Chapter 1

Introduction

Cosmology is defined as *"The study of the physical universe considered as a totality of phenomena in time and space."*[5] As one might expect from this lofty definition, the exploration of the nature of the universe has long been the province of poets, philosophers and religious thinkers – indeed, for the majority of the history of humanity, the field of cosmology has been dominated by the attempt to understand mankind's role in the universe and his relationship with a god or gods. Most religions have some sort of creation myth that explain how the earth and the universe came to be and how all forms of life appeared. Typically these myths describe the universe as being created by a deity of some sort, who is also responsible for the creation of the earth and of mankind. These myths often foretell the end of the universe in great (and often gory) detail.

In the past century, physics has come to play a central role in shaping our understanding of the universe (though not necessarily our place in it). The development of the field of "physical cosmology" has been driven almost entirely by the improvement in technology used in astronomical observations and by Einstein's theory of general relativity. The theory of "Big Bang" cosmology (described in Section 1.1) was proposed by Georges Lemaître, building upon Einstein's ideas, and was later confirmed by Hubble's observations of the recession of distant galaxies in 1924 [6] and by the discovery of the cosmic microwave background (CMB) by Penzias and Wilson in 1964 [7, 8].

Despite these advances, the field of cosmology was starved for data until quite recently. In the past decade, massive statistical surveys of galaxies and large-scale structure such as the Two-Degree Field (2dF) survey and the Sloan Digital Sky Survey (SDSS), combined with high-resolution observations of the cosmic microwave background by the Wilkinson Microwave Anisotropy Probe (WMAP) satellite and of distant supernovae, have allowed us to constrain essentially all of the cosmological parameters, such as the amount of matter in the universe, the rate of expansion, and the existence and rough properties of a cosmological constant, to within a few percent.

This new epoch of "precision cosmology" has also fostered a renaissance in compu-

tational structure formation. In the past, numerical simulations of large-scale structure (such as galaxies and clusters of galaxies) have been primarily used to constrain cosmological parameters and to rule out ideas such as the concept of "hot dark matter." However, with the rapid advances in observations and the corresponding constraint of the basic cosmological parameters, numerical simulations of large-scale structure formation can now be used in a predictive sense, to study the formation of distant and highly nonlinear objects which are too complicated to approach purely analytically.

My thesis presents the results of high-resolution numerical simulations of structure formation in the early universe. In order to verify that Enzo, the cosmology simulation code used for the work presented here, is working correctly, I perform a comparison between it and the SPH code GADGET. I then predict properties of the first generations of stars in both the fiducial cold dark matter cosmology and also in a universe with a generic "warm dark matter" cosmology. I also show how the first generation of stars in the universe affects following generations of star formation, and present constraints on how much of an impact these "first stars" can have on the feedback of metals into the low-density intergalactic medium. In this chapter, I will review the basic principles of cosmology and cosmological structure formation, and also discuss the current state of literature on the formation of the first generation of stars and their effects on the universe via feedback processes.

1.1   Big-Bang cosmology and the FRW universe

The Big Bang theory of cosmology rests on two theoretical pillars: Einstein's theory of General Relativity and what is known as the Cosmological Principle. Einstein's theory provides a mathematical framework for describing gravity as a distortion of space and time and is a generalization of Newton's theory of gravity. The Cosmological Principle assumes that, on very large scales, the universe is homogeneous and isotropic – there is no preferred reference frame, and the universe looks the same no matter where an observer is within it. Additionally, it is generally assumed that the laws of physics are the same at all places and at all times.

The content of the universe is described by the "standard model" of particle physics. This model, coupled with the understanding of how the universe expands from general relativity, provides predictions of the primordial composition of the universe (via Big Bang Nucleosynthesis, or BBN) and has been observationally confirmed to very high precision. Observations indicate that the universe is mostly composed of some sort of vacuum energy ("dark energy"), and a form of matter that only appears to interact with baryonic matter via gravitational coupling ("dark matter"). These observations indicate that at the present epoch baryons comprise approximately 4% of the total energy density of the universe, dark matter comprises approximately 23%, and vacuum energy comprises

roughly 73% of the total. The total energy density adds up to a "critical density" which suggests that the universe is geometrically flat (as discussed below).

This combination of theory and observations forms the entire theoretical basis of Big Bang cosmology, and produces very specific predictions for observable properties of the universe. These predictions have been heavily tested and appear to be accurate, suggesting that the Big Bang cosmological model is an accurate description of the universe. Given this model of the universe as a starting point, we can then make predictions about the nonlinear processes that follow, such as the formation of large-scale structure.

In principle one can use the theory of general relativity to predict the properties of any kind of universe. However, when one assumes that the universe is isotropic and homogeneous, the only sort of movement that is allowed is a uniform expansion of the universe as a whole. Under these assumptions, Einstein's field equations reduce to the following pair of independent equations:

$$\left(\frac{\dot{a}}{a}\right)^2 - \frac{8\pi G}{3}\rho = -\frac{kc^2}{a^2} + \frac{\Lambda c^2}{3} \tag{1.1}$$

$$\frac{\ddot{a}}{a} = -\frac{4\pi G}{3}\left(\rho + \frac{3p}{c^2}\right) + \frac{\Lambda c^2}{3} \tag{1.2}$$

where a is the cosmological expansion parameter, G is the gravitational constant, ρ and p are the mass-energy density and pressure of the universe, c is the speed of light, k is the curvature constant, and Λ is the cosmological constant. Equation 1.1 is commonly referred to as *Friedmann's equation*, and has the general form of an energy equation. Equation 1.2 has the form of a force equation, and is sometimes referred to as *Friedmann's acceleration equation*.

These equations bear further examination. The first and second terms on the left hand side of Equation 1.1 look like kinetic and gravitational potential energies, respectively, and the right hand side is effectively a total energy. Before continuing further, it is useful to define the "Hubble parameter," $H \equiv \dot{a}/a$, which has the value H_0 at the present epoch. Similarly, we define a "critical density," which is the matter density at the present epoch in a universe with $k = 0$ (a geometrically flat universe), and is defined as $\rho_c \equiv 3H_0^2/8\pi G$ (with a cgs value at the present day of 1.8788×10^{-29} h^2 g cm^{-3}, where h is the Hubble parameter in units of 100 km/s/megaparsec), and relative densities $\Omega_i \equiv \rho_i/\rho_c$. At the present epoch ($a = 1$ and $\dot{a} = H_0$) with $\Lambda = 0$ and $\rho \equiv \Omega\rho_c/a^3$, we get $H_0^2 = \Omega H_0^2 - kc^2$, or $k = H_0^2/c^2(\Omega - 1)$. This provides a clear relationship between the curvature of the universe and the total mass-energy density of the universe: if $k = 0$, $\Omega = 1$. Likewise, if $k < 0$, $\Omega < 1$ and if $k > 0$, $\Omega > 1$. Also, it can be shown that for large values of the scale factor ($a \to \infty$) Equation 1.1 reduces to:

$$\dot{a}^2 = \frac{H_0^2}{c^2}(1 - \Omega) \tag{1.3}$$

In the absence of a cosmological constant, the curvature parameter k determines whether the universe has a net positive, negative or zero energy. If $k = +1$ ($\Omega > 1$) the universe is said to have "positive curvature," meaning that the universe is effectively closed – the kinetic energy term is always dominated by the potential energy term. Practically speaking, this results in a universe that expands, attains some maximum size, and then contracts again to a point, or a "Big Crunch." If $k = -1$ ($\Omega < 1$), the universe is said to have "negative curvature" and the kinetic energy term on the left hand side of Equation 1.1 always dominates. This means, effectively, that the universe will expand forever with some positive kinetic energy. This is referred to as an "open" universe. If $k = 0$ the universe is geometrically flat and (from a strict interpretation of Equations 1.1 and 1.3) its expansion will coast to a halt as $a \to \infty$.

