# A. Aykutalp

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## The Impact of Metallicity on Early Star Formation Supervisor: Prof. M. Spaans

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"We should be unwise to trust scientific inference very far when it becomes divorced from opportunity for observational test" - Sir Arthur Eddington

## Abstract

In this research we study the formation of a multi-phase ISM and early star formation in the universe by using the N-body hydrodynamical simulation code Enzo. We follow the collapse and cooling of minihalos with different metallicities. We use the star formation algorithm from Cen & Ostriker (1992) and include the chemical network of Spaans & Meijerink (2008); Meijerink & Spaans (2005). In our simulations we use 128<sup>3</sup> grid cells on the top grid with two nested subgrids, each refining by a factor of two. The box size of the simulations is  $0.25 \text{ h}^{-1}\text{Mpc}$  and  $1\text{h}^{-1}\text{Mpc}$  for cases with and without star formation, respectively. We run simulations over a redshift range of 70 to 5 for non-star formation case and 99 to 5 for the star formation case and use three different cooling prescriptions for the metallicities of  $10^{-3}$ ,  $10^{-2}$ , and  $10^{-1} \text{ Z}_{\odot}$ .

We have found that metallicity impacts the star formation by allowing minihalos to cool to lower temperatures, which makes them collapse and evolve faster than the zero metallicity case. Due to the lack of resolution in our simulations we cannot address the fragmentation of the cloud.

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### 1 Introduction

The Cosmological Principle states that on average the Universe is homogeneous and isotropic. Although this is the case for large scales (>  $100h^{-1}$  Mpc) on smaller scales the Universe contains a lot of structure. One of the important questions in cosmology is how the stars, galaxies, and clusters formed from a homogeneous and isotropic Universe. The theory that explains the formation of structure in the Universe is called the 'gravitational instability theory'. According to the gravitational instability theory the Universe has small fluctuations in the beginning and these density fluctuations are amplified under the influence of gravity. The structures that we observe today are the result of the gravitational growth of those primordial fluctuations. The observed fluctuations in the temperature of the cosmic microwave background radiation (CMB),  $\frac{\Delta T}{T} < 10^{-5}$  (T = 2.725 K), support the idea of these small density perturbations. The origin of these small perturbations are thought to be the result of quantum fluctuations during the inflationary stage of the big bang.



Figure 1: Gravitational instability theory

In the last two decades, cosmological simulations have become an important tool for theoreticians to simulate the structure formation in the Universe from the primordial fluctuations. To interpret the observations of the CMB we need a cosmological model. The cosmological model that currently matches the observations best is the so called Cold Dark Matter (CDM) model. According to the ACDM model the Universe consists of 73% cosmological constant (dark energy), 23% dark matter, and 4% baryonic matter. Primordial density perturbations on a small scale appear to have a much higher amplitude than those on large scales. This leads to the conclusion that small clumps are the first to collapse and form structures and then they build up larger structures by mergers and the accretion of matter. This process is called hierarchical structure formation.



Figure 2: Power Spectrum

A powerful model of hierarchical structure formation is the Press-Schechter theory (Press & Schechter 1974). The Press-Schechter formalism is used to estimate the number of collapsed objects as a function of mass at any given time. In this formalism it is assumed that the dense objects that we observe today are the results of the peaks in the initial density field. This formalism states that the number of halos per co-moving volume with masses in the range (M, M+dM) is

$$n(M,z)dM = \sqrt{\frac{2}{\pi}} \frac{\rho_0}{M} \frac{d\nu}{dM} exp(-\frac{\nu^2}{2})dM$$
(1)

where z is the redshift,  $\rho_0$  is the background density. In this equation  $\nu$  is defined as:

$$\nu = \frac{\delta_c}{D(z)\sigma(M)} \tag{2}$$

with  $\delta_c$  the critical overdensity, D(z) the linear growth factor and  $\sigma(M)$  is the root variance of the primordial density field in spheres containing mass M on average, which is extrapolated to z = 0 by using linear theory. In the Press-Schechter formalism it is assumed that density peaks are perfectly spherically symmetric, although in reality this is not the case. She thet al. (2001) generalized the Press-Schechter formalism to incorporate homogeneous ellipsoidal density perturbations. Then equation (1) becomes

