

Numerical simulations have shown that the very first stars invariably formed in isolation and were much more massive than the sun, due mainly to the inability of primordial gas to efficiently cool at low temperatures (Abel et al. 2002; Bromm et al. 2002; Yoshida et al. 2006). Tumlinson et al. (2004) have suggested that the Pop III IMF was not dominated by very massive stars ($M > 140 \ M_\odot$), but instead by stars with $M = 8-40 \ M_\odot$. Even this IMF, though, is still remarkably distinct from that observed for the local universe, which peaks at less than one solar mass (Miller & Scalo 1979; Scalo 1986, 1998; Kroupa 2001, 2002; Chabrier 2003).

The deaths of the first stars produced and distributed copious amounts of metals into their surroundings, through either core-collapse ($M > 10 \ M_\odot$) or pair-instability ($M > 140 \ M_\odot$) supernovae (Heger & Woosley 2002). These metals provide additional avenues for radiative cooling of the ambient gas, through fine-structure and molecular transitions, as well as continuum emission from dust formed from the supernova ejecta, permitting the gas that will form the next generation of stars to reach temperatures lower than what is possible for metal-free gas. Fragmentation of collapsing gas will continue so long as the gas can keep decreasing in temperature as the density increases (Larson 2005), or until the gas becomes optically thick to its own emission (Low & Lynden-Bell 1976). The minimum fragment mass is determined by the local Jeans mass,

$$M_J \simeq 700 \ M_\odot (T/200K)^{3/2} (n/10^4 \text{cm}^{-3})^{-1/2} (\mu/2)^{-2},$$

where $T$, $n$, and $\mu$ are the temperature, number density, and mean molecular weight, at the end of fragmentation (Larson 2005). For metal-free gas, a minimum temperature of $\sim 200$ K is reached at $n \simeq 10^4$ cm$^{-3}$ when $\text{H}_2$ cooling becomes inefficient, yielding a Jeans mass, $M_J \simeq 10^3 \ M_\odot$ (Abel et al. 2002; Bromm et al. 2002). At some certain chemical abundance, it is conjectured that metals provide sufficient cooling, so that the temperature of the gas continues to decrease as the density increases past the stalling point for metal-free gas, allowing the collapsing gas-cloud to undergo fragmentation and form smaller and smaller clumps. The enrichment of gas to some critical metallicity, $Z_{cr}$, will trigger the formation of the first low-mass (Pop II) stars in the universe, as the gas can cool to lower temperatures at higher metallicity, in general. The value of $Z_{cr}$ can be estimated by calculating the metallicity required to produce a cooling rate equal to the rate of adiabatic compression heating at a given temperature and density. This has been carried out for individual alpha elements, such as C and O, by Bromm & Loeb (2003b),
and C, O, Si, Fe, as well as solar abundance patterns by Santoro & Shull (2006), yielding roughly, $10^{-3.5} \lesssim Z_{\odot} \lesssim 10^{-3} \lesssim Z_{\odot}$.

Aside from the minimum clump mass, however, not much more can be said about the spectrum of clump masses produced during fragmentation. Omukai et al. (2005) use one-zone models with very sophisticated chemical networks to follow the evolution of temperature and density in the center of a collapsing gas cloud, for a range of metallicities. The predictions of fragmentation from this work, though, are based solely on statistical arguments of elongation in prestellar cores and do not capture the complex processes of interaction and accretion associated with the formation of multiple stars (Bate et al. 2003). Tsuribe & Omukai (2006) simulate the high density ($n \geq 10^{10} \text{ cm}^{-3}$) evolution of extremely low-metallicity gas ($Z < 10^{-4} \lesssim Z_{\odot}$), but the conclusions of this work are limited by the fact that the simulations are initialized at an extremely late phase in the evolution of the prestellar core. The numerical simulations by Bromm et al. (2001), which use cosmological initial conditions, show fragmentation in gas with $Z = 10^{-3} \lesssim Z_{\odot}$, but a mass resolution of 100 $M_{\odot}$ prevents this study from saying anything conclusive about the formation of sub-stellar mass objects.

In this paper, we present the results of three-dimensional hydrodynamic simulations of metal-enriched star-formation. These simulations are similar in nature to those of Bromm et al. (2001), but with vastly improved numerical methods and updated physics. We describe the setup of our simulations in §3.2, with the results in §3.3 and a discussion of the consequences of this work in §3.4.

### 3.2 Simulation Setup

We perform a series of four simulations, with constant metallicities, $Z = 0$ (metal-free), $10^{-4} \lesssim Z_{\odot}$, $10^{-3} \lesssim Z_{\odot}$, and $10^{-2} \lesssim Z_{\odot}$, using the Eulerian adaptive mesh refinement hydrodynamics/N-body code, Enzo (Bryan & Norman 1997a; O’Shea et al. 2004). The metallicity is held constant throughout each simulation in order to isolate the role of heavy element concentration in altering the dynamics of collapse compared to the identical metal-free case. In reality, metals will be injected over time into star forming gas by Pop III supernova blast waves, and the mixing of those metals with the gas will not be completely uniform. Here we focus on an idealized approximation in order to capture the essential physics of collapse and fragmentation.

Each simulation begins at $z = 99$, in a cube, 300 $h^{-1}$ kpc comoving per side, in a $\Lambda$CDM universe, with the following cosmological parameters: $\Omega_M = 0.3$, $\Omega_\Lambda = 0.7$, $\Omega_B = 0.04$, and Hubble constant, $h = 0.7$, in units of 100 km s$^{-1}$ Mpc$^{-1}$. We initialize all the simulations identically, with a power spectrum of density fluctuations given by Eisenstein & Hu (1999), with $\sigma_8 = 0.9$ and $n = 1$. The computation box consists of a top grid, with $128^3$ cells, and three static subgrids, refining by a factor of 2 each. This gives the central refined region, which is 1/64 the total computational volume, an effective top grid resolution of $1024^3$ cells. The grid is centered on the location of a $\sim 5 \times 10^5 M_{\odot}$ dark matter halo that is observed to form at $z \sim 18$ in a prior dark-matter-only simulation, as is done similarly in Abel et al. (2002); O’Shea et al. (2005). Refinement occurs during the simulations whenever the gas, or dark matter, density is greater than the mean density by a factor of 4, or 8, respectively. We also require that the local
Jeans length be resolved by at least 16 grid cells at all times in order to avoid artificial fragmentation as prescribed by Truelove et al. (1997).

To include the radiative cooling processes from the heavy elements, we use the method described in Smith et al. (2007). The nonequilibrium abundances and cooling rates of H, H$^+$, H$^-$, He, He$^+$, He$^{++}$, H$_2$, H$_2^+$, and e$^-$ are calculated internally, as in Abel et al. (2002); Anninos et al. (1997). Meanwhile, the metal cooling rates are interpolated from large grids of values, precomputed with the photoionization software, Cloudy (Ferland et al. 1998). We ignore the cooling from dust and focus only on the contribution of gas-phase metals in the optically-thin limit. Unlike other studies of the formation of the first metal-enriched structures, we do not assume the presence of an ionizing UV background. In our model, the singular Pop III star that was associated with the dark matter halo in which our stars form has already died in a supernova. We also assume any other Pop III stars are too distant to affect the local star-forming region and that QSOs have yet to form. We use the coronal equilibrium command when constructing the cooling data in Cloudy to simulate a gas where all ionization is collisional. The metal cooling data was created using the Linux cluster, Lion-xo, run by the High Performance Computing Group at The Pennsylvania State University. As a consequence of our choice to ignore any external radiation, we do not observe the fine-structure emission of [C II] (157.74 μm) that was reported by Santoro & Shull (2006) to be important. Instead, cooling from C comes in the form of fine-structure lines of [C I] (369.7 μm, 609.2 μm). The cooling from [C I] in our study dominates in the same range of densities and temperatures as the cooling from [C II] in Santoro & Shull (2006). We observe the contributions of the other coolants studied by Santoro & Shull (2006), [O I], [Si II], and [Fe II], to be in agreement with their work. In addition, we find that emission from [S I] (25.19 μm) dominates the cooling from metals at $n \sim 10^{7}$ cm$^{-3}$ and $T \sim 1\text{–}3 \times 10^3$ K. The absence of UV radiation in our simulations also allows H$_2$ to form, differentiating this study from Bromm et al. (2001). This allows for a more direct comparison between the metal-free and metal-enriched cases.

The simulations are run until one or more dense cores form at the center of the dark matter halo and a maximum refinement level of 28 is reached for the first time, giving us a dynamic range of greater than $10^{10}$. Only the simulation with $Z = 10^{-2} Z_\odot$ reached 28 levels of refinement. The three other simulations were stopped after reaching 27 refinement levels, since their central densities were already higher than the simulation with $Z = 10^{-2} Z_\odot$. Table 3.1 summarizes the final state of each simulation, where $z_{col}$ is the collapse redshift, $l_{max}$ is the highest level of refinement, $n_{max}$ is the maximum gas density within the box, and $\Delta t_{col}$ is the time difference to collapse from the metal-free simulation.

### 3.3 Results

As can be seen in Table 3.1, the runs with higher metallicities reach the runaway collapse phase faster. The relationship between metallicity relative to solar and $\Delta t_{col}$ is well fit by a power-law with index, $n \simeq 0.22$. Gas-clouds with more metals are able to radiate away their thermal energy more quickly, and thus, collapse faster. An inverse relation between metallicity and the number of grids and grid-cells exists because the
low-density, background gas evolves at roughly the same rate in all simulations, yet has more time, in the runs with lower metallicities, with which to collapse to higher density, requiring additional refinement.