The addition of a cosmological constant (Λ term) complicates matters somewhat. Einstein originally added this constant to maintain a steady-state universe. However, with Hubble's announcement of the observation of an expanding universe, Einstein abandoned the idea of a cosmological constant, referring to it as "the greatest blunder of my life." [9]. However, current observations suggest that roughly 70% of the energy density of the universe at the present epoch is due to a mysterious "dark energy" that behaves like a positive cosmological constant, making the cosmological constant an issue once again.

Examination of Equation 1.2 shows that, even in the absence of any other source of mass-energy (e.g. $\rho = p = 0$), the existence of a positive cosmological constant indicates that the expansion of the universe is accelerating – essentially, the vacuum energy is acting as a repulsive force. Also, if $k = 0$, Equations 1.1 and 1.2 can be reworked to show that at the present epoch $\Omega_{tot} = 1.0$, where $\Omega_{tot} = \Omega_m + \Omega_{rad} + \Omega_\Lambda$, the sum of all of the constituents of the mass-energy density of the universe. Here Ω_m is the total matter content of the universe, Ω_{rad} is the total relativistic particle content (including photons), and Ω_Λ is the energy density of the cosmological constant, all in units of the critical density. At the present epoch the approximate values of Ω_{rad}, Ω_m and Ω_Λ are $\sim 10^{-4}, 0.27$ and 0.73, respectively (with $\Omega_m = \Omega_b + \Omega_{dm}$, where $\Omega_b = 0.04$ and $\Omega_{dm} = 0.23$).

For the purposes of clarity, we can simplify Equation 1.1 to be in terms of the components of the mass-energy contents of the universe at the present epoch. The proper energy density of matter scales with the cosmological constant as a^{-3} due to pure geometrical dilution. The proper energy density of relativistic particles such as photons scales as a^{-4} – a factor of a^{-3} due to geometric dilution and an additional factor of $1/a$ due to the redshifting of a particle's momentum. The proper energy density of the cosmological constant is unchanged at all times, by definition. Refactoring Equation 1.1 gives us:

$$\left(\frac{\dot{a}}{a}\right)^2 + \frac{kc^2}{a^2} = H_0^2 \left(\frac{\Omega_{rad}}{a^4} + \frac{\Omega_m}{a^3} + \Omega_\Lambda\right) \tag{1.4}$$

The different scaling factors for each of the terms on the right hand side suggest that each one dominates at different epochs, with radiation dominating first (at very small

a), then matter, then finally the cosmological constant at late times (the epoch that we are currently entering into). The universe expands as $a(t) \sim t^{1/2}$ during the radiation-dominated epoch, $a(t) \sim t^{2/3}$ during the matter-dominated epoch, and $a(t) \sim e^t$ during the cosmological constant-dominated epoch.

For more detailed discussion of general relativity, big bang nucleosynthesis and related topics, the following references may be of use: [10, 11, 12, 13, 14].

1.2 Cosmological structure formation

The current paradigm describing the formation of large-scale structure is referred to as "hierarchical structure formation." During the epoch of inflation, quantum mechanical effects manifested themselves as very tiny density perturbations in an otherwise homogeneous universe. As the universe expanded these perturbations grew via gravitational instability and eventually became gravitationally bound halos, which grew by a sequence of mergers into the galaxies and other large scale structure observed today.

This scenario is demonstrated analytically by the Press-Schechter (PS) formalism [15, 16, 17]. The PS formalism very accurately describes many properties of the dark halo population in the ΛCDM cosmology, and has been verified both observationally and numerically to be accurate on large scales. An example of the use of the PS formalism to describe the growth of large-scale structure is shown in Figure 1.1. This is a plot of cumulative dark matter halo mass functions for several redshifts. At very early times the universe is sparsely populated with gravitationally bound objects. As time goes by (redshift decreases), dark matter halos grow more numerous and the maximum halo mass increases via merger of smaller halos. It is intriguing to note that at the current epoch ($z = 0$) there are actually *fewer* low mass halos than at higher redshifts (earlier times). This supports the idea of hierarchical mergers of dark matter halos.

Though the PS formalism provides a good description of the dark matter halo properties in a ΛCDM cosmology, it only tells the simplest part of the story, and only in a purely statistical sense. Also, by definition dark matter is not directly observable. Baryons in stellar and gaseous form comprise all of the visible matter in the universe, and are much more complicated to model. It is difficult, if not impossible, to analytically model the effects that halo mergers would have on the properties of the baryons that are gravitationally bound to the dark matter halos. The range of physics that is involved – radiative cooling, star formation, the feedback of radiation and metals – combine together with the unique merger histories of individual halos to produce the galaxies, groups and clusters that are observed in the universe today.

It is for this reason that three-dimensional numerical simulations of the formation and evolution of large scale structure are exceedingly useful. Essentially all of the baryon physics described above can be modeled, either from first principles or through con-
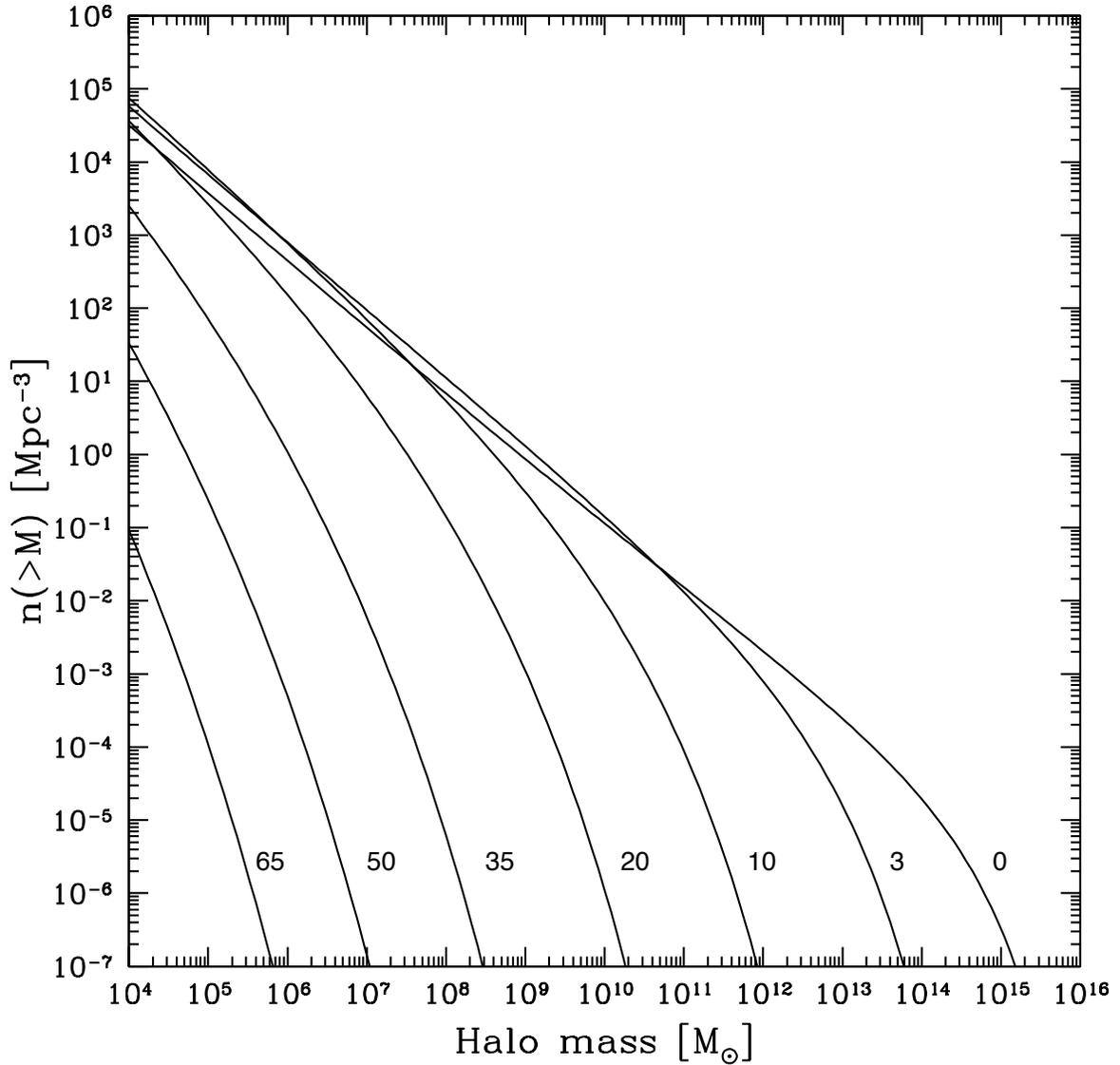
Figure 1.1: Cumulative halo dark matter mass function calculated using the Press-Schechter formalism for a cosmology with fiducial cosmological parameters ($\Omega_m = 0.3, \Omega_\Lambda = 0.7, h = 0.7, \sigma_8 = 0.9, n = 1$). Plot is of comoving number density of halos greater than a given mass M vs. mass for several redshifts. The number to the right of each line indicates the redshift at which the mass function is calculated.