$$n(M,z)dM = A(1+\frac{1}{\nu'^{2q}})\sqrt{\frac{2}{\pi}}\frac{\rho_0}{M}\frac{d\nu'}{dM}exp(-\frac{\nu'^2}{2})dM$$
(3)

where  $\nu' = \sqrt{a\nu}$ 

Due to the lack of observations of the period in which the first stars and galaxies formed we use cosmological simulations to investigate how the Universe evolved between the recombination and re-ionization era (Dark Ages). Given the initial conditions, a cosmological model with a composition of the Universe (matter, radiation), and primordial fluctuations one can compute the further structure formation from the big bang to the present day with numerical simulations.

In our research we study the collapse and evolution of minihalos  $(10^6 M_{\odot})$ under the influence of metallicity to address early star formation and their impacts on the surroundings by using the adaptive mesh refinement code Enzo (N-body + Hydrodynamics). So far, cosmological simulations which are based on the CDM models of hierarchical structure formation predict that the first stars have formed at redshifts  $z \sim 20 - 30$ , in dark matter halos of mass  $\sim 10^6 M_{\odot}$  (Tegmark et al. 1997; Yoshida et al. 2003), at the end of the cosmic dark ages. Due to a lack of observational data we do not know their physical properties or their impact on their surroundings. Also the initial mass function (IMF) of the first stars remains an open question.

Theoretically the physics of the first stars is rather simple compared to the physics of present day star formation (Abel et al. 2002). We know that the primordial gas in the early Universe was metal free and there were no magnetic fields that could effect the formation of structure. Also, there were no dust grains to couple the gas to radiation emitted by the protostar or winds from other stars. The efficiency of radiative cooling is determined by the density and the chemical composition of the gas. Therefore cooling depends mostly on the abundances of atomic and molecular H, and HD. Neutral atomic hydrogen, HI, is the major coolant for temperatures  $T \geq 10^4 K$ , and molecular hydrogen,  $H_2$ , dominates cooling in a metal free gas for  $200 < T < 10^4$  (Saslaw & Zipoy 1967; Peebles & Dicke 1968). On the other hand, heavy hydrogen, HD, becomes the dominant coolant for gas of metallicity,  $Z < 10^{-3}$  and temperatures T < 200 K (Flower et al. 2000; Omukai et al. 2005). Here the challenge is what happens to this gas when it collapses. Does it fragment and form binary systems or even cluster of stars, or does it form a single massive star?

The very first stars are the stars whose metallicity is so low that metal cooling does not have any effect, either on the formation or the evolution of the stars. Nowadays, in the literature, the first stars are called Pop III stars. These stars might have formed in various environments and this might have caused different modes of Pop III star formation. Indeed, it has become evident that Pop III star formation might have two distinct modes: Pop III.1 and Pop III.2 stars (McKee & Tan 2008). Pop III.1 stars are the first generation of stars that are formed from the collapse of the primordial gas into DM minihalos whereas Pop III.2 stars are the second generation of these stars that are affected by the radiation of previously formed stars. Early on, Pop III.2 stars were called Pop II.5 stars (Mackey et al. 2003; Greif & Bromm 2006; Johnson & Bromm 2006). Pop III.2 stars will be less massive than Pop III.1 stars because when the gas is ionized by the previous generation of stars, HD cooling can become important and this allows the gas to cool more efficiently and therefore lowers the mass of these stars through the Jeans mass criterion as explained below. (see Figure 3)



Figure 3: The characteristic mass of stars as a function of redshift (Johnson & Bromm 2006). Pop III.1, Pop III.2 (Pop II.5) and Pop II stars with characterized masses of the order of  $100M_{\odot}$ ,  $10M_{\odot}$ , and  $1M_{\odot}$ , respectively.