Our simulations, shown in Figure 3.1, display a qualitative transition in behavior between metallicities of $10^{-4} \ Z_\odot$ and $10^{-3} \ Z_\odot$. In the runs with the highest metallicities (Figures 3.1C and 3.1D), the central core is extremely asymmetric, and multiple density maxima are clearly visible. All four runs display similar large-scale density profiles (Figure 3.2A). Radiative cooling from H$_2$ becomes extremely inefficient below $T \sim 200$ K, creating the temperature floor, visible in Figure 3.2B for the metal-free case (Abel et al. 2002; Bromm et al. 2002). At $n \sim 10^4 \ \text{cm}^{-3}$, the rotational levels of H$_2$ are populated according to LTE, reducing the cooling efficiency and causing the temperature to increase (Abel et al. 2002; Bromm et al. 2002). In the isothermal collapse model of Shu (1977), the accretion rate is proportional to the cube of the sound speed. The increase in temperature leads to an increase in the accretion rate, causing the density, and thus, the enclosed mass (Figure 3.2C), to be slightly higher inside the central $\sim 0.1$ pc in the metal-free case. A similar situation occurs further within for the $Z = 10^{-4} \ Z_\odot$ and, later, the $10^{-3} \ Z_\odot$ cases, as the metal cooling is overwhelmed by adiabatic compression heating and the temperature begins to rise with density. The presence of metals at the level of $10^{-4} \ Z_\odot$ enhances the cooling enough to lower the gas temperature to $\sim 75$ K. Metallicities greater than $10^{-3} \ Z_\odot$ provide sufficient cooling to bring the gas down to the temperature of the cosmic microwave background, where $T_{CMB} \simeq 2.7$ K $(1 + z)$. The gas temperatures are in general agreement with the calculations of Omukai et al. (2005) that include a CMB spectrum at $z = 20$. Fragmentation requires that the cooling time be less than the dynamical time. Figure 3.2D shows that this criterion is essentially never met in the zero metallicity case, and only marginally in the $Z = 10^{-4} \ Z_\odot$ case. However, the fragmentation criterion is more than satisfied in the $Z = 10^{-3} \ Z_\odot$ and $10^{-2} \ Z_\odot$ cases over a wide mass-range.

In order to locate fragments within our simulations, we employ an algorithm, based on Williams et al. (1994), that works by identifying isolated density countours. Before we search for clumps, we smooth the density field by assigning each grid-cell the mass-weighted mean density of the group of cells including itself and its neighbors within one cell-width. This serves to eliminate small density perturbations that would be misidentified as clumps by the code. In order to directly compare the fragmentation from each simulation, we limit the search for clumps to the 1 $M_\odot$ of gas surrounding the cell with the highest density. On larger scales, all of the runs display a filamentary structure that is qualitatively similar. No other region in any of the simulation boxes has collapsed to densities comparable to those found within the region where the clump search is performed. The results are shown in Figure 3.3. A single clump exists in the metal-free and $10^{-4} \ Z_\odot$ simulations, containing 99.7% of the total mass within the region of interest. In the simulation with $Z = 10^{-3} \ Z_\odot$, 91% of the mass is shared between two clumps with 0.52 $M_\odot$ and 0.39 $M_\odot$. In the same simulation, we also find two smaller clumps 0.06 $M_\odot$ and 0.02 $M_\odot$. Finally, in the $Z = 10^{-2} \ Z_\odot$ simulation, we see two clumps with 0.79 $M_\odot$ and 0.21 $M_\odot$.
3.4 Discussion

We have shown, through three-dimensional hydrodynamic simulations, that fragmentation occurs in collapsing gas with metallicities, \( Z \geq 10^{-3} Z_\odot \). Our results indicate that star-formation occurs in exactly the same manner at metallicity, \( Z = 10^{-4} Z_\odot \), as it does at zero metallicity. The similarities between the simulations with metallicities, \( Z = 10^{-3} Z_\odot \) and \( 10^{-2} Z_\odot \), suggest that the transition to low-mass star-formation is complete by \( 10^{-3} Z_\odot \), implying that the entire transition occurs over only one order of magnitude in metal abundance. More simulations, bracketing the metallicity range, \( 10^{-4} \) to \( 10^{-3} Z_\odot \), will test how abrupt the transition truly is. We will also explore the effect of non-solar abundances on the low metallicity IMF. It has been recently argued that dust cooling at high densities (\( n \geq 10^{13} \text{ cm}^{-3} \)) can induce fragmentation for metallicities as low as \( 10^{-6} Z_\odot \) (Schneider et al. 2006). In light of the work by Frebel et al. (2007), who note the absence of stars with \( D_{\text{trans}} < -3.5 \), where \( D_{\text{trans}} \) is a measure of the combined logarithmic abundance of C and O, it seems unlikely that \( Z_{\odot} \) is this low. While the fragmentation mode discussed in Schneider et al. (2006), and also Omukai et al. (2005), may truly exist, it is possible that metal yields from Pop III supernovae overshoot this metallicity, for realistic mixing scenarios, leaving almost no star-forming regions with such a low concentration of heavy elements. Similar to our results, Omukai et al. (2005) note that only high-mass fragments are produced when \( Z = 10^{-4} Z_\odot \). If Pop III supernovae are able to immediately enrich the local universe to \( Z = 10^{-4} Z_\odot \), the high-density dust cooling fragmentation mode would be skipped altogether, and the high-mass stars that formed via the mode observed at \( 10^{-4} Z_\odot \) would leave no record in the search for low-metallicity stars in the local universe.

We have limited the search for fragments to the dense \( 1 M_\odot \) core at the center of each simulation. Within this region, it is unlikely that any more fragments will form in any of the simulations. In all of the cases presented, the cooling has begun to be overwhelmed by compression heating such that the central temperature is now increasing with increasing density, which was indicated by Larson (2005) to be the end of hierarchical fragmentation. Fragmentation may continue in the surrounding lower density gas in the cases of \( Z = 10^{-3} Z_\odot \) and \( 10^{-2} Z_\odot \). The final stellar masses of these objects will also be affected interaction and accretion that will occur in later stages of evolution. In the two lowest metallicity cases, the gas immediately surrounding the central core evolves slowly enough that it will not have sufficient time to reach high densities before the UV radiation from the central, massive star dissociates all of the \( \text{H}_2 \). As was shown by Bromm et al. (2001), clouds with metallicities, \( Z \leq 10^{-4} Z_\odot \) are unable to collapse without the aid of \( \text{H}_2 \) cooling.

In the two simulations in which significant fragmentation is observed, \( Z = 10^{-3} \) and \( 10^{-2} Z_\odot \), the gas is able to cool rapidly to the temperature of the CMB. Wise & Abel (2005) predict that the rate of Pop III supernovae peaks at a redshift, \( z \sim 20 \), and then drops off sharply, implying that metal production from Pop III stars is effectively finished at this point. In this epoch, the characteristic mass-scale for metal-enriched star formation will be regulated by the CMB, as is predicted in Bromm & Loeb (2003b). Thus, the first Pop II stars will be considerably more massive, on average, than stars observed today, as was suggested by Larson (1998). Observations of low-mass prestellar
cores in the local universe reveal them to have temperatures of about 8.5 K (Evans 1999), implying that the IMF may not become completely 'normal' until $z < 3$ when the CMB fell below this temperature.
Table 3.1. Final States

<table>
<thead>
<tr>
<th>$Z$ ($Z_\odot$)</th>
<th>$z_{col}$</th>
<th>$l_{max}$</th>
<th>Grids</th>
<th>Cells</th>
<th>$n_{max}$ (cm$^{-3}$)</th>
<th>$\Delta t_{col}$ (Myr)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>18.231519</td>
<td>27</td>
<td>8469</td>
<td>$4.82 \times 10^7$</td>
<td>$4.11 \times 10^{13}$</td>
<td>-</td>
</tr>
<tr>
<td>$10^{-4}$</td>
<td>18.83816</td>
<td>27</td>
<td>8060</td>
<td>$4.64 \times 10^7$</td>
<td>$3.90 \times 10^{13}$</td>
<td>9.19</td>
</tr>
<tr>
<td>$10^{-3}$</td>
<td>19.33657</td>
<td>27</td>
<td>7911</td>
<td>$4.56 \times 10^7$</td>
<td>$1.65 \times 10^{13}$</td>
<td>16.21</td>
</tr>
<tr>
<td>$10^{-2}$</td>
<td>20.032518</td>
<td>28</td>
<td>7521</td>
<td>$4.42 \times 10^7$</td>
<td>$1.50 \times 10^{13}$</td>
<td>25.33</td>
</tr>
</tbody>
</table>
Fig. 3.1 Slices through gas density for the final output of simulations with $Z = 0$ (A), $10^{-4} \ Z_\odot$ (B), $10^{-3} \ Z_\odot$ (C), and $10^{-2} \ Z_\odot$ (D). Each slice intersects the grid-cell with the highest gas density and has a width of $2 \times 10^{-8}$ of the computation box, corresponding to a proper size of $\sim 4 \times 10^{-4} \ pc$ (84 AU). The color-bar at bottom ascends logarithmically, from left to right, spanning exactly four orders of magnitude in density.
Fig. 3.2 Spherically averaged, mass-weighted quantities for the final output of each simulation: \( Z = 0 \) (red), \( 10^{-4} \) \( Z_{\odot} \) (green), \( 10^{-3} \) \( Z_{\odot} \) (blue), and \( 10^{-2} \) \( Z_{\odot} \) (violet). A: Number density vs. radius. B: Temperature vs. enclosed mass. C: Enclosed gas mass vs. radius. D: Ratio of crossing time to cooling time vs. enclosed mass. The classical criterion for fragmentation is met when the ratio of the crossing time to the cooling time is greater than 1.
Fig. 3.3 Masses of clumps found within the final output of each simulation. The location on the x and y axes corresponds to the log of the clump mass and the metallicity of the simulation. Colors are the same as in Figure 3.2. The radii of the circles are proportional to the masses of the clumps they represent. A factor of 10 in mass is equivalent to a factor of 2 in radius. The search for clumps is limited to the 1 $M_\odot$ surrounding the grid cell with the highest gas density. Only clumps with at least 1000 cells are plotted.
Chapter 4