strained phenomenological models, within a cosmological framework. The entire scope of cosmological structure formation simulations is vast and continually expanding with increases in computing power and the creation of new simulation techniques. For a somewhat dated review, see the 1998 Bertschinger Annual Reviews article [18].

1.3 Formation of the first generation of stars

The first generation of stars (also known as Population III stars or Pop III stars) formed in a very different, and far simpler, physical environment than present-day stars. According to BBN, the primordial gas consisted of primarily hydrogen and helium (76.2%/23.8% by mass, respectively) and trace amounts of deuterium and lithium - an extremely simple mix of elements with well-understood and easily modeled gas chemistry! [19]. Unlike the present-day universe, there were no metals or dust grains - two factors which complicate the solution of the modern-day star formation problem tremendously. The main source of cooling in the early universe was molecular hydrogen, which is inefficient below 200 K, as opposed to current star formation, where cooling via the heavier elements allows temperatures in the molecular clouds where star formation takes place to drop to $\simeq 10$ K [20, 21].

The universe during the epoch of formation of the first stars was a very dull place. By definition, there were no other stars – meaning that there were no sources of radiation, winds or supernovae that could affect star formation in any way. Significantly, this also means that there were no sources of intense ultraviolet radiation to disrupt the formation of molecular hydrogen and no cosmic rays to ionize hydrogen. Also, there were no sources to sustain turbulent motion, as long as the density perturbations remained linear. Only after the explosion of the first supernovae, and the associated input of mechanical and thermal energy, was this state of quiescence bound to change [22, 23].

1.3.1 A brief history of research regarding the first stars

The history of research regarding the first generation of stars is long and full of conflicting results. Peebles & Dicke [24] were among the pioneers in the field. They suggested in 1968 that globular clusters may have originated as gravitationally bound gas clouds before the galaxies form. Their idea follows from what was then called the primitive-fireball picture (and is now referred to as the Big Bang theory) and they showed that the first bound systems to have formed in the expanding universe were gas clouds with mass and shape similar to the globular star clusters observed around the Milky Way and nearby galaxies. They also argued that only a small fraction of the total cloud mass would fragment into stars and they also discussed the influence of molecular hydrogen on cooling and fragmentation. A year later, Hirasawa [25] performed similar calculations but claimed

that his results suggested that collapsing hydrogen clouds would result in supermassive black holes.

Palla, Salpeter & Stahler published an important work in 1983 discussing the role of molecular hydrogen (H_2) in star formation [20]. They discuss (as I will in Section 1.3.2) the cooling of a collapsing cloud of hydrogen gas via molecular hydrogen (H_2) formation and explore the importance of the three-body reaction for creating H_2. They also suggest that the Jeans mass is higher for stars without metals to cool them but argue that cooling leads to a rapidly dropping Jeans mass, resulting in fragmentation which would lead to low-mass stars regardless. In the same year, Silk published a work on Population III stars showing that large density fluctuations of ~ 0.1 $M_\odot$ ($M_\odot$ = "solar mass") arise in any collapsing cloud with extremely low metallicity ($Z_{cloud} \leq 10^{-3} Z_\odot$) [26]. Gravitational instability ensures that many of the clumps coagulate to form protostars of masses extending up to the Jeans mass at the time when the fluctuations start to develop, roughly ~ 100 $M_\odot$. He argues that the primordial IMF would have spanned the mass range from $\sim$0.1-100 $M_\odot$ but could have been dominated by the more massive stars.

This disagreement in theoretical studies seems quite surprising. However, the first bound objects in the universe formed via the gravitational collapse of a thermally unstable reactive medium, which naturally makes conclusive analytical calculations difficult.

1.3.2 The role of molecular hydrogen

Molecular hydrogen (H_2) in primordial gas clouds is produced at low densities primarily by these coupled gas-phase reactions:

$$H + e^- \rightarrow H^- + \gamma \tag{1.5}$$

$$H^- + H \rightarrow H_2 + e^- \tag{1.6}$$

This pair of reactions depends on free electrons to act as a catalyst, and even a small mass fraction of molecular hydrogen ($f_{H2} \sim 10^{-3}$) can contribute significantly to the cooling of a cloud via the rotational and vibrational transitions of the hydrogen molecule, allowing primordial gas to cool efficiently below $\sim 10^4$ K, which is the lowest temperature gas can radiatively cool to due to atomic hydrogen line transitions. Significant amounts of molecular hydrogen can cool gas down to $\simeq 200$ K. Below this temperature it is relatively ineffective as a coolant, as can be seen from Figure 1.2, which shows the molecular hydrogen cooling function for gas at three different densities. At all densities, the cooling rate of a gas of primordial composition decreases sharply below $\simeq 200$ K. Metal-enriched gas can cool to much lower temperatures efficiently, due to the presence of many closely-spaced line transitions in the various molecules and dust grains that exist.

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At high densities in primordial gas ($n \geq 10^8$ cm^{-3}) the 3-body reaction for the formation of molecular hydrogen becomes dominant:

$$H + H + H \rightarrow H_2 + H \tag{1.7}$$

$$H + H + H_2 \rightarrow H_2 + H_2 \tag{1.8}$$

and is so efficient that virtually all of the atomic hydrogen at that density or above can be converted to molecular hydrogen before it is dissociated, allowing rapid cooling and contraction of the gas cloud [20, 21].

The properties of the hydrogen molecule are extremely important in studying the formation of the first stars. In the absence of metals, the properties of H_2 completely control the size and formation times of the first objects. Therefore, it is extremely important to include the effects of H_2 formation in simulations of the formation of the first stars.