From observations of the nearby Universe we know that the present day stellar mass scale is  $\sim 1 M_{\odot}$ . There are two important processes that define the final mass of a star. The initial mass of the core and the accretion rate. The accretion rate can be estimated as follows

$$\dot{M}_{acc} \sim \frac{c_s^3}{G} \propto T^{3/2} \tag{4}$$

Here  $c_s$  is the sound speed, G is the gravitational constant, and T is the temperature. Because the temperature of the star forming regions in the early Universe ( $T \sim 100 - 300$ K) is different from those we see today ( $T \sim 10$ K), we expect to have a different mass scale for the first stars. Also, the lack of metals in the early Universe lets the first stars be more massive than present day stars because of insufficient cooling. We can see this easily from the Jeans mass criterion. The Jeans mass gives a maximum mass value for a cloud that can be in an equilibrium

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

If  $M_{cloud} > M_J$  then the cloud will collapse. It has been suggested that the first stars have  $M \ge 100 M_{\odot}$  (Bromm et al. 1999; Nakamura & Umemura 2001; Abel et al. 2000) but more recent studies show that the first stars are not necessarily that massive and they can be  $10 M_{\odot} - 100 M_{\odot}$  (Heger & Woosley 2008).

When the first stars form they will influence their surroundings, this is called a feedback effect. Feedback is a back reaction of a process on itself or on the causes that have produced it. It can be negative or positive. We can classify the feedback effects from the first stars into three groups: mechanical, chemical and radiative feedback.

Mechanical Feedback: Mechanical feedback affects the subsequent star formation process in different ways. At the end of their life, massive first stars can explode as supernova explosions (SNe). This feedback can be either negative or positive. SNe might blow away the gas (Bromm et al. 2003; Springel & Hernquist 2003; Whalen et al. 2008). This has a negative effect on the star formation. On the other hand, shocks can compress gas and increase the density so that gas cools down more efficiently and give rise to star formation. This way it has a positive effect.

*Chemical Feedback*: Chemical feedback is related to the critical metallicity of the gas which leads to a transition in the star formation history. SNe of the first stars are crucial for understanding the metal enrichment of the ISM and the faith of the structure and star formation. Metal enriched primordial gas enhances cooling and is therefore believed to govern the underlying physics of the transition from Pop III to Pop II stars, since the cooling enhanced the Jeans mass of protostars is lowered significantly, thus resulting in less massive stars. Chemical feedback has recently been studied by several authors Bromm et al. (2001); Schneider et al. (2002); Omukai et al. (2005); Clark et al. (2008); Smith & Sigurdsson (2007). These studies have shown that metal line cooling is important in a non-zero metallicity gas, compared to  $H_2$  and HD, for metallicities of the order of  $10^{-3}$  (Bromm & Loeb 2003) or even  $10^{-5} - 10^{-6}$  (Jappsen et al. 2007). In the paper of Bromm et al. (2001), the critical metallicity for the transition between Pop III and Pop II stars was reported as  $10^{-3.5}Z_{\odot}$  but other studies have shown that this threshold is the point where metal line cooling becomes more important than  $H_2$  cooling. There is also an important contribution to the cooling by the collisional coupling of warm gas and cool dust grains, provided the density exceeds  $10^4/[Z/Z_{\odot}]$  cm<sup>-3</sup>.

The epoch of the Pop II stars depends on the number of Pop III stars that explode as pair instability supernovae (PISN), the metal ejection efficiency, and mixing in the intergalactic medium (IGM), as well as on the initial mass function. So it is a local process and therefore the use of a single critical metallicity can be misleading.

Radiative Feedback: The radiation from the first stars will influence their surroundings by heating and ionizing the gas, leading Pop III.2 stars. Also the radiation will photodissociate hydrogen molecules within the larger Lyman-Werner (LW) bubbles that surround the first stars. Radiative feedback effects can be either negative or positive according to the energy of the radiation. If the radiation is soft UV then this will destroy  $H_2$ . In the absence of  $H_2$  gas cannot cool efficiently and collapse, so in this case the feedback has a negative effect. On the other hand if the radiation is in the form of X-ray photons this feedback effect will be positive. This is because, gas phase  $H_2$  formation is related to the abundance of free electrons and any process that temporarily enhances their abundance, will also tend to increase the  $H_2$  fraction. So the cloud will cool down and start collapsing. In the paper of Whalen et al. (2004), they argue, for a given smooth density distribution, that the H II ionization front expels gas when Pop III stars are formed in a minihalo of  $10^6 M_{\odot}$ .