Simulations II

4.1 Introduction

The formation of the first stars in the universe is, in principle, a well-posed problem. The required ingredients consist of (1) the proper cosmological parameters, e.g., Spergel et al. (2007), (2) the chemical composition of primordial gas, e.g., Smith et al. (1993), and (3) the non-equilibrium chemistry and cooling rate of that gas, e.g., Abel et al. (1997); Galli & Palla (1998). As such, numerical simulations have been able to accurately characterize the formation process of primordial stars from the assembly of their dark-matter halos through the end of optical thinness of the collapsing protostar (Abel et al. 2002; Bromm et al. 2002; Bromm & Loeb 2004; Yoshida et al. 2006; O'Shea & Norman 2007; Gao et al. 2007). Currently, theory and simulations estimate that the first stars had masses of roughly 30–300 M⊙ (Abel et al. 2002; Tan & McKee 2004; Yoshida et al. 2006; O'Shea & Norman 2007). A direct calculation, however, involves simulating the complex processes of accretion and radiative feedback, a capability just beyond the state of the art. In contrast, the challenge of the understanding the second generation of stars is exceedingly complex. While the initial conditions of the first stars essentially depend only on the principles of cold dark matter cosmology, the initial conditions of the second stars require a complete solution to the formation and evolution of their predecessors. The chemical composition and physical conditions of second-generation star-forming environments depend heavily on the exact mass of the first stars (Heger & Woosley 2002; Maeder et al. 2005; Nomoto et al. 2006; Rockefeller et al. 2006) and the mechanics of their supernovae (Greif et al. 2007).

At the heart of the problem of the second stars is understanding how the star-formation process is altered by the introduction of the first metals in the universe. The chemistry of a gas determines the efficiency with which that gas can cool radiatively. Metal-free gas cools solely through ro-vibration lines of H₂, whose lowest-lying transition has an energy equivalent temperature of ~ 512 K, resulting in a minimum achievable temperature of ~ 200 K. In addition, the energy levels of H₂ become thermalized at rather low densities, n ~ 10³–⁴ cm⁻³, above which the cooling rate only scales as n, instead of n². Numerical simulations have shown that this creates a stalling point in the star-formation process, where the free-fall collapse of metal-free gas comes to a halt as the cooling time rises well above the dynamical time (Abel et al. 2002; Bromm et al. 2002). Entry into this ‘loitering’ phase marks the end of hierarchical fragmentation that occurs during the free-fall period, as the temperature is able to continually decrease with increasing density. The final fragmentation mass-scale is then set by the Jeans mass at the temperature and density corresponding to the point where the gas can no longer
cool as the density increases (Larson 1985, 2005). In the metal-free case, this yields a mass-scale of $\sim 1000 M_\odot$, resulting in the high-mass, singular nature of the first star.

The addition of metals enhances the cooling rate at low temperatures, as shown in Figure 4.1. In extremely low abundances, metals only elevate the cooling rate significantly above that of H$_2$ alone at the very lowest of temperatures ($T < 200$ K). Gas-clouds at these metallicities ($Z \lesssim 10^{-5} Z_\odot$) evolve similarly to the metal-free case, as the cooling is still not sufficient to lower the cooling time below the dynamical time at the stalling point (Omukai 2000; Bromm et al. 2001; Omukai et al. 2005). At higher metallicities, however, the cooling time becomes shorter than the dynamical time, allowing the gas-cloud to bypass the loitering phase and to undergo continued fragmentation (Bromm et al. 2001; Bromm & Loeb 2003b; Santoro & Shull 2006; Smith & Sigurdsson 2007). In the context of star-formation in the early universe, the arrival at this critical metallicity, $Z_{\text{cr}}$, at which fragmentation phase can persist past that of primordial gas, is predicted to be the point where universal mode of star-formation shifts permanently from the high-mass, solitary mode of the first stars, to the low-mass, multiply-producing mode that is presently observed (Bromm & Loeb 2003b; Santoro & Shull 2006; Smith & Sigurdsson 2007).

The protostellar collapse of metal-enriched gas-clouds has been studied extensively with one-zone models coupled to large chemical networks by Omukai (2000); Schneider et al. (2003); Omukai et al. (2005); Schneider et al. (2006). These studies have produced insight into the evolution in density and temperature of protostars with finite metallicities, but one-zone models cannot speak to the actual process of fragmentation, which requires an attention to complex cloud geometries that can only be given by full, three-dimensional hydrodynamic simulations (Larson 2007). The first of such simulations were carried out by Bromm et al. (2001), who included cooling from C, N, O, Fe, S, and Si, but not H$_2$, finding that clouds with metallicities, $Z \geq 10^{-3} Z_\odot$ are able to fragment with mass-scales lower than in the metal-free case. These simulations had a mass-resolution of only $100 M_\odot$ and were, therefore, unable to investigate the formation of solar-mass stars. More recently, Smith & Sigurdsson (2007) have performed a series of high-resolution simulations of metal-enriched gas-collapse that were able to follow the evolution of gas-fragments to sub-solar mass-scales. They, too, find that gas with metallicities, $Z \geq 10^{-3} Z_\odot$ will fragment into multiple clumps, while gas with $Z \leq 10^{-4} Z_\odot$ will produce only one object. However, Smith et al. (2007) reported the existence of regions in density and temperature that are thermally unstable in gas with metallicities as low as $10^{-4} Z_\odot$. Fragmentation is traditionally thought to happen when the cooling time is less than the dynamical, but fragments can also grow out of thermal instabilities (Field 1965). In the adaptive mesh refinement simulations of Smith & Sigurdsson (2007), grid refinement was performed based on baryon and dark-matter overdensities and the Truelove criterion (Truelove et al. 1997), $l_J < \Delta x$, where $l_J$ is the local Jeans length and $\Delta x$ is the grid-cell size. Refinement was not performed, though, when the cooling time was less than the hydrodynamic time-step. While this was not explicitly wrong, since the radiative cooling solver iterates with time-steps that are no larger than 10% of the cooling time, it may have suppressed the growth of thermal instabilities that could have formed extra fragments.
We rerun the simulations of Smith & Sigurdsson (2007) with the additional refinement criterion maintaining that the hydrodynamic time-step be less than the cooling time. In addition, we extend the series of simulations to lower metallicities and to metallicities between $10^{-4} \ Z_\odot$ and $10^{-3} \ Z_\odot$. We describe the setup of our simulations and the improvements over Smith & Sigurdsson (2007) in §4.2, present the results in §4.3, and conclude with a discussion of the nature of the second generation of stars in §4.4.

### 4.2 Simulation Setup

We perform a series of six simulations, with constant metallicities, $Z = 0 \ (Z0)$, $10^{-6} \ Z_\odot \ (Z-6)$, $10^{-5} \ Z_\odot \ (Z-5)$, $10^{-4} \ Z_\odot \ (Z-4)$, $10^{-3.5} \ Z_\odot \ (Z-3.5)$, and $10^{-3} \ Z_\odot \ (Z-3)$, using the Eulerian adaptive mesh refinement hydrodynamics/N-body code, Enzo (Bryan & Norman 1997a; O'Shea et al. 2004). As in Smith & Sigurdsson (2007), we confine the simulations to constant metallicities, saving the more realistic, and far more complicated, simulations of true second-generation star-forming environments, with heterogeneous metal-mixing and nonsolar abundance patterns, for a later paper.

The initial conditions for our simulations are identical to those used in Smith & Sigurdsson (2007). The simulation box has a width of $300 \ h^{-1} \ kpc$ comoving, with $128^3$ grid cells on the top grid, with three nested subgrids, each refining by a factor of 2, for an effective top-grid resolution of $1024^3$ cells. The cosmological parameters have the following values: $\Omega_M = 0.3$, $\Omega_\Lambda = 0.7$, $\Omega_B = 0.04$, and Hubble constant, $h = 0.7$, in units of $100 \ km \ s^{-1} \ Mpc^{-1}$. The power spectrum of initial density fluctuations is given by Eisenstein & Hu (1999), with $\sigma_8 = 0.9$ and $n = 1$. Refined grids are created during the simulations when the baryon (dark matter) density becomes 4 (8) times greater than the mean density. The local Jeans length is resolved by a minimum of 16 grid-cells at all times, as per the Truelove criterion (Truelove et al. 1997). In addition, grid-refinement will occur whenever the cooling time drops below the integration time-step of the hydrodynamic solver. This final refinement criterion was not used in Smith & Sigurdsson (2007).

We use the third implementation of the optically-thin metal cooling method of Smith et al. (2007). The Cloudy/ROCO metal cooling data-grid (Smith et al. 2007) was created with the Linux computer cluster, Lion-xo, operated by the High Performance Computing Group at The Pennsylvania State University. Similar to the precursor to this work, we do not assume the existence of an ionizing UV background. The Population III stars responsible for the enrichment of the gas in our simulations have, of course, died, and any living Pop III stars are, most likely too distant to contribute significant amounts of radiation. A major difference between our simulations and those of Smith & Sigurdsson (2007) is the choice of H$_2$ cooling rates. We use the updated H$_2$ cooling rates of Galli & Palla (1998), whereas Smith & Sigurdsson (2007) used the older rates of Lepp & Shull (1984). The rates of Galli & Palla (1998) are generally lower than those of Lepp & Shull (1984), causing the gas to take longer to cool in the newer simulations. As a result, the moment of runaway-collapse in our simulations is systematically delayed by $\sim 70 \ Myr$ from those of Smith & Sigurdsson (2007).

Each simulation runs from $z = 99$ until the point where at least one dense, protostellar core forms in the center of a $5 \times 10^5 \ M_\odot$ dark-matter halo, located in the middle
of the simulation box. The simulations are stopped when a maximum refinement of 24 levels below the top-grid has been reached. The typical central density of the dominant clump is $\sim 10^{11}$ cm$^{-3}$, or roughly $3 \times 10^{-13}$ g cm$^{-3}$. A summary of the final state of each simulation is given in Table 4.1, where $z_{\text{col}}$ is the redshift at the onset of runaway collapse, $l_{\text{max}}$ is the maximum level of refinement, $n_{\text{max}}$ is the maximum baryon density within the box, and $\Delta t_{\text{col}}$ is the time difference to runaway collapse from the metal-free case.