For an excellent review of the chemistry of the early universe (including all deuterium and lithium chemistry, which we have ignored here) see the paper by Galli & Palla [27], and for analysis of the effects of H_2 cooling on structure formation, see Tegmark et al. [28].

1.3.3 The role of magnetic fields

It is believed that the magnetic fields that existed at the epoch of first star formation were dynamically unimportant at large scales (though they may be relevant to angular momentum transport in primordial protostars). This stands in sharp contrast to the local universe, where magnetic fields play a critical role in star formation. Observations of the cosmic microwave background (CMB) provide a strong upper limit of B $\leq$ 3 x 10^{-8} G (as measured at the present epoch) for large-scale (megaparsec) coherent magnetic fields at the time of recombination [29], with theory suggesting that limits could be obtained which are as stringent as $\sim$ 1 nG [30]. This limit is poor enough that it does not disprove that magnetic fields are dynamically important at the epoch of Population III star formation – see Section 4.5 for more discussion of this issue. An examination of the possible (known) sources of magnetic fields in the pre-structure formation era provides two likely candidates. A discontinuous (i.e., first order) phase transition at the time of the QCD or electroweak phase transitions could create significant coherent magnetic fields before recombination. However, the mechanisms involved are highly speculative and predictions of the possible magnetic field strengths are unreliable [31]. Intriguingly, the standard picture of cosmology predicts that large-scale magnetic fields were created at recombination due to Thompson scattering differentially accelerating electrons and ions. However, the strengths of the resulting fields are on the order of 10^{-20} G [32]. More recent work was done by Matarrese et al. [33], who derive the *minimum* magnetic field that invariably arises prior to recombination. They show that a weak magnetic field is
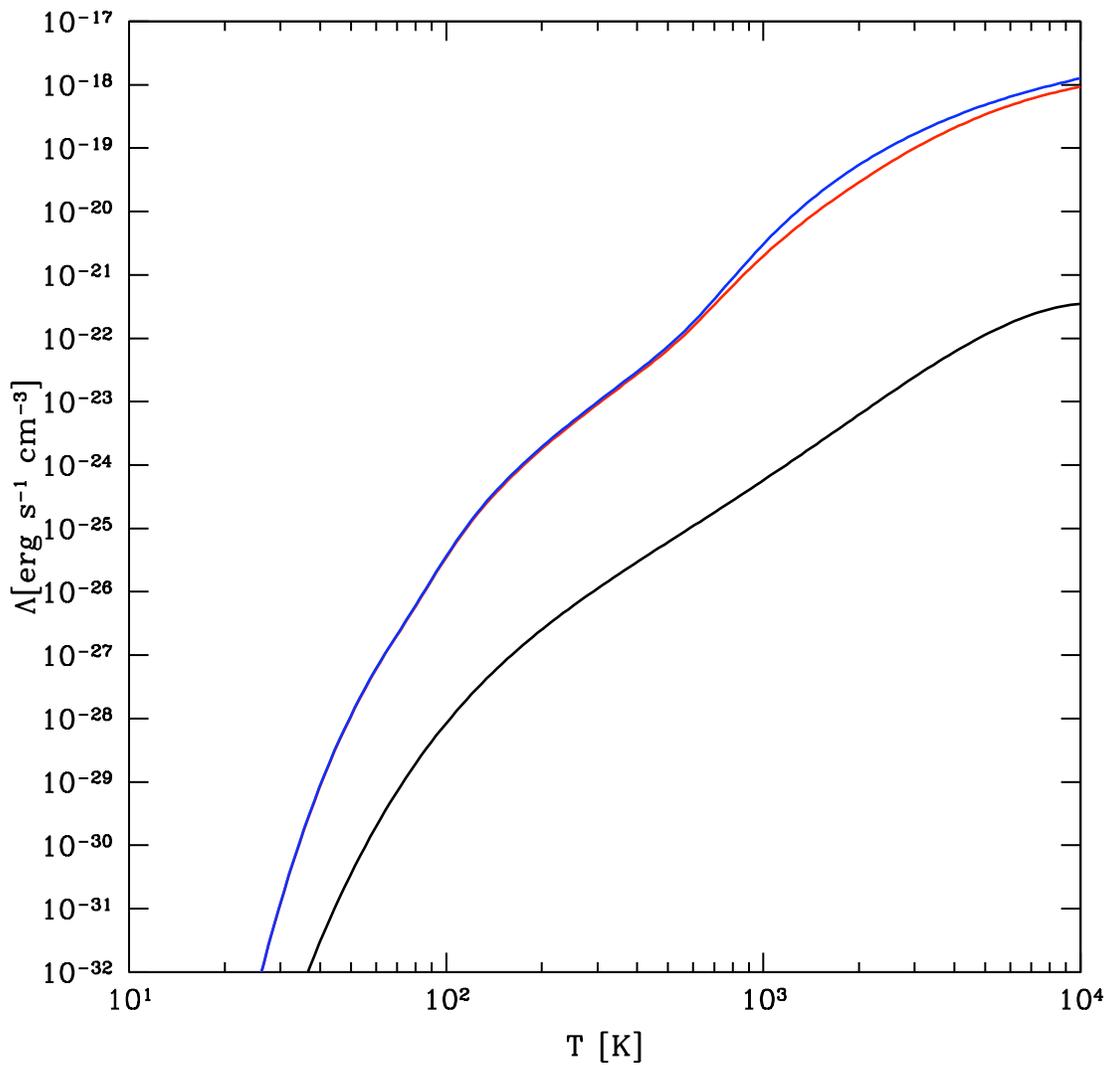
Figure 1.2: Molecular hydrogen cooling rate as a function of temperature for gas at three different densities. Black line: $n = 1$ cm^{-3} (proper). Red line: $n = 10^4$ cm^{-3} (proper). Blue line: $n = 10^8$ cm^{-3} (proper).

generated in the radiation dominated era by Harrison's mechanism [124], which occurs in regions of non-vanishing vorticity. They show that this vorticity is generated by the 2nd order nonlinear coupling of primordial density fluctuations, resulting in a differential rotational velocity between ions and electrons that produces a small magnetic field. The power spectrum of this field is determined entirely by the power spectrum of primordial density perturbations. The RMS amplitude of this field at recombination is predicted to be $B \simeq 10^{-23} \, (\lambda/\mathrm{Mpc})^{-2}$ G on comoving scales $\lambda \geq 1$ Mpc. The magnetic fields are suppressed at smaller scales via Silk damping, which is simply diffusion of photons on sub-horizon scales from high density regions to low density regions prior to recombination. Electrons are "dragged" with the photons via Compton interactions and then proceed to carry protons along with them via the Coulomb interaction. This smoothes out the matter density at small scales, which has the effect of damping out CMB fluctuations (and thus B-field creation) on those scales. The estimated B-fields, while not strong enough to be dynamically important in the formation of the first stars, could be amplified via the dynamo effect during protogalaxy formation to strengths that are significant today [35].