In the near future new telescopes, such as the James Webb Space Telescope (JWST), the Atacama Large Millimeter/submillimeter Array (ALMA), and the Square Kilometer Array (SKA) will open up the epoch of re-ionization for observations. When this happens valuable information about the formation of first stars will become available and make it possible to distinguish between the different theories of first star formation.

This thesis is structured as follows, in section 2 we will first discuss the dynamics of the cosmological simulation code Enzo. Section 3 will explain the modifications we have done to the code, and give an overview of the cooling processes and star formation criteria that are used. In section 4 we will give the setup of our simulations. Finally in section 5 we will present our results and in § 6 we will give the summary of this research and discuss future work.

### 2 The Code -Enzo-

We have used the cosmological adaptive mesh refinement code Enzo (Bryan & Norman 1997) for our research. Enzo is a grid based code which allows you to zoom in on the region of interest and keep the rest of the simulation at low resolution. Therefore, it saves computational time and allows a more detailed view of the physics. Enzo is developed and maintained by the Laboratory for Computational Astrophysics at the University of California in San Diego. It is written in a mixture of C++ and Fortran 77. Enzo uses the hierarchical data format (HDF5), to write out and restart files in a platform-independent format. It is a parallelized code using the Message Passing Interface (MPI) which enables it to run on multiple processors. Although it has been designed to simulate cosmological structure formation, it also allows hydrodynamical and N-body simulations in one, two, and three dimensions.

Enzo simulates both the baryonic and non-baryonic (dark matter) matter components of the Universe. Due to the different nature of baryonic and nonbaryonic matter this requires different numerical algorithms. Baryonic matter is evolved using a finite volume discretization of the Euler equations of gas dynamics in an expanding Universe. On the other hand, dark matter is assumed to behave as a collisionless phase fluid, obeying the Vlasov-Poisson equation and its evolution is solved by using particle-mesh algorithms for collisionless Nbody dynamics. Baryonic matter and dark matter interact only through their self-consistent gravitational field. The gravitational potential is computed by solving the Poisson equation on the uniform or adaptive grid hierarchy using Fast Fourier Transform and multigrid techniques. In this section we will discuss the main features of Enzo in detail.

#### 2.1 Adaptive Mesh Refinement

Enzo uses the structured adaptive mesh refinement technique (SAMR) which was developed by Berger and Oliger (1984) for hyperbolic partial differential equations. Later on, Berger and Collela used it for conservation laws, and demonstrated that the method is also successful for gas dynamics in two dimensions. Saltzmann and Welcome (1991) extended the methodology to three dimensions.



Figure 4: coarse and ghost grids

Adaptive mesh refinement (AMR) is a grid based method. It first puts a coarse grid which has the same size as the simulation box. Then it scans the whole box volume to see if there is something interesting going on. In the algorithm, one can define criteria that tell Enzo to refine the grid. In Enzo, one can set a value for the mass of a cell (either baryonic or particle) so that whenever a cell has a mass value bigger than the one given, Enzo will make higher refinement to that point. Also one can tell Enzo to make higher refinement to the cells if the Jean's length is to be resolved, if there is a shock present, if the cell's cooling time is less than the cell's width divided by the speed of sound, or if the density of the cell (baryon) is higher than the value you set. So whenever one or a combination of these criteria is matched Enzo puts a second grid (called child grid) inside the coarse grid's cell with a higher refinement. Afterwards it starts scanning this child grid to look if there is a region where the criteria are matched. If it finds cells in the child grid that match the criteria then it will put another grid into the child grid with even better refinement. Enzo can go on doing this as much as one wants. Refinement can occur anywhere in the volume or at a subvolume that is defined by the user. However, the resolution of the simulation is limited by the size of these cells. If the physics you are interested in are occurring on smaller scales than the size of a cell, then nothing can be resolved. In our work we use mass criteria (for both baryonic and non-baryonic particles) for increasing the refinement.