4.3 Results

The critical metallicity, $Z_{\text{cr}}$, has been estimated analytically by calculating the chemical abundance required for the cooling time to equal the dynamical time at the stalling point for metal-free gas, $n \sim 10^{3-4}$ cm$^{-3}$ and $T \sim 200$ K. Bromm & Loeb (2003b) performed this exercise with C and O, and Santoro & Shull (2006) did so with C, O, Fe, and Si, and including cooling from H$_2$. Santoro & Shull (2006) considered densities above and below the stalling point as well. The general consensus from these studies is that $Z_{\text{cr}} \approx 10^{-3.5}$ $Z_\odot$ at $n = 10^{4}$ cm$^{-3}$. Using the cooling rates from Smith et al. (2007), we estimate $Z_{\text{cr}}$ at $n = 10^{3}$ cm$^{-3}$ and $10^{4}$ cm$^{-3}$ in Figure 4.2. Our calculation of the critical metallicity, $10^{-4.6} Z_\odot \leq Z_{\text{cr}} \leq 10^{-4.2} Z_\odot$, is significantly lower than previous calculations. This is due to the fact that the cooling method we use includes all atomic species from H to Zn, not simply C, O, Fe, and Si. The main extra contributor to the cooling is fine-structure emission from S, which was shown by Smith et al. (2007) to be important. In addition, the cooling contribution from H$_2$, which was not included at all in Bromm & Loeb (2003b), is likely higher than in Santoro & Shull (2006) since we have computed the H$_2$ fraction by integrating the H/He chemical network of Abel et al. (1997) for a time-period equivalent to that between $z = 99$ and $z = 20$. This is appropriate for this work, since it more accurately approximates the fraction of H$_2$ that will be present when the star-forming cloud reaches the metal-free stalling point.

We see a trend with metallicity and collapse redshift that is similar to what was reported by Smith & Sigurdsson (2007), where simulations with higher metallicities reach the runaway collapse phase earlier. The only deviation from this trend occurs for run Z-5, which collapsed approximately 300,000 years after the simulation with $Z = 10^{-6}$ $Z_\odot$. Similarly, the simulations collapsing later have a higher number of total grids and grid-cells in their final output, since the lower-density envelope gas has had more time to evolve and reach higher densities.

In Figures 4.3–4.8, we display density slices through the final output of each simulation, intersecting the cell of maximum density. Runs Z0 (Figure 4.3) and Z-6 (Figure 4.4) appear qualitatively similar. Their central cores are slightly elongated, and there are a few smaller density maxima present, but no concrete evidence of fragmentation can be seen. The central core in run Z-5 (Figure 4.5) appears more uniform than the two cores of lower metallicity. In contrast, run Z-4 (Figure 4.6) presents the strongest case for the occurrence of fragmentation. This is not unexpected, however, since this metallicity is above the value of $Z_{\text{cr}}$ calculated earlier in §4.2 (Figure 4.2). Surprisingly, run Z-3.5 (Figure 4.7) appears the most uniform of the entire series, with absolutely no
indication of any fragmentation. Finally, run Z-3 (Figure 4.8), shows only minor evidence for fragmentation, but noticeably less than run Z-4.

In Figure 4.9, we plot the spherically-averaged gas density and mass as a function of radius from the central density peak for the final output of each simulation. At large radii from the density peak, \( r \gtrsim 10^{-3} \) pc, the gas density scales roughly as \( n \propto r^{-2.2} \). The gas density and mass at the center vary by almost an order of magnitude, with the lowest metallicity simulations having the highest central densities and masses. Each simulation with \( Z \geq 10^{-5} Z_\odot \) has a region where the slope of the density profile is slightly shallower than the average slope over the entire range of radii. In each case, this coincides with a drop in the gas temperature (Figure 4.10A and B) when moving radially inward. The accretion rate in the isothermal collapse model of Shu (1977) is proportional to the cube of the sound speed. In this framework, the drop in temperature decreases the accretion rate, resulting in the lower density and mass with radius. In Figure 4.11, we plot the instantaneous accretion rate, given by

\[
\dot{M} = 4\pi r^2 \rho(r) v_r(r),
\]

vs. radius and enclosed mass. As predicted, a decrease in the accretion rate occurs simultaneously with a drop in temperature and the flattening of the density profile. Mass can be transferred no faster than the sum of the bulk velocity plus the local sound speed. The two lowest metallicity simulations, Z0 and Z-6, with maximum temperatures of \( \sim 1000 \) K, have the highest infall velocities. The peak in the infall velocities (Figure 4.10E and F), at \( r \sim 10^{-2} \) pc, occurs exactly where the gas is hottest.

In runs Z-4, Z-3.5, and Z-3, which all have \( Z > Z_{cr} \), the classical fragmentation criterion is satisfied for all of the gas within 1 pc of the core (Figure 4.10C). The cooling time is only lower than the dynamical time in run Z-5 briefly at \( r \sim 2 \times 10^{-2} \) pc, corresponding to the peak in the metal cooling efficiency that occurs at \( n \sim 10^6 \) cm\(^{-3}\) (Figure 2.13). Within the central \( 10^{-2} \) pc, the cooling time drops just below the dynamical time in runs Z0 and Z-6. This is due to the onset of 3-body \( \text{H}_2 \) formation at \( n \sim 10^9 \) cm\(^{-3}\), which rapidly converts all of the H into \( \text{H}_2 \), creating a weak thermal instability (Abel et al. 2002). Since the cooling rate of \( \text{H}_2 \) is roughly 1000 times higher at 1000 K than it is at 300 K (Figure 2.2), the significant increase in the \( \text{H}_2 \) fraction from the 3-body process is unable to lower the gas temperature in the simulations with \( Z \geq 10^{-5} Z_\odot \).

At first glance, the picture created by Figures 4.3–4.8 is somewhat puzzling. Intuitively, one would expect all of the simulations above the critical metallicity to exhibit conclusive evidence of fragmentation. Fragmentation, however, can only continue as long as the temperature decreases with increasing density (Larson 1985, 2005). In Figure 4.12, we plot the number density vs. gas temperature for the final output of each simulation. Due to the self-similar nature of the collapse, Figure 4.12 can also be used to understand the evolution of the central core throughout the collapse. Runs Z-3.5 and Z-3 are able to cool very quickly to the temperature of the CMB. In fact, the cooling proceeds so efficiently that the gas has not had sufficient time to reach high densities before hitting the temperature-floor of the CMB. For runs Z-3.5 and Z-3, the Jeans masses at the point where the temperature evolution becomes flat from the CMB are 184 \( M_\odot \) and 360 \( M_\odot \),
respectively. In runs Z0, Z-6, and Z-5, the cooling is too low to prevent the temperature from rising at the H\textsubscript{2} thermalization density, \(n \sim 10^3 \text{cm}^{-3}\). The Jeans mass at their respective density minima are 7,861 \(M_\odot\), 5,597 \(M_\odot\), and 5,402 \(M_\odot\). In run Z-4, the cooling is just strong enough to bypass the loitering phase without any increase in temperature. On the other hand, the cooling is not efficient enough to cool all the way to the CMB. The core continues to slowly cool to about 60 K at \(n \sim 10^8 \text{cm}^{-3}\), where the Jeans mass is only 3 \(M_\odot\). Run Z-5 undergoes a second cooling phase, from \(n \sim 10^6 \text{cm}^{-3}\) to \(10^8 \text{cm}^{-3}\). This does not result in renewed fragmentation, because the earlier heating phase has homogenized the core to the point where no density perturbations exist that can grow into fragments, as was predicted by Larson (2005) and also observed in the models of Omukai et al. (2005).

To confirm our explanation of the suppression of fragmentation in runs Z-3.5 and Z-3, we examine density slices of outputs from before and after the gas temperature has reached a minimum. In Figures 4.13 and 4.14, we plot density slices through outputs from each of the six runs, taken when the maximum number density is \(n \sim 10^2 \text{cm}^{-3}\). The core in each simulation is still in free-fall collapse, and appears extremely non-uniform. In contrast, when the cores have reached maximum densities of \(n \sim 10^5 \text{cm}^{-3}\) (Figures 4.15 and 4.16), they have all become significantly more uniform, with the exception, of course, of run Z-4. In Figures 4.17 and 4.18, we examine this process in more detail for runs Z-3.5 and Z-3. From left to right, the slices in Figure 4.17 show the core in run Z-3.5 when the maximum number density is \(n \sim 10^3, 10^4,\) and \(10^5 \text{cm}^{-3}\). We perform the same exercise for run Z-3 in Figure 4.18, with slices when the maximum number density is \(n \sim 10^2, 10^3,\) and \(10^4 \text{cm}^{-3}\). In each case, the central core becomes noticeably more uniform after its temperature has reached the CMB temperature. Further evidence that fragmentation is suppressed when the core temperature reaches the CMB \(T=200\) K is provided in Figure 4.19, where we show the results of a simulation with metallicity, \(Z = 10^{-3} Z_\odot\), but with the CMB removed. In the absence of the CMB, the cooling phase can continue to much higher densities, allowing extensive fragmentation to occur.