There is no observational evidence against strong magnetic fields at the time of recombination (only strong upper limits), but there are also no theoretical arguments demanding strong fields, so it seems reasonable to assume that magnetic fields are negligible for the first treatment of the problem. As a side note, I would direct the reader who is interested in speculations of the origin of the magnetic fields that are of such great importance in present day star formation to a paper by Kulsrud et al. [36], who discuss one possible scenario for the creation and amplification of dynamically important magnetic fields during the epoch of protogalaxy formation. In addition, Gnedin et al. [37] discuss the generation of magnetic fields by the Biermann battery mechanism in cosmological ionization fronts propagating through a dense, irregular medium. Though their estimates suggest that the magnetic fields generated are small ($\sim 10^{-19} - 10^{-18}$ G), this is a lower bound and could be amplified significantly during the following epochs of structure formation. Similar work by Langer et al. [38] presents a model of magnetic field generation based on local charge separation provide by an anisotropic, inhomogeneous radiation pressure. This process would also take place during reionization ($z \geq 7$), and would produce fields on the order of $\sim 10^{-12} - 10^{-11}$ G. They also show that these fields are generated preferentially on large (> 1 kpc) scales, and strongly suppress coherent B-fields on smaller scales. Though this is interesting, and a reasonable seed mechanism for galactic magnetic fields, it occurs at far too late of an epoch to be useful for Population III stars.

1.3.4 Numerical simulations of Pop III star formation

The most detailed *ab initio* simulations to date have been done by Abel, Bryan & Norman, henceforth referred to as ABN [39]. They perform a cosmological simulation of

the collapse of a cosmological density perturbation into a protostellar core utilizing the adaptive mesh refinement (AMR) technique to obtain very high dynamical range. They discover that the collapsing halo is initially characterized by a period of rapid cooling and infall. This corresponds to an increase in H_2 mass fraction in the center of the halo to $\sim 0.1\%$, which is sufficient to rapidly cool the gas down to ~ 200 K. Following this, the central density of the halo increases to 10^4 cm^{-3} and, at which point the cooling time becomes density-independent, so the temperature again increases coupled with a rise in the cooling rate. This causes an increase in inflow velocities, and by z $\simeq 18.5$, the central 100 $M_\odot$ of gas exceeds the Bonnor-Ebert critical mass at that radius, which is indicative of unstable collapse [40, 41]. Interestingly enough, it is found that the collapsing cloud does not fragment into multiple cores, which is the result expected by analytical treatment. [26, 20] Instead, they find that a single protostar of ~ 1 $M_\odot$, made completely of molecular hydrogen, forms at the center of the 100 $M_\odot$ core. In addition, the core is not rotationally supported, meaning that it will collapse on a timescale determined by the cooling processes of the gas. The final mass of the star remains unclear, since the simulations lack the necessary physics to compute how much of the available cool material surrounding the protostar will accrete or at what point feedback from the protostar will limit further accretion. At the rate of infall when the simulation stopped, roughly 70 $M_\odot$ of matter would be accreted in the following 10^4 years, with a maximum of 600 $M_\odot$ in the following 5 x 10^6 years. Though the maximum value of 600 $M_\odot$ is exceedingly unlikely (the main-sequence lifetime of a star weighing ~ 100 $M_\odot$ is much less than 5 x 10^6 years), this does point towards a top-heavy initial mass function for Population III stars.

Bromm, Coppi & Larson [42] pursue the same avenue of research with a complementary method (smoothed particle hydrodynamics) and find somewhat different results. They initialize their simulations with a top-hat overdensity using similar cosmological parameters to ABN, and set this initial top-hat configuration into rigid-body rotation with a given angular velocity in order to simulate tidal interactions with nearby clumps. They find that their gas clumps evolve similarly to those of ABN, which is unsurprising as the dynamics of the halo collapse is dominated by the physics of H_2 formation and cooling. However, they find that their halo develops a very lumpy, filamentary substructure with several sub-clumps, each of which which individually evolve in a manner comparable to the single halo in ABN and end up with a ~ 100 $M_\odot$ core of cool gas in a state of semi-free fall in the center of each sub-clump. More detailed information on the core is unavailable due to lack of simulation resolution. Bromm et al. also suggest that Population III star formation might have favored very massive stars.

More recently, Gao et al. [43] and Reed et al. [44] have performed a series of dark matter-only simulations where they use a sequence of nested N-body simulations to follow the growth of progenitors of the most massive object in a ~ 500 Mpc/h volume. They use a sequence of nested re-simulations to "zoom in" on this object to study the environment

and merger history of the halos in that area. The first object capable of forming stars is believed to collapse at $z \simeq 47$, when the mass of this halo is $\simeq 2.4 \times 10^5$ M$_\odot$ h^{-1}. Halos forming in this environment are significantly overabundant and also undergo rapid mergers compared to a more "average" part of the universe. This leads to the rapid growth of halos in this region – the largest reaches a mass of $\sim 5 \times 10^7$ M$_\odot$ at $z = 29$. These authors suggest that by $z = 30$ a substantial population of primordial objects are capable of forming Population III stars, and that by this time small "galaxies" with $T_{vir} > 10^4$ K (that are able to cool effectively by atomic hydrogen) will also exist. These authors also note that halo populations, merger rates and correlation scales in their simulations are well-modeled by the extended Press-Shechter formalism at all times, which is promising.

It should be noted that, as stated above, the simulations discussed by Gao et al. and Reed et al. are N-body calculations and do not contain baryonic physics. The results that predict, e.g., the redshift of first star formation, should be taken to be approximations only. An important lesson, however, is that the simulations which include baryonic physics use box sizes that are most likely too small to adequately model the scatter in star formation times (which will be discussed in later sections of this work). This is a reasonable and correct issue, and is investigated in this thesis.

The reader desiring a more thorough review of Population III star formation is directed to reviews by Bromm & Larson [45] and Ciardi & Ferrara [46].

1.3.5   The Initial Mass Function of primordial stars

One of the most interesting open questions relating to the issue of primordial stars concerns their initial mass function (IMF). If these stars are very massive, they will be copious emitters of UV radiation and produce large amounts of metals, as discussed in Section 1.4. This problem, however, is a very difficult one to solve, owing to the range of physics involved.

Abel et al. [39] are unable to follow the evolution of the fully molecular protostar that forms in the center of their halo to the point where it moves onto the main sequence. Their simulations are terminated due to a lack of appropriate physics – namely, the optically thin radiative cooling approximation for primordial gas breaks down at $\sim 10^{14}$ cm^{-3}. This can be extended another few orders of magnitude using analytical approximations to the primordial cooling function [47], but eventually full radiation transport will be necessary. Regardless, Abel et al. estimate the mass range of the protostar by examining the spherically-averaged accretion rate onto the 1 M$_\odot$, fully molecular protostar that had formed by the end of their simulation. Based on the observed accretion rates, they observe that at least 30 M$_\odot$ of gas will have accreted onto the central core in a few thousand years, which is much shorter than expected protostellar evolution times. Approximately 200 M$_\odot$ of gas will accrete in $\sim 10^5$ years, and a total of 600 M$_\odot$ will accrete in 5×10^6

years. It is implausible that this mass will be reached, since the lifetime of primordial stars in the mass range of hundreds of solar masses is only $2 - 3$ million years. They suggest that a more reasonable mass range is $30 - 300$ $M_\odot$, and no attempt is made to state the possible distribution of masses in this range.

The other 3D simulations that have been performed are by Bromm et al. Their earlier simulations do not have the mass and spatial resolution to estimate the masses of these stars – however, they suggest that the first generation of stars may have been with massive, with $m_* \geq 100$ $M_\odot$ [42]. A later simulation by Bromm & Loeb [48] improves upon this calculation and follows the evolution of a primordial protostar down to a scale of ~ 100 AU. They find a conservative upper limit of $m_* \leq 500$ $M_\odot$ and suggest that the actual stellar mass is likely to be significantly lower than that due to feedback from the protostar.