In the end we obtain a hierarchical structure with cells inside bigger cells as shown in Figure 5. These cells in the grids are treated as individual objects. They can contain both field variables and particle data. The code uses a simple dynamic load-balancing scheme to distribute the workload within each level of the AMR hierarchy evenly across all processors. The advantage of this is that the computational time is reduced by distributing different grids among the processors on parallel machines. Each processor stores the entire distributed AMR hierarchy, but not all processors contain all the grid data. If a grid's data is allocated to a processor then it is a real grid on that processor and on all other processores it is a ghost grid. The values in the cells at the boundary of the grid depend on the values of the neighboring grids. Real grids are used to store the data grid values, and ghost grids are used to temporarily store neighboring grid values, so that these values can be used for updating real grids when required. The ghost grid layer is three zones deep in order to make calculations of the hydrodynamics solver properly. These three zone deep ghost grid layers cost a lot of computational time and cause storage problems. Especially for the region with the highest refinement.



Figure 5: Adaptive mesh refinement structure with 5 levels of refinement

#### 2.2 Hydrodynamics

On large scales, dark matter dominates the gravitational evolution of the universe. However, on the scales of galaxy formation baryonic matter, which is dissipative in nature, takes over and dominates the formation of structure. Therefore, the hydrodynamics of the collisional particles has to be included in the simulations. In cosmological simulations there are two common hydrodynamical methods: Lagrangian schemes, and Eulerian schemes. In the Lagrangian schemes, the observer moves with the fluid while in Eulerian schemes, the observer stands still as fluid moves by. This is shown in the Figure 6.

So in Eulerian schemes fluid quantities are functions of position x and time t while in Lagrangian schemes fluid quantities are functions of initial position  $x(t_0)$  and time t.

Enzo uses the Eulerian scheme for simulating the hydrodynamics. There are two different formulations of Eulerian hydrodynamics in Enzo to solve the equations of gas dynamics: The Piecewise Parabolic Method (PPM) (Colella & Woodward 1984), and a three-dimensional implementation of the artificial viscosity-based scheme used in the magnetohydrodynamics code ZEUS (Stone & Norman 1992). Although ZEUS is implemented into Enzo, the preferred scheme is the PPM method.

PPM is a higher order, more accurate version of Godunov's method. The



Figure 6: On the left a visualization of the Eulerian scheme, and on the right the Lagrangian scheme.

Godunov method treats the solution of the problem as piecewise constants. Then it solves the time evolution over  $[t_n, t_{n+1}]$  for this piecewise function exactly. The exact solution can then be used to produce fluxes. The time evolution is determined by the exact solution of the Riemann problem (shock tube) at the inter-cell boundaries (Hirsch, 1990). The idea behind Godunov's method consists of solving analytically the Riemann problems arising at each cell interface of a cell-wise constant finite-volume scheme as shown in Figure 7. The problem of a one-dimensional initial discontinuity with constant left and right states is called the Riemann problem.



Figure 7: Godunov scheme

The baryonic content of the Universe can be described approximately as an ideal gas. To follow the evolution of the gas one has to solve the equations of hydrodynamics:

$$\frac{\partial \rho}{\partial t} + \nabla \rho u = 0 \quad \text{Continuity equation} \tag{6}$$

$$\frac{\partial \rho u}{\partial t} + (\nabla . u)u) = -\nabla p - \rho \nabla \phi \quad \text{Momentum conservation} \tag{7}$$

$$\frac{\partial E}{\partial t} + \nabla [(E+P)u] = -\rho u \cdot \nabla \phi \quad \text{Energy conservation} \tag{8}$$

where  $\rho$  is the mass density, u is the fluid velocity, P is the thermal pressure, E is the total energy per unit volume. Together with the equation of state (see below) and the Poisson equation they close the hierarchy of the hydrodynamic equations:

$$\epsilon = \frac{1}{\gamma - 1} \frac{P}{\rho} \quad \text{Equation of state} \tag{9}$$

When additional physics are taken into account, like adding cooling into the simulation, cooling and heating parameters should be included to the right hand side of the energy conservation equation as follows:

$$\frac{\partial E}{\partial t} + \nabla [(E+P)u] = -\rho u \nabla \phi + (\Gamma - \Lambda) \quad \text{Energy conservation}$$
(10)

where  $\Gamma$  is the heating and  $\Lambda$  is the cooling term in erg s<sup>-1</sup>.