4.4 Discussion

We have shown that gas-clouds with metallicities, \(Z \geq 10^{-4} Z_\odot\), are able to continue to cool past the onset of the loitering phase in metal-free gas-collapse, which we observe to occur at \(n \sim 10^3 \text{cm}^{-3}\) and \(T \sim 200\) K. This agrees nicely with our calculation of the critical metallicity, \(Z_{\text{cr}} = 10^{-4.2} Z_\odot\). When \(Z \geq Z_{\text{cr}}\), the period in which fragmentation can occur is prolonged, reducing the characteristic mass-scale. When the metallicity is above \(10^{-3.5} Z_\odot\), however, the gas cools quickly to the CMB temperature, halting fragmentation at low densities. This results in a mass-scale that is much smaller than in gas-clouds with \(Z \leq Z_{\text{cr}}\), but still over 100 \(M_\odot\) for redshifts, \(Z \sim 15\). For fragmentation to continue to solar-mass scales, the metallicity must be greater than the critical metallicity, but low enough so as not to cool the gas down to the CMB temperature.

This implies the existence of three distinct metallicity regimes for star-formation. In the first regime, \(Z \leq Z_{\text{cr}}\), metals do not provide enough additional cooling to allow the gas temperature to continue to decrease monotonically with increasing density when the
core reaches the H$_2$ thermalization density. In this case, the collapse proceeds similar to metal-free collapse, resulting in the formation of a single, massive object. At the other extreme, we define $Z_{\text{CMB}}$ as the metallicity at which the gas can cool to the CMB temperature. When $Z \gg Z_{\text{CMB}}$, the cloud-core will efficiently cool to the temperature of the CMB when the central density is still relatively low. As we have shown in runs Z-3.5 and Z-3, fragmentation is suppressed by cooling rapidly to the CMB temperature, as the mass-scale is determined by the Jeans mass at the density when the core first reaches the CMB temperature. Finally, our simulations have shown that there exists a special range in metallicity, $Z_{\text{cr}} \leq Z < Z_{\text{CMB}}$, where the core does not reheat at the metal-free stalling point, but also cannot cool all the way to the CMB temperature. The core collapses to much higher densities before reaching its minimum temperature, which is set only by the balance of radiative cooling and adiabatic heating. Run Z-4, whose metallicity is within this special regime, is able to cool up to a number density of $9.5 \times 10^7$ cm$^{-3}$, setting the mass-scale at only 3 $M_{\odot}$. In this specific case, the mass-scale is not regulated externally by the CMB, but rather internally by the metallicity-dependent gas-cooling.

In Figure 4.20, we present an estimate of the mass-scale as a function of metallicity. For $Z < Z_{\text{cr}}$, the mass-scale is approximately constant, as fragmentation comes to an end at the beginning of the loitering phase. The transition from $Z < Z_{\text{cr}}$ to $Z \geq Z_{\text{cr}}$ should be extremely sharp, as the core is now able to slowly cool without ever reaching the CMB floor, as in run Z-4. This matches the general predictions of Clarke & Bromm (2003), who note the large difference in characteristic stellar mass between clouds cooling by H$_2$ and those cooling by CO. Between $Z_{\text{cr}}$ and $Z_{\text{CMB}}$, the mass-scale will decrease slightly, as a small increase in metallicity will cool the gas to marginally lower temperatures and higher densities. When $Z = Z_{\text{CMB}}$, the gas will be able to cool to the CMB floor for the first time. As $Z$ rises above $Z_{\text{CMB}}$, the point at which the gas temperature reaches that of the CMB will occur at lower and lower densities, resulting in an increase in mass-scale with metallicity. It is important to note that the placement of $Z_{\text{CMB}}$ in Figure 4.20 is merely an illustration, as we can only constrain it to $10^{-4} < Z_{\odot} < 10^{-3.5}$ at this time. Future simulations within this metallicity range will allow us to more tightly constrain $Z_{\text{CMB}}$, and better understand the behavior of the mass-scale very near this special metallicity. Clearly, $Z_{\text{CMB}}$ is also dependent on redshift. $Z_{\text{cr}}$ is constant in time, as it only depends on the radiative cooling physics of heavy elements. At higher redshifts, $Z_{\text{CMB}}$ will decrease, since lower metallicities are required to reach the higher CMB temperatures. Eventually, $Z_{\text{CMB}}$ will approach $Z_{\text{cr}}$, and the low-mass formation mode observed in run Z-4 will be eliminated, and the evolution will resemble runs Z-3.5 and Z-3. At lower redshifts, the low-mass mode of run Z-4 will grow toward the right in Figure 4.20 as $Z_{\text{CMB}}$ increases with the slowly decreasing CMB temperature. The mass-scale for stars forming with $Z \geq Z_{\text{CMB}}$ will also be dependent on redshift. Since the CMB temperature is lower at later times, the Jeans mass at a given density will also be lower. This type of evolution of the stellar mass-scale with the CMB was predicted by Larson (1998). Eventually, the CMB regulated mode of star-formation, where $Z \geq Z_{\text{CMB}}$, will vanish, as the CMB temperature drops below the minimum temperature achievable via radiative cooling. In the current epoch, prestellar cloud-cores are observed...
with temperatures averaging $\sim 8.5$ K (Evans 1999), implying that the CMB regulated star-formation mode only dies out at $z \sim 2$.

It was claimed recently, by Tumlinson (2006), that an IMF for the first stars that is dominated by stars in the pair-instability supernova range ($140 M_\odot \leq M \leq 260 M_\odot$) is unable to produce the observed metallicity distribution in the Galaxy, in models of hierarchical formation of the Milky Way that include chemical enrichment. If very early metal-enriched stars were also rather massive, although less massive than the first stars, then it is possible that they were responsible for a significant portion of the high-redshift metal production. In this scenario, there could have been a brief period very early in the universe where the first stars existed in the pair-instability supernova mass-range. If metal-production from massive, second-generation stars was high-enough, then it could have erased any trace of the very-massive first stars. In that case, the models of Tumlinson (2006) could be tracing chemical enrichment that began with massive second stars, but missing the brief phase of very massive first stars. This explanation could potentially reconcile the conclusions of first-star theorists, who claim that the first stars must be very massive, with those of the observers, who find no evidence of the existence of very massive stars in the chemical abundance data.

The case presented above is an idealized one, in which the first metals exist in solar abundance patterns. In this instance, the value of \([Fe/H] \equiv \log_{10}(n_X/n_H) - \log_{10}(n_X/n_H)_\odot\), is an exact measure of the metallicity, Z. It seems quite clear, however, based both on predicted yields of Population III supernovae (Heger & Woosley 2002; Heger et al. 2003), and the observed abundance patterns of the most metal-poor stars (Christlieb et al. 2002; Frebel et al. 2005; Beers & Christlieb 2005; Frebel et al. 2007), that alpha elements, particularly C and O, were of primary importance in triggering the formation of the first low-mass stars in the universe. The two most iron-poor stars known, HE0107-5240 (Christlieb et al. 2002), and HE1327-2326 (Frebel et al. 2005), both with \([Fe/H] < -5\) and referred to as hyper metal-poor (HMP) stars (Beers & Christlieb 2005), are extremely overabundant in C and O. It is, therefore, a possibility that the very low-metallicity gas out of which the second stars formed was generally over-enriched with C and O, which would drastically alter what we think of as the critical metallicity, $Z_{cr}$. In nonsolar abundance patterns, the concept of metallicity loses some of its meaning, as it cannot be directly tied the abundance of any single element. Ideally, metallicity should be quantified by the total radiative cooling from all of the heavy elements present. Under this definition, HE0107-5240 and HE1327-2326 do not qualify as the most metal-poor stars. Observationally, metallicity is generally related to the value of \([Fe/H],\) regardless of the abundance pattern. Adopting the observational definition of metallicity, we estimate the effect of C/O overabundance on the value of $Z_{cr}$ by calculating the increase in cooling resulting from an enhancement of C and O above a given mean metallicity. We include the cooling from $H_2$ in the manner described in §2.2.2. In Figures 4.24–4.26, we illustrate the effective increase in metallicity resulting from a C/O enhancement by a factor of 3, 10, and 100 over mean metallicities of $10^{-6}$, $10^{-5}$, $10^{-4}$, and $10^{-3} Z_\odot$. For low metallicities and high temperatures, additional C and O does not increase the effective metallicity because the cooling in those regimes is dominated by $H_2$, e.g., Figure 2.2. Additionally, cooling from C becomes less important at higher densities and temperatures, e.g., Figures 2.3–2.11. Defining $\Delta Z_{eff}(Z,n,T)$ as the effective logarithmic increase in metallicity at
number density, $n$, and temperature, $T$, from a value, $Z$, due to C/O enhancement, we approximate a new $Z_{cr}$ by finding the metallicity, $Z_{cr}^{\text{new}}$, such that

$$\log_{10}(Z_{cr}^{\text{new}}) = \log_{10}(Z_{cr}^{\text{old}}) + \Delta Z_{\text{eff}}(Z_{cr}^{\text{new}}, 10^3 \text{ cm}^{-3}, 200 \text{ K}).$$

We estimate the new value of $Z_{CMB}$ using the same method with $T \sim 100$ K. The value of $n$ is less important in this case, as $\Delta Z_{\text{eff}}$ is roughly constant at low temperatures. In Figures 4.24–4.26, we show the expected mass-scale/metallicity relation, shown originally in Figure 4.20, after C/O enhancement. An overabundance of C and O decreases the value of $Z_{cr}$, but decreases the value of $Z_{CMB}$ even more. As a result, the special regime of $Z_{cr} \leq Z < Z_{CMB}$ shrinks as more C and O are added. Given, the uncertainty in $Z_{CMB}$, it is entirely possible that the low-mass star-formation mode has completely vanished for C/O enhancement of 100. If this is to be believed, then the observed abundances of HE0107-5240 and HE1327-2326, with $[\text{C/Fe}] \sim 4$, cannot be indicative of the their original chemical abundances, but are, instead, a result of their peculiar stellar evolution, e.g., mass transfer from a binary companion, as laid out recently by Tumlinson (2007).
Table 4.1. Final States