Though useful in many ways, and the final arbiter of the Population III IMF, 3D calculations of Pop III star formation in a cosmological context are limited by computational costs and the physics packages currently implemented in them. Fully 3D calculations of accretion onto the primordial protostar, including all relevant physics such as multifrequency radiation transport, accurate models of the primordial protostar, magnetohydrodynamics, and a full nonequilibrium chemical reaction network are in principle technically feasible, but the computational cost for doing such a calculation is prohibitive at best. One could wait for computational resources to increase to the point where this sort of calculation is reasonable, but more impatient (and practical) researchers have resorted to analytical and one and two-dimensional numerical models.

Tan & McKee and Tan & Blackman [49, 50] have created theoretical models of the evolution of the Population III protostar as it moves onto the main sequence. They combine a range of assumptions about the strength of magnetic fields generated in the protostellar disk (as well as their efficiency in transporting angular momentum) with estimates of the disk structure, gas infall rates and protostellar evolution models to gain some understanding of the radiative feedback from the protostar and its role in shutting off accretion. Based on accretion rates from Abel et al. [39] and from their calculations showing feedback is dynamically unimportant for protostars with masses < 30 $M_\odot$, they conclude that the masses of these primordial stars should be at least 30 $M_\odot$.

Omukai & Nishi [51] performed calculations modeling the hydrodynamical evolution of primordial, spherically symmetric clouds taking into account chemistry as well as continuum and molecular hydrogen line radiative transfer. They find (similarly to Abel et al.) that a ~ 1 $M_\odot$, fully molecular protostar forms in the inner region of their calculation. However, they see that as accretion continues and central densities climb, the molecular hydrogen in the core dissociates and a hydrostatic core with mass $M_{core} \sim 5 \times 10^{-3}$ $M_\odot$ forms at the center of the cloud, with gas accreting onto it at $\sim 10^{-2}$ $M_\odot$/year. The accretion rate declines with time. They make no estimate of the final range of stellar masses. Later work by Omukai and various collaborators [52, 53, 54] predict upper mass

limits for massive primordial stars that range from $300 - 1000$ M$_\odot$. All of these works assume spherical symmetry and high, time-dependent accretion rates ($\sim 10^{-2}$ M$_\odot$/year initially, decreasing as a function of time), with the upper limit depending strongly on assumptions regarding the evolution of the protostar, the strength and efficiency of radiation from the star in halting accretion, and the accretion rates onto the stars.

The results of Omukai et al. are in sharp contrast to the calculations of Nakamura & Umemura [55, 56, 57]. They perform one and two-dimensional hydrodynamic simulations coupled with nonequilibrium primordial chemistry and follow the evolution of the clouds from a central density of $\sim 10^2$ cm^{-3} up to $\sim 10^{13}$ cm^{-3}. They observe that the star-forming clouds tend to fragment out of filaments, and therefore choose to simulate these objects using cylindrical symmetry. In their earlier work [55] they perform one-dimensional cylindrically symmetric hydrodynamic calculations that neglect all deuterium-related chemistry and cooling and observe that the typical mass of their central object is ~ 3 M$_\odot$ (though they state that it could grow to be approximately five times that mass via accretion) over a wide range of input assumptions about cloud temperature and other properties. Later calculations [56] were performed in both 1D and 2D, again assuming axial symmetry, and improve upon the previous result. These calculations show that the initial density of the filaments in their problem setup strongly affects the scale at which fragmentation occurs, and they posit that the IMF of Population III stars is likely to be bimodal, with peaks at ~ 1 and ~ 100 M$_\odot$, with the relative numbers of stars in each peak possibly being a function of the collapse epoch. They also perform 1D calculations including deuterium chemistry [57] and show that due to the enhanced cooling from the HD molecule there is still a bimodal distribution with a low-mass peak of $\sim 1 - 2$ M$_\odot$, though the high mass peak can now be somewhere between $10 - 100$ M$_\odot$, depending on the initial filament density and H$_2$ abundance.

This section has shown that there is both agreement and disagreement between different groups' results. All of the research discussed here indicates that the IMF of Population III stars is wildly different than the IMF of stars in our galaxy at the present day, with the mean stellar mass being significantly higher in primordial stars than at the present epoch. The disagreement lies in both the shape of the Population III IMF and in the mean mass of the primordial stars.

What is the root of this discrepancy? The simulations performed by Abel et al. [39] (and myself, as discussed later in this thesis) show that the accretion onto the protostar is not inherently one-dimensional – we typically see the formation of a generally spherical core forming in the center of the halo, though there is evidence for angular momentum-transporting turbulence within this core. Also, the cosmological structures that these halos form out of are inherently aspherical. This suggests that 1D models are missing crucial physics. Additionally, it seems apparently that modeling the interplay between radiation from the growing protostar and the accreting gas is going to be very important, and this must be done carefully. It also appears that complete modeling of

the primordial gas (including deuterium, lithium and the various molecules they form between themselves and with hydrogen) may be important in 2D and 3D simulations. It may be that magnetic fields also play a significant role in angular momentum transport at scales corresponding to the size of the forming protostar, so they must be included in simulations and analytical models. Though expensive, these calculations are possible in 2D, and will be feasible in 3D in a few years, assuming that the power and availability of computing resources continues to grow at similar rates to today. At that point, accurately predicting the IMF of primordial stars may be a tractable problem.

1.4   Feedback from the first generation of stars

The formation of the first stars marks the transformation of the universe from its almost completely smooth initial state to its clumpy, complicated current state. As the first luminous objects to form in the universe, Population III stars play an extremely important role by fundamentally changing the environment that later cosmological structures form in, through radiative, mechanical, and chemical feedback. The literature discussing the feedback properties of Population III stars is vast and rapidly evolving. This section will provide only a brief overview of these properties, and the interested reader is encouraged to refer to the 2001 review article by Barkana & Loeb [58] or the much more recent review by Ciardi & Ferrara [46].

1.4.1   Physical properties of Population III stars

As discussed in Section 1.3, recent analytical work and numerical simulations using a range of initial conditions and assumptions about relevant physics suggest that Population III stars may have an exceedingly top-heavy IMF compared to stars in our galaxy. Massive primordial stars are believed to have several interesting properties that distinguish them from stars with a significant fraction of metals: these stars are extremely compact and, as a result, have very high effective temperatures (approximately 10^5 K). As a result, Population III stars have rather hard spectra and produce large numbers of both hydrogen and helium-ionizing photons. Additionally, due to the lack of metals in these objects, they are expected to have little mass loss near the end of their main-sequence lifetime due to line-driven winds. See Schaerer [59] and references therein for a more complete review.

The final fate of these stars is also quite remarkable. Recent one-dimensional, nonrotating simulations of the evolution of massive primordial stars suggest that at the end of their lives, the more massive of these stars ($M_* \geq 30M_\odot$) which typically collapse directly into a black hole ($M_* \sim 30 - 100$, $M_* > 260M_\odot$) or explode in a massive pair instability supernova (PISN; $M_* \sim 140 - 260$ $M_\odot$), which would completely destroy the star, leaving no compact remnant behind. These supernovae can be almost two orders of magnitude

more energetic than a standard Type II supernovae and also leave behind a very distinct nucleosynthetic signature [60]. A middle range of extremely massive stars is believed to have an energetic pulsational instability that causes the ejection of much of its envelope before collapsing into a black hole. The low-mass end of the Population III stellar IMF would see behavior more comparable to that seen by dying stars in the local universe – collapse to a white dwarf preceded by asymptotic giant branch-type activity or a Type II supernova resulting in a neutron star or black hole compact remnant. See Heger et al. [61] and Figure 1.3 for more information on the the fates of Population III stars over a large mass range. The black hole remnants of extremely massive Population III stars have been suggested as seeds for the super massive black holes (SMBHs) that have been observed in the centers of essentially all large galaxies [62, 63].