In the original Godunov method variables were assumed to be constant in each cell and at each cell interface the fluxes of variables are computed by solving the Riemann boundary problem. To be able to solve the gas dynamics we need to find a set of intermediate states (one for each characteristic) that connect the left and right states and that satisfy the physical conditions (e.g. shock jump conditions).

Given the boundary conditions on the left and on the right of the cell



Figure 8: Boundary condition problem.

interface (see Figure 8) one can solve the conservation equations to obtain the flux.

Shocks occur when the velocity of a fluid becomes comparable with or exceeds that of the sound speed in the surrounding medium. This will lead the

medium to heat up, compress and accelerate. There are two types of shocks: Continuous shocks (C-shock) and Jump shocks (J-shock).

The C-shocks are magnetized shocks and are weak compared to the J-shocks. In general C-shocks occur in gas with a low degree of ionization, high density and molecular fraction. C-shocks have velocity's of less than  $\sim 40$  km s<sup>-1</sup>. The shock front here is thicker than the cooling length scale. This means that once the shock propagates into the medium it sweeps up the material and heats it up but this material will cool back down even before the shock is completely passed.

In the J-shock, the shock front is much thinner than the post-shock relaxation layer. It is a fast shock with velocities ( $\geq 40 \text{ km s}^{-1}$ ) and there is a big difference between the pressure and temperature properties of the medium before and after the shock. Therefore this causes a big jump in the properties of the medium. We can relate the physical quantities of the medium before and after the shock by using the conservation laws. These are called jump conditions and are given by:

$$\rho_1 u_1 = \rho_2 u_2 \quad \text{Mass conservation} \tag{11}$$

$$P_1 + \rho_1 u_1^2 = P_2 + \rho_2 u_2^2 \quad \text{Momentum conservation} \tag{12}$$

$$\frac{1}{2}u_1^2 + \frac{\gamma}{\gamma - 1}\frac{P_1}{\rho_1} = \frac{1}{2}u_2^2 + \frac{\gamma}{\gamma - 1}\frac{P_2}{\rho_2} \quad \text{Energy conservation} \tag{13}$$

Enzo uses a non-linear Riemann solver for shock capturing. It conserves energy (by using a dual energy formalism), mass flux, and momentum. In the dual energy formalism, the thermal energy and the total energy are computed for each time step and therefore it can estimate the entropy jump at shock fronts and correct the temperature and pressure in hypersonic flows with a high accuracy (O'Shea et al. 2005).

Another issue is the time step of the calculations. If one takes a time step too small than it will result in the calculations being unfeasibly small. On the other hand, if the time step is chosen too large than this might lead the material flow from a grid cell x to grid cell x+2 without its effect being calculated at the grid cell x+1 which causes instability in the simulation. To prevent these problems one can calculate the minimum possible time step by using the Courant number which is given by

$$C_r = \frac{c_s \Delta t}{\Delta x} \tag{14}$$

where  $C_r$  is the Courant number,  $\Delta t$  is the time step,  $\Delta x$  is the length of a grid cell, and  $c_s$  is the speed of sound. Here  $C_r$  should not be greater than one. In practise the time step is usually chosen in such that  $C_r$  is 0.6.

#### 2.3 N-body dynamics

N-body codes are algorithms that enable us to follow the motion of a large number of masses under the influence of gravitational interaction. Enzo is a collisionless N-body code. Collisionless N-body codes are used to model systems over much shorter time scales than the relaxation time. N-body simulations use a finite set of particles to sample the underlying phase-space distribution function. The system is simulated as a set of N particles moving with a velocity  $v'_i$  in co-moving coordinates. In cosmological N-body simulations co-moving coordinates and periodic boundary conditions are needed and the gravity is assumed to be the only force acting on a particle. In N-body simulations it is assumed that the Universe is homogeneous and isotropic. With these assumptions we can define the distance and location of an object in co-moving coordinates. This allows distances, and locations, in an expanding homogeneous and isotropic cosmology to be related only in terms of a scale factor. This means that in co-moving coordinates the distance and location of an object do not change as the Universe expands. Figure 9 and 10 show the co-moving coordinates in the Eulerian and Lagrangian scheme.