<table>
<thead>
<tr>
<th>Run</th>
<th>Z ($Z:\odot$)</th>
<th>$z_{col}$</th>
<th>$l_{max}$</th>
<th>Grids</th>
<th>Cells</th>
<th>$n_{max}$ (cm$^{-3}$)</th>
<th>$\Delta t_{col}$ (Myr)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Z0</td>
<td>0</td>
<td>14.761203</td>
<td>24</td>
<td>13790</td>
<td>6.49 $\times 10^{7}$</td>
<td>5.96 $\times 10^{11}$</td>
<td>-</td>
</tr>
<tr>
<td>Z-6</td>
<td>$10^{-6}$</td>
<td>15.070589</td>
<td>24</td>
<td>13369</td>
<td>6.30 $\times 10^{7}$</td>
<td>6.16 $\times 10^{11}$</td>
<td>7.81</td>
</tr>
<tr>
<td>Z-5</td>
<td>$10^{-5}$</td>
<td>15.058936</td>
<td>24</td>
<td>13387</td>
<td>6.32 $\times 10^{7}$</td>
<td>2.93 $\times 10^{11}$</td>
<td>7.52</td>
</tr>
<tr>
<td>Z-4</td>
<td>$10^{-4}$</td>
<td>15.122490</td>
<td>24</td>
<td>13406</td>
<td>6.34 $\times 10^{7}$</td>
<td>1.06 $\times 10^{11}$</td>
<td>9.08</td>
</tr>
<tr>
<td>Z-3.5</td>
<td>$10^{-3.5}$</td>
<td>15.234573</td>
<td>24</td>
<td>13060</td>
<td>6.21 $\times 10^{7}$</td>
<td>7.09 $\times 10^{10}$</td>
<td>11.8</td>
</tr>
<tr>
<td>Z-3</td>
<td>$10^{-3}$</td>
<td>16.313200</td>
<td>24</td>
<td>11758</td>
<td>5.72 $\times 10^{7}$</td>
<td>7.12 $\times 10^{10}$</td>
<td>35.7</td>
</tr>
</tbody>
</table>
Fig. 4.1 Top: Cooling rate vs. temperature for gases with hydrogen number densities, $n_H = 10^3 \text{ cm}^{-3}$ (left) and $10^4 \text{ cm}^{-3}$ (right), with metallicities, $Z = 0$ (black), $10^{-6} Z_\odot$ (red), $10^{-5} Z_\odot$ (yellow), $10^{-4} Z_\odot$ (green), $10^{-3.5} Z_\odot$ (blue), and $10^{-3} Z_\odot$ (violet). Bottom: Cooling time vs. temperature for same densities and metallicities. The corresponding dynamical time is indicated by the dashed, black line.
Fig. 4.2 The solid lines show the cooling time vs. metallicity at $T = 200$ K and $n = 10^3$ cm$^{-3}$ (blue) and $10^4$ cm$^{-3}$ (red). The dotted lines indicate the dynamical time for $n = 10^3$ cm$^{-3}$ (blue) and $10^4$ cm$^{-3}$ (red). The intersection of the solid and dotted lines for each color gives the critical metallicity, $Z_{cr}$, at the respective densities.
Fig. 4.3 Density slices of the final output of the simulation with $Z = 0$ (metal-free) in x (top), y (middle), and z (bottom). Each slice intersects the densest point in the simulation box and has a width of $5 \times 10^{-6}$ (left), $5 \times 10^{-7}$ (center), and $2 \times 10^{-7}$ (right) of the full box ($300 \, h^{-1} \, \text{kpc comoving}$).
Fig. 4.4 Density slices of the final output of the simulation with $Z = 10^{-6} \, Z_\odot$ in x (top), y (middle), and z (bottom). Each slice intersects the densest point in the simulation box and has a width of $5 \times 10^{-6}$ (left), $5 \times 10^{-7}$ (center), and $2 \times 10^{-7}$ (right) of the full box ($300 \ h^{-1} \ kpc$ comoving).
Fig. 4.5 Density slices of the final output of the simulation with $Z = 10^{-5} \, Z_\odot$ in x (top), y (middle), and z (bottom). Each slice intersects the densest point in the simulation box and has a width of $5 \times 10^{-6}$ (left), $5 \times 10^{-7}$ (center), and $2 \times 10^{-7}$ (right) of the full box ($300 \, h^{-1} \, \text{kpc comoving}$).
Fig. 4.6 Density slices of the final output of the simulation with $Z = 10^{-4} Z_\odot$ in $x$ (top), $y$ (middle), and $z$ (bottom). Each slice intersects the densest point in the simulation box and has a width of $5 \times 10^{-6}$ (left), $5 \times 10^{-7}$ (center), and $2 \times 10^{-7}$ (right) of the full box ($300 \ h^{-1} \ kpc$ comoving).
Fig. 4.7 Density slices of the final output of the simulation with $Z = 10^{-3.5} \ Z_\odot$ in $x$ (top), $y$ (middle), and $z$ (bottom). Each slice intersects the densest point in the simulation box and has a width of $5 \times 10^{-6}$ (left), $5 \times 10^{-7}$ (center), and $2 \times 10^{-7}$ (right) of the full box ($300 \ h^{-1}$ kpc comoving).
Fig. 4.8 Density slices of the final output of the simulation with $Z = 10^{-3} \ Z_\odot$ in $x$ (top), $y$ (middle), and $z$ (bottom). Each slice intersects the densest point in the simulation box and has a width of $5 \times 10^{-6}$ (left), $5 \times 10^{-7}$ (center), and $2 \times 10^{-7}$ (right) of the full box ($300 \ h^{-1} \ kpc$ comoving).
Fig. 4.9 Spherically averaged, mass weighted quantities for the final output of each simulation: $Z = 0$ (black), $10^{-6} \ Z_\odot$ (red), $10^{-5} \ Z_\odot$ (yellow), $10^{-4} \ Z_\odot$ (green), $10^{-3.5} \ Z_\odot$ (blue), and $10^{-3} \ Z_\odot$ (violet). A: Number density vs. radius. B: Enclosed gas mass vs. radius.
Fig. 4.10 Spherically averaged, mass weighted quantities for the final output of each simulation: $Z = 0$ (black), $10^{-6} Z_\odot$ (red), $10^{-5} Z_\odot$ (yellow), $10^{-4} Z_\odot$ (green), $10^{-3.5} Z_\odot$ (blue), and $10^{-3} Z_\odot$ (violet). A: Temperature vs. radius. B: Temperature vs. enclosed mass. C: Ratio of dynamical time to cooling time vs. radius. D: Ratio of dynamical time to cooling time vs. enclosed mass. E: Radial velocity vs. radius. F: Radial velocity vs. enclosed mass.
Fig. 4.11 The instantaneous accretion rate (Equation 4.1) vs. radius (A) and enclosed gas mass (B) for the final output of each simulation: $Z = 0$ (black), $10^{-6} \ Z_\odot$ (red), $10^{-5} \ Z_\odot$ (yellow), $10^{-4} \ Z_\odot$ (green), $10^{-3.5} \ Z_\odot$ (blue), and $10^{-3} \ Z_\odot$ (violet).
Fig. 4.12 Number density vs. temperature for final output of each simulation: $Z = 0$ (black), $10^{-6} \, Z_{\odot}$ (red), $10^{-5} \, Z_{\odot}$ (yellow), $10^{-4} \, Z_{\odot}$ (green), $10^{-3.5} \, Z_{\odot}$ (blue), and $10^{-3} \, Z_{\odot}$ (violet). The dashed lines indicate lines of constant Jeans mass. The dotted line illustrates the CMB temperature floor at 45 K ($z \sim 15.5$).
Fig. 4.13 Density slices of the simulations with $Z = 0$ (left), $10^{-6} Z_\odot$ (center), and $10^{-5} Z_\odot$ (right) in x (top), y (middle), and z (bottom). Each dataset was chosen such that the maximum number density in the simulation is $\sim 10^2 \text{ cm}^{-3}$. Each slice intersects the densest point in the simulation box and has a width of $10^{-3}$ of the full box ($300 \ h^{-1} \text{ kpc}$ comoving).
Fig. 4.14 Density slices of the simulations with $Z = 10^{-4} Z_\odot$ (left), $10^{-3.5} Z_\odot$ (center), and $10^{-3} Z_\odot$ (right) in x (top), y (middle), and z (bottom). Each dataset was chosen such that the maximum number density in the simulation is $\sim 10^2$ cm$^{-3}$. Each slice intersects the densest point in the simulation box and has a width of $10^{-3}$ of the full box ($300 \, h^{-1}$ kpc comoving).
Fig. 4.15 Density slices of the simulations with $Z = 0$ (left), $10^{-6} \, Z_\odot$ (center), and $10^{-5} \, Z_\odot$ (right) in x (top), y (middle), and z (bottom). Each dataset was chosen such that the maximum number density in the simulation is $\sim 10^5 \, \text{cm}^{-3}$. Each slice intersects the densest point in the simulation box and has a width of $10^{-4}$ of the full box (300 $h^{-1}$ kpc comoving).
Fig. 4.16 Density slices of the simulations with $Z = 10^{-4} Z_\odot$ (left), $10^{-3.5} Z_\odot$ (center), and $10^{-3} Z_\odot$ (right) in x (top), y (middle), and z (bottom). Each dataset was chosen such that the maximum number density in the simulation is $\sim 10^5$ cm$^{-3}$. Each slice intersects the densest point in the simulation box and has a width of $10^{-4}$ of the full box ($300 \, h^{-1}$ kpc comoving).
Fig. 4.17 Density slices of the simulation with $Z = 10^{-3.5} Z_\odot$ when the maximum number density is $\sim 10^3 \text{ cm}^{-3}$ (left), $\sim 10^4 \text{ cm}^{-3}$ (center), and $\sim 10^5 \text{ cm}^{-3}$ (right) in $x$ (top), $y$ (middle), and $z$ (bottom). Each slice intersects the densest point in the simulation box and has a width of $5 \times 10^{-4}$ (left), $2.5 \times 10^{-4}$ (center), and $1.25 \times 10^{-4}$ (right) of the full box ($300 h^{-1}$ kpc comoving).
Fig. 4.18 Density slices of the simulation with $Z = 10^{-3} Z_{\odot}$ when the maximum number density is $\sim 10^2 \text{ cm}^{-3}$ (left), $\sim 10^3 \text{ cm}^{-3}$ (center), and $\sim 10^4 \text{ cm}^{-3}$ (right) in x (top), y (middle), and z (bottom). Each slice intersects the densest point in the simulation box and has a width of $2 \times 10^{-3}$ (left), $4 \times 10^{-4}$ (center), and $4 \times 10^{-4}$ (right) of the full box ($300 \, h^{-1} \, \text{kpc comoving}$).
Fig. 4.19 Density slices of the final output of the simulation with $Z = 10^{-3} \, Z_{\odot}$ and without a CMB temperature floor in x (top), y (middle), and z (bottom). Each slice intersects the densest point in the simulation box and has a width of $5 \times 10^{-5}$ (left), $5 \times 10^{-6}$ (center), and $2 \times 10^{-6}$ (right) of the full box (300 $h^{-1}$ kpc comoving) Note: The slices shown have widths 10 times larger than Figures 4.3–4.8.
Fig. 4.20 The diamonds show the Jeans mass at the end of the fragmentation phase for each of the simulations. The vertical, dashed blue line indicates the critical metallicity, $Z_{cr} = 10^{-4.2} Z_{\odot}$. The cyan rectangle indicates the approximate value of $Z_{CMB}$, somewhere between $10^{-4} Z_{\odot}$ and $10^{-4.5} Z_{\odot}$. The red, dashed line shows the expected trend of mass-scale with metallicity.
Fig. 4.21 Contours over number density and temperature of the equivalent logarithmic increase in metallicity resulting from an enhancement of the C and O abundances by a factor of 3 over base metallicities of $Z = 10^{-6} Z_{\odot}$ (top-left), $10^{-5} Z_{\odot}$ (top-right), $10^{-4} Z_{\odot}$ (bottom-left), and $10^{-3} Z_{\odot}$ (bottom-right). An enhancement of all metal species by a factor of 3 is equivalent to $\log_{10}(\Delta Z) = 0.5$. 
Fig. 4.22 Contours over number density and temperature of the equivalent logarithmic increase in metallicity resulting from an enhancement of the C and O abundances by a factor of 10 over base metallicities of $Z = 10^{-6} \ Z_\odot$ (top-left), $10^{-5} \ Z_\odot$ (top-right), $10^{-4} \ Z_\odot$ (bottom-left), and $10^{-3} \ Z_\odot$ (bottom-right). An enhancement of all metal species by a factor of 10 is, of course, equivalent to $\log_{10}(\Delta Z) = 1$. 
Fig. 4.23 Contours over number density and temperature of the equivalent logarithmic increase in metallicity resulting from an enhancement of the C and O abundances by a factor of 100 over base metallicities of $Z = 10^{-6} \, Z_\odot$ (top-left), $10^{-5} \, Z_\odot$ (top-right), $10^{-4} \, Z_\odot$ (bottom-left), and $10^{-3} \, Z_\odot$ (bottom-right). An enhancement of all metal species by a factor of 100 is, of course, equivalent to $\log_{10}(\Delta Z) = 2$. 
Fig. 4.24 The red, dashed line approximates the behavior of mass-scale with metallicity when C and O abundances are enhanced above the mean metallicity by a factor of 3. The vertical, dashed blue line indicates the critical metallicity, $Z_{cr} \approx 10^{-4.5} Z_{\odot}$. The cyan rectangle indicates the approximate value of $Z_{CMB}$. All metallicities, $Z$, refer to the base metallicity, before enhancement of C and O.
Fig. 4.25 The red, dashed line approximates the behavior of mass-scale with metallicity when C and O abundances are enhanced above the mean metallicity by a factor of 10. The vertical, dashed blue line indicates the critical metallicity, $Z_{cr} \approx 10^{-4.8} Z_\odot$. The cyan rectangle indicates the approximate value of $Z_{CMB}$. All metallicities, $Z$, refer to the base metallicity, before enhancement of C and O.
Fig. 4.26 The red, dashed line approximates the behavior of mass-scale with metallicity when C and O abundances are enhanced above the mean metallicity by a factor of 100. The vertical, dashed blue line indicates the critical metallicity, $Z_{cr} \approx 10^{-5.8} Z_\odot$. The cyan rectangle indicates the approximate value of $Z_{CMB}$. All metallicities, $Z$, refer to the base metallicity, before enhancement of C and O.
Chapter 5