1.4.2   Radiative feedback

As mentioned in Section 1.4.1, recent numerical work indicates that Population III stars are copious emitters of ultraviolet radiation. In addition, it has been noted that the black hole remnants from these stars may produce large amounts of x-rays. What are the possible effects of the radiative feedback from these stars and their remnants?

Observations of the polarization of the cosmic microwave background by the Wilkinson Microwave Anisotropy Probe (WMAP) satellite have detected excess power on large angular scales compared to predictions based solely on the temperature power spectrum. This result is consistent with a period of partial reionization of the intergalactic medium taking place at redshifts of $11 < z < 30$ [64]. Observations of high-redshift quasars have shown that the universe was fully ionized at z=5.8 [65]. Recent calculations suggest that complete reionization occurred some time between $z = 7$ and $z = 12$ [66, 67, 68], though the exact epoch of reionization in these simulations is sensitive to a number of highly uncertain parameters, such as the formation efficiency of stars and quasars and the escape fraction of ionizing photons produced by these sources. Also, it is apparent that the topology of reionization is very complex - the epoch of reionization starts as "patches" of ionized material around the first stellar objects and spreads as structure evolves and more UV-emitting massive stars form [68]. In addition, the regions of highest gas density (which harbor the stars producing ionizing radiation) also contain significant amounts of neutral gas. Though the first stars to form are prodigious UV emitters, they are relatively few in number and quite short-lived. This makes the most likely scenario one where Population III stars are responsible for a partial reionization of the universe, and the structures that form from material polluted by these stars, namely, the first galaxies and pre-galactic objects (PGOs), is responsible for the final reionization of the universe, an idea that was first put forth by Cen [69] and supported by Hui & Haiman, who show that an early epoch of reionization would have to be followed by some cooling and recombination, or else the IGM would have a significantly different temperature than is
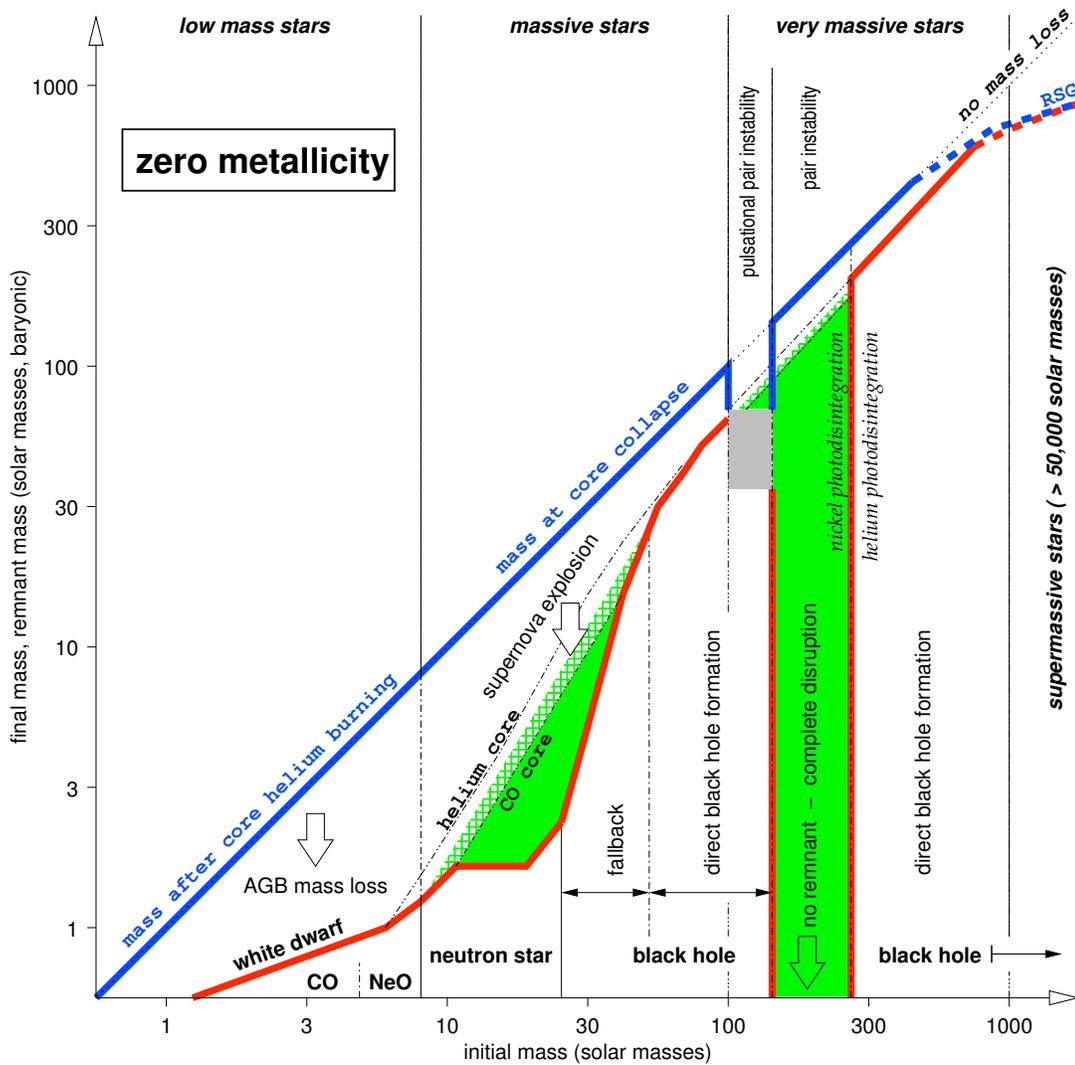
Figure 1.3: Stellar endpoints for zero metallicity stars, as a function of mass. This images were calculated using the 1D stellar evolution code KEPLER, and were done assuming a nonrotating model. Results may quantitatively change when rotation, convection and other physical effects are added. Figure courtesy of Alex Heger (Theoretical Astrophysics (T-6), Los Alamos National Laboratory).

observed today [70].

The primary cooling agent in the formation of massive primordial stars is molecular hydrogen. This molecule is quite fragile – its formation is dependent on the availability of H^-, the formation of which in turn depends on the availability of free electrons, and it can be easily destroyed by radiation in the Lyman-Werner band, which ranges from 11.18 to 13.6 eV (corresponding to the soft UV band). Since this is below the ionization threshold of atomic hydrogen, photons in this energy band can propagate great distances in the IGM. Also, since Population III stars appear to be prolific emitters of UV radiation, they will build up a background of this soft UV light, which may cause the overall dissociation of molecular hydrogen, halting the epoch of Population III star formation until more massive halos, whose virial temperatures are high enough that the gas can cool effectively by atomic hydrogen (e.g. $T_{vir} > 10^4$ K) have time to form [72, 73]. At this point, the clouds can continue to collapse and eventually produce primordial stars [74], which may have a different mass spectrum than Population III stars that form in minihalos with masses of $\sim 10^6$ M$_\odot$ [75]. Simulations have shown at this soft UV radiation is quite effective in suppressing the formation of Population III stars in halos with masses of $\sim 10^5 - 10^6$ M$_\odot$ [71].

The HII regions produced by massive primordial stars may also have a significant effect on star formation. Whalen et al. [76] show that the I-fronts from massive primordial stars can propagate several proper kpc in the high-redshift intergalactic medium, ionizing large volumes of space. These stars will also heat the gas in their parent halo, typically resulting in the majority of the baryons in a 10^6 M$_\odot$ halo to be driven out of the halo at speeds of up to ten times the escape velocity of that halo. Oh & Haiman [77] suggest that these HII regions will suppress the formation of any further stars in that region. However, work presented in this thesis shows that the high electron fraction produced as a result of ionization actually promotes the formation of molecular hydrogen, and in halos with a density above some critical density this can actually result in a positive feedback process where stars would form in halos that otherwise would not experience star formation. It has also been demonstrated that HD (deuterium hydride) can be a significant source of cooling in star-forming sites in fossil HII regions, allowing the gas temperature to drop even lower than via cooling due to molecular hydrogen alone would allow (below 100 K) and possibly resulting in low mass Population III stars [78].

Accretion onto the black holes formed by the collapse of Population III stars may be a source of significant x-ray radiation in the early universe. It has been suggested that this radiation is at least partially responsible for the WMAP polarization result [79, 80, 81]. Additionally, the soft x-ray background will produce a significant free electron fraction, that may result in a positive feedback effect on the formation of Population III stars by spurring the creation of molecular hydrogen [82]. This is not a certainty – depending on assumptions about the associated soft UV background and the hardness of the x-ray spectrum from the Population III black holes, the feedback effects may only be a weak

positive effect, or even negative [83, 77].

1.4.3   Chemical feedback

Observations of quasar absorption spectra show that the universe at the present day is uniformly polluted with metals, even at the lowest observed column densities, which correspond to regions of very low overdensity commonly referred to as the Lyman-α forest [84, 85]. The primordial composition of the universe is well understood, and post-BBN nucleosynthesis is believed to take place only in stars and the cataclysmic events associated with them. Because of this, it is apparent that this period of enrichment must have taken place between the epoch of first star formation and the present day.

As with reionization, it is unclear which objects are responsible for the majority of metals in the low-overdensity universe: The most massive galaxies in the early universe, often referred to as Lyman Break Galaxies (LBGs), are sites of vigorous star formation and metal production and characterized by strong, metal-rich galactic outflows and high luminosities [86]. However, being massive, they have deep potential wells which might serve to trap the ejected materials. Also, since these objects are the most massive bound objects in the early universe, the theory of hierarchical structure formation tells us (and observations support the assertion) that these galaxies are few and far between, so metals produced by them would have to be transported cosmologically significant distances in order to be as homogeneously distributed (as indicated by observations). The other possible candidate for homogeneous metal enrichment in a ΛCDM scenario would be pre-galactic objects and the first dwarf galaxies. While they are much smaller than LBGs, with correspondingly smaller star formation rates, they have shallower potential wells which would allow outflowing material to escape much more easily [87]. In addition, these smaller objects begin to form much earlier and there are many more of them than LBGs, so metal outflowing as winds from these galaxies or released via ram pressure stripping during the frequent galaxy mergers demanded by the hierarchical structure formation scenario would have more time to be distributed and also be required to travel a much more reasonable distance from their point of origin to obtain the observed relatively homogeneous distribution of metals [88].

The metals produced by Population III supernovae would have a very important effect on the following generations of stars. They enhanced the cooling properties of the gas significantly – molecular hydrogen is a relatively poor coolant compared to dust grains, which are believed to be produced in significant quantities by both primordial Type II supernovae and pair-instability supernovae, with the fractional quantity of dust increasing as the stellar mass increases [89, 90, 91]. Very little metal is required for gas to cool efficiently – analytical work and simulations suggest that the presence of carbon and oxygen at levels $10^{-4} - 10^{-3}$ Z$_\odot$ would be sufficient for enhanced fragmentation of collapsing gas clouds, signifying a change from the top-heavy Population III IMF to

a mass function resembling that observed in the galaxy today [93, 94]. As with their HII regions, the metals ejected from Population III supernovae, particularly if the stars fall into the mass range that produces highly energetic pair-instability supernovae, can propagate to great distances – simulations indicate that the ejecta from a massive PISN can eject metal into a sphere of ~ 1 kpc diameter at $z \sim 20$, producing a metallicity floor above that needed for enhanced cooling to take place [95].

It is doubtful that individual Population III stars can be observed directly during their main sequence lifetime, even by the James Webb Space Telescope (JWST), which is scheduled to be launched in 2011. However, it has been suggested that extremely massive Population III stars may be the progenitors of gamma ray bursts, and as such may be observable to very high redshifts [96]. The predicted rates of Population III supernovae suggest that their gamma ray bursts may be observable by the SWIFT satellite at the rate of approximately one per year, and that Population III supernovae may be observable by JWST at the rate of 4 $\deg^{-2}$ year^{-1} at $z \sim 15$, with a high level of uncertainty in these calculations [97, 98]. The nucleosynthetic yields of these stars may have already been detected in observations of the abundance ratios of two extremely metal poor stars, which have Fe/H ratios of $\sim 10^{-5.5}$ [99, 100]. Both of these stars show extreme overabundances of carbon and nitrogen with respect to iron, which suggests a similar origin of the abundance patterns. However, these abundance patterns do not agree with theoretical predictions for yields of Population III supernovae, so their origin is uncertain, though it has been suggested that these results can be naturally explained as the concurrent pollution of at least two supernovae of relatively low mass [101]. Finally, the coalescence of black hole remnants of Population III stars may be directly detected by gravitational interferometers such as Advanced LIGO [102], and indirectly by their contribution to the near-infrared background excess [103, 104].

1.5   Flaws in the ΛCDM paradigm

It is acknowledged that there appear to be flaws in the ΛCDM scenario. Observations of gravitational lensing by galaxy clusters indicate that the dark matter profile in the center of these clusters forms a smooth core, while theory and simulations using the ΛCDM model suggest that there should be a dark matter 'cusp' [105]. This cusp is also predicted to be seen in galaxies, but has not been observed [106, 107]. In addition, the CDM model predicts the formation of a large number of dwarf galaxies, and also suggests that these tiny galaxies will form in the cosmic voids - a prediction that has not been verified observationally [108, 109]. In addition, there have been observations of significant numbers of dwarf galaxies forming after the larger Lyman break galaxies, which is not what one would expect in a hierarchical clustering scenario [110].

This is not to say, however, that the CDM model is fatally flawed. The model has

done an excellent job of predicting the formation and evolution of large scale structure [111], as shown in recent years by extensive surveys of the local universe (such as the 2dF and SDSS surveys). The flaws in the dark matter models are on the sub-galactic scale [106, 112] – too small to affect the formation and evolution of large-scale structure, but certainly significant for the evolution of the first structures in the universe. Also, some work has been done recently which shows that the dark matter cusp issue in galaxies can be resolved [113]. A complete abandonment of the CDM paradigm seems premature.

There are several proposed solutions to the problems with the ΛCDM model, which include decaying dark matter [114], warm dark matter [115], collisional dark matter [116], annihilating dark matter [117] and fuzzy dark matter [118]. The essential feature of the majority of these models is that they suppress the formation of low-mass cosmological halos and can significantly alter predictions for early structure formation. The impact of the suppression of small-scale power by a generic warm dark matter model on cosmic structure formation in the early universe is explored in Chapter 5.