Conclusion

5.1 Summary

The creation of the first heavy elements in the supernovae of the first stars added a level of complexity to the universe that forever changed the way baryonic structure formed and evolved. Likewise, the need to include the physical processes associated with these metals in numerical simulations has created new challenges for computational astrophysics. In this work, we have taken the next step toward meeting these challenges by introducing a method to include the radiative cooling from a complete set of heavy elements through Zn in large-scale, three-dimensional simulations of cosmic structure formation. We have utilized the highly sophisticated radiation transport machinery of Cloudy to create a metal cooling method that is physically valid for an extremely wide range of physical conditions, which will allow this work to be applied to the simulation of many astrophysical systems from, large scale to small, and from the early universe to the present day.

We have used this method to study the very first objects to form with some level of metal-enrichment, the second generation of stars in the universe. In the case of solar abundance patterns and a full complement of metals, we calculate the critical metallicity, $Z_{\text{cr}}$, to be $10^{-4.2} Z_\odot$. While it is unlikely that the first metals were present in solar abundance patterns, our calculation serves as an estimate of the cooling rate required to begin the transition to the low-mass star-formation mode. When considering nonsolar abundance patterns, we will have to be wary of how we calculate the metallicity of a gas. The measure of [Fe/H], which is commonly used interchangeably with the metallicity, $Z$, is very misleading, especially in the context of iron-poor stars with large alpha enhancements, such as HE0107-5240 and HE1327-2326. In cases such as these, it would be more accurate to define the metallicity, $Z$, as the metallicity required to create an equivalent cooling function in a gas with a solar abundance pattern. This will be nontrivial, as each element makes a unique contribution to the aggregate cooling function. One possible remedy to this situation would be to compare cooling rates at one density and temperature. Since the point, $n = 10^4$ cm$^{-3}$, $T = 200$ K, is often used for the calculation of $Z_{\text{cr}}$ (Bromm & Loeb 2003b; Santoro & Shull 2006), this may be the ideal case for calculating the effective metallicity for a nonsolar abundance pattern.

Analysis of cooling rates as a function of density and temperature helps to pinpoint the evolutionary phase during which fragmentation occurs in a collapsing gas-cloud. In addition to the classical fragmentation criterion, $t_{\text{cool}} < t_{\text{dyn}}$, we have studied the ability of metals to induce fragmentation through the formation of thermal instabilities. We have found that regions in density and temperature exist where the gas is both thermally unstable and satisfies the classical fragmentation criterion. These doubly unstable
regions, we have called them, provide the physical conditions most likely to produce fragmentation. We have observed doubly unstable regions to exist for metallicities as low as $10^{-4} \ Z_\odot$, which fits very well with our calculation of $Z_{cr} = 10^{-4.2} \ Z_\odot$. The presence of the CMB, however, limits the doubly unstable regions to temperatures, $T \gg T_{CMB}$. At very high redshift ($Z \gtrsim 10$), this effect will be appreciable, and may result in a unique IMF for the earliest generations of Population II stars, as was suggested by Larson (1998).

Using the metal cooling method we created, we have performed two series of numerical simulations of pre-enriched primordial star-formation, using the adaptive mesh refinement code, Enzo. Our first set of simulations, performed for metallicities, $Z = 0, 10^{-4} \ Z_\odot, 10^{-3} \ Z_\odot$, and $10^{-2} \ Z_\odot$, showed a sharp transition in behavior between metallicities, $Z = 10^{-4} \ Z_\odot$ and $10^{-3} \ Z_\odot$. For simulations with $Z \leq 10^{-4} \ Z_\odot$, we observed the formation of a single a single, central object. In those with $Z \geq 10^{-3} \ Z_\odot$, we observed multiple, however only a few, isolated density maxima in the very center.

Our second set of simulations incorporated updated $\text{H}_2$ cooling rates, as well as the additional refinement criterion requiring refinement to occur wherever the cooling time was less than the integration timestep. For this series, we eliminated the run with $Z = 10^{-2} \ Z_\odot$, but added runs with $Z = 10^{-6} \ Z_\odot, 10^{-5} \ Z_\odot$, and $10^{-3.5} \ Z_\odot$. This time, our results were noticeably different. The simulations with $Z \leq 10^{-5} \ Z_\odot$ proceeded much like the metal-free case. However, significant fragmentation was observed in the run with $Z = 10^{-4} \ Z_\odot$. Even more surprising, though, was the fact that little or no fragmentation occurred for the simulations with $Z = 10^{-3.5} \ Z_\odot$ and $10^{-3} \ Z_\odot$. The explanation for this is quite clear when considering the evolution in density and temperature of the central core, shown in Figure 4.12. Fragmentation can only occur as long as the gas temperature continues to decrease with increasing density. For the three lowest metallicity simulations, this cessation occurred at the traditional stalling point of metal-free gas, and the resulting mass-scales were of the order of $10^4 \ M_\odot$. For the two highest metallicity simulations, this happened when the gas cooled down to the temperature of the CMB. Since the cooling was so efficient for these two cases, this took place when the central density was still quite low, resulting in a mass-scale of a few $\times \ 10^2 \ M_\odot$. Only in the simulation with $Z = 10^{-4} \ Z_\odot$ was the gas able to continue to cool past the metal-free stalling point, but unable to reach the CMB temperature. In this particular case, fragmentation continued to a mass-scale of roughly $3 \ M_\odot$. From this, we have identified a second metallicity of interest, $Z_{CMB}$, defined as the metallicity at which the gas is first able to reach the CMB temperature. Unlike $Z_{cr}$ which is only dependent on physics, $Z_{CMB}$ will clearly evolve with time, as the CMB temperature evolves. At lower redshift, $Z_{CMB}$ will be higher, as a higher metallicity is required to reach lower temperatures. In Figure 4.20, we painted a portrait of the approximate behavior of the mass-scale with respect to metallicity, denoting three distinct regimes of star-formation. For $Z < Z_{cr}$, star-formation proceeds as in the metal-free case. For $Z_{cr} \leq Z < Z_{CMB}$, the minimum achievable gas temperature is determined by metallicity-dependent cooling. Cooling is able to continue to relatively high densities, resulting in a mass-scale of a few $M_\odot$. Finally, for $Z \geq Z_{CMB}$, fragmentation is halted early when the temperature hits the CMB floor, resulting in a mass-scale that is, at least, higher than the second case. The mass-scale of the third case will decrease at later times, as the CMB temperature
is lower. This suggests that at very early times, even metal enriched stars were much more massive than they are today. This would have a profound effect on the luminosity functions of high-redshift galaxies.

We have also examined how this portrait would change if the earliest metal-enriched environments had enhanced abundances of C and O. For these cases, we considered the metallicity to be the value $\text{[Fe/H]}$, which is what is quoted in observation of low-metallicity stars. C/O enhancement shifts both $Z_{cr}$ and $Z_{CMB}$ to lower metallicities, but shifts $Z_{CMB}$ more than $Z_{cr}$. When C and O are enhanced by a factor of 100, $Z_{cr}$ and $Z_{CMB}$ are approximately the same, and the low-mass mode of star-formation has all but vanished.

Finally, the above scenario does not explain the marked difference in results between the first and second set of simulations. The explanation for this lies with the addition of the cooling-time based refinement criterion. In theory, the runs with $Z = 10^{-4} \ Z_\odot$ should show fragmentation since it is above the critical metallicity. However, Figures 3.2D and 4.10C and D indicate that the fragmentation criterion is only weakly satisfied by a factor peaking at roughly 2. The inclusion of cooling-time based refinement was required to allow the weak thermal instabilities to grow into fragments. In both of the simulations with $Z = 10^{-3} \ Z_\odot$, roughly the same level of weak fragmentation was observed.

### 5.2 Future Work

The work presented here represents only the initial steps on the path to fully understanding the nature of the first metal-enriched stars. More simulations with metallicities close to $Z_{cr}$ will explore the abruptness of this transition. Perhaps, clouds with metallicities only slightly below $Z_{cr}$ will only experience a small temperature increase at the metal-free stalling point, but then quickly resume cooling. If the heating phase is short, fragmentation might not be fully suppressed by the homogenization of the core, as in the simulation with $Z = 10^{-5} \ Z_\odot$. In the second set of simulations, $Z_{CMB}$ could only be constrained within a factor of 3, somewhere between $10^{-4} \ Z_\odot$ and $10^{-3.5} \ Z_\odot$. More simulations within this metallicity range will tighten the constraint on $Z_{CMB}$, as well. Also, it will be important to understand the evolution of $Z_{CMB}$ with redshift, as this will determine the epoch at which all star-formation takes place within the low-mass mode. In collaboration with Dr. Jason Tumlinson, of the Yale Center for Astronomy and Astrophysics, I will perform a much larger series of simulations, varying both metallicity and collapse redshift, so as to determine the evolution of both CMB and metallicity regulated star-formation throughout the history of the universe. It will also be necessary to perform more simulations at the same metallicities as above, and collapsing at the same redshifts, but with entirely different sets of initial conditions. As more results are amassed, I will be able to create statistical mass spectra for the clumps within the simulations. With these mass spectra, I will be able to make predictions of the stellar IMF at low metallicities and high redshifts. It still remains to be seen when and where the IMF finally becomes normal (Salpeter).

Another relatively unstudied component of star-formation is the effect of rotation. Most primordial star-formation simulations have used halos with low spin-parameters ($\lambda$
Recently, simulations by Clark et al. (2007), which use a different methodology, have found that higher angular momentum leads to fragmentation for metallicities as low as $10^{-5} Z_\odot$. As the precise initial conditions for the formation of the second stars are essentially unknown, it would be useful to investigate the influence of rotation on the fragmentation of the gas-clouds currently studied.

Currently, these simulations must come to a halt when the most massive clump has evolved to the point where we can no longer follow its evolution. This provides a limited view of the evolution of clumps that are slightly less massive. One solution to this problem is the creation of sink particles in clumps that reach high densities. The use of sink particles will allow the simulation to continue after the most massive clump has reached high densities.

Predicted yields of Population III supernovae (Heger & Woosley 2002; Heger et al. 2003) have shown that nonsolar abundances patterns will be important for characterizing the first generations of metal-enriched stars. Within reason, I will investigate nonsolar abundances with more simulations. An ideal place to start will be with the mass-integrated mean metal yields for Population III stars of Tumlinson et al. (2004). Recently, Frebel et al. (2007) have suggested, in the spirit of the critical abundances of C and O calculated by Bromm & Loeb (2003b), that the transition to low-mass star formation occurs when $D_{\text{trans}} = -3.5$, where

$$D_{\text{trans}} = \log_{10}(10^{[C/H]} + 0.3 \times 10^{[O/H]}).$$  \hspace{1cm} (5.1)

Essentially, this argument suggests that the critical metallicity is degenerate with C and O abundances. Figure 5.1 displays the thermal instabilities and associated doubly unstable regions for gases with C only and O only, but each with $D_{\text{trans}} = -3.5$. For the same value of $D_{\text{trans}}$, the two gases have completely different regions of instability. These results suggest that C and O cannot be considered interchangeable, and one simulation at each of these abundances will most likely confirm it. It should also be noted that the thermal instability produced in the C-only gas exist primarily at low densities and temperatures. As Figure 2.16 shows, this thermal instability is erased at high redshifts by the CMB. This may imply that the C abundance has little or no influence on the very first generations of metal-enriched stars.

In the work presented here, the assumption of constant metallicity has been made to isolate the physics involved in fragmentation. In reality, however, metals will be injected into star-forming environments in a heterogeneous way by supernova blast-waves. In the coming months, I will take part in a collaboration with Dr. Brian O’Shea, of Los Alamos National Laboratory, in which we will simulate a Population III supernova blastwave using the metal cooling methodology introduced here. We will study the efficiency of metal-mixing and the subsequent star-formation in the heterogeneously enriched gas. In this work, we will be able to truly simulate the formation of the second generation of stars.

Finally, our current methodology is limited by the assumption of ionization equilibrium, the lack of any treatment of dust-grains and chemical heating from $H_2$ formation. In the fall, I will work in collaboration with Prof. Mike Shull, of the University of Colorado, Boulder to implement new, non-equilibrium chemical networks, such as the one
described in Santoro & Shull (2006), as well as a treatment of dust physics, in the Enzo simulation code.
Fig. 5.1 Top: Contours of the instability parameter, \((\alpha - \beta)\) over number density and temperature, for C-only gas with \([\text{C/H}] = -3.5\) (left) and O-only gas with \([\text{O/H}] = -3.0\) (right). Both abundances correspond to \(D_{\text{trans}} = -3.5\). Bottom: Double unstable regions associated with the thermal instability contours above.
Bibliography

—. 2002, Science, 295, 93
Alpher, R. A. & Herman, R. C. 1950, Reviews of Modern Physics, 22, 153
Berger, M. J. & Colella, P. 1989, Journal of Computational Physics, 82, 64


Burbidge, E. M., Burbidge, G. R., Fowler, W. A., & Hoyle, F. 1957, Reviews of Modern Physics, 29, 547


Ferland, G. J. 2006, Hazy, A Brief Introduction to Cloudy 06.02 (University of Kentucky Internal Report, 565 pages)


Gamow, G. 1948, Physical Review, 74, 505


Glover, S. 2005, Space Science Reviews, 117, 445


Grevesse, N. & Sauval, A. J. 1998, Space Science Reviews, 85, 161


Hirasawa, T. 1969, Progress of Theoretical Physics, 42, 523


Matsuda, T., Satô, H., & Takeda, H. 1969, Progress of Theoretical Physics, 42, 219


O'Shea, B. W. 2005, PhD thesis, University of Illinois at Urbana-Champaign


—. 1980, The large-scale structure of the universe (Research supported by the National Science Foundation. Princeton, N.J., Princeton University Press, 1980. 435 p.)


Rybicki, G. B. Escape probability methods (Methods in Radiative Transfer), 21–64


Scalo, J. M. 1986, Fundamentals of Cosmic Physics, 11, 1


Schwarzschild, M. & Spitzer, L. 1953, The Observatory, 73, 77


Takeda, H., Satō, H., & Matsuda, T. 1969, Progress of Theoretical Physics, 41, 840


Vita
Britton Devon Smith

Education

*The Pennsylvania State University* University Park, Pennsylvania 2001–Present
Ph.D. in Astronomy & Astrophysics, expected in December 2007
Area of Specialization: Numerical Simulations of Structure Formation

*(University of Wisconsin)* (Madison), (WI) 1997–2001
B.S. in Astronomy, Mathematics, and Physics

Awards and Honors

Astronomy T.A. of the Year 2003
Graduate Assistant Outstanding Teaching Award 2004

Research Experience

*Doctoral Research* The Pennsylvania State University 2004–Present
Thesis Advisor: Steinn Sigurdsson
Numerical simulations of the transition from the first to the second stars.

*Graduate Research* The Pennsylvania State University 2001–2004
Research Advisor: Prof. Tom Abel
Metal cooling in numerical simulations of cosmic structure formation.

*Undergraduate Research* University of Wisconsin 1998–2001
Research Advisor: Prof. Dan McCammon
Non-linear effects in low-temperature semiconductors.

Teaching Experience

Taught introductory labs, graded and delivered substitute lectures for introductory and upper-level courses, and supervised upper-level lab.