Figure 9: Co-moving coordinates in Eulerian scheme



Figure 10: Co-moving coordinates in Lagrangian scheme

The basic theory behind N-body simulations is computing the gravitational force at a given time on each particle. This force is determined by the relative positions of the particles. After estimating the force that acts on every particle, the new position and momentum of each particle for some time interval can be computed.

The major problem in determining the gravitational force on a particle is the large number of particles that exert a force on this particle. N-body simulations use Poisson solvers to compute the gravitational force on each particle. There is a dilemma about deciding the number of particles to use in the simulation: On one hand large numbers of particles are needed to be able to represent the universe properly, on the other hand using a large particle masses leads to a resolution problem of underlying physics.

There are several Poisson solvers such as Particle-Particle (PP), Particle-Mesh (PM), Particle-Particle/ Particle-Mesh (P3M), Particle Multiple Mesh (PM2), and Tree code Particle Mesh (TPM). The Poisson solver method that is used in N-body simulations depends on the purpose of the simulation. Here we will explain the steps that are involved in computing the gravitational force exerted on a particle by other particles in grid based simulation codes.

The basic method of calculating the gravitational force that is exerted on a particle by other particles is the Particle-Particle method. The gravitational force between two particles is calculated simply by using Newton's gravitational law

$$F_{ij} = -G \frac{m_i m_j}{(x_i - x_j)^2}$$
(15)

Here  $F_{ij}$  is the force that acts on particle *i* by particle *j*,  $m_i$  and  $m_j$  are the masses of the particles i and j respectively, G is the universal gravitational constant (G= 6.67300  $10^{-11}$  m<sup>3</sup> kg<sup>-1</sup> s<sup>-2</sup>), and  $x_i$  and  $x_j$  are the positions of the particles *i* and *j* respectively. In a system with N particles the total gravitational force that is exerted by N-1 particles on a particle is then computed as follows

$$F_i = Gm_j \sum_{j=1, j \neq i}^{N} \frac{x_j - x_i}{|x_j - x_i|^3}$$
(16)

and the acceleration of the particle  $m_i$  is:

$$a_i = -G\sum_{j=1, j \neq i}^N m_i \frac{x_j - x_i}{|x_j - x_i|^3}$$
(17)

When we integrate this over a time interval we get the equations of motion for a particle  $m_i$ 

$$\frac{dx_i}{dt} = v_i \tag{18}$$

$$a_i = \frac{dv_i}{dt} = -\nabla\phi \tag{19}$$

This way of computing the gravitational force costs a lot of computational time. This is because in the PP method the distance between particle i and j is

used twice, once for the contribution of particle j to the force on particle i and once for the force from particle i on particle j. So the number of computations per timestep increases with N as  $N^2$ . Eventhough, it is easy to implement this method is not used much because of costing too much computational time.

Another method for computing the gravitational force is the PM method. In the PM method the number of computations per timestep increases with N as NlogN. Therefore in Enzo the PM method is used. In the PM method a grid is put onto the computational box. Phase-space is divided up into a mesh of equal sizes. Afterward it assigns each particles mass onto the grid using a specific mass assignment scheme. The process of estimating the density on the grid from the positions of a large number of particles that trace the density is called mass assignment. There are several mass assignment schemes like Nearest Grid Point (NGP), Cloud-in-Cell (CIC), and Triangular Shaped Cloud (TSC). In the NGP assignment scheme the mass of each particle  $m_i$  is assigned to the meshpoint that is closest to the particle. NGP is also referred to as zero-order interpolation.

In the CIC assignment scheme, the mass of each particle is weighted over the four (in 2D) closest mesh points (mass is splitted over  $2^D$  cells, where D is the dimension of the grid) which is called a cloud; the weighting is proportional to the intersection of the cloud surrounding the particle and the cell (see Figure 11).

The idea of the TSC assignment scheme is the same as the CIC scheme, but the TSC scheme differs in the size of interaction cloud. In the TSC scheme mass is splitted over  $3^D$  cells. So the number of cells that the mass of each particle is spread over is different in the TSC scheme.

After estimating the densities on the grid from the particle distribution the potential is solved at the meshpoints using the Poisson equation. Forces at the meshpoints can then be obtained by calculating the gradient of the potential. If a particle is not located at a meshpoint then the force on that particle can be computed either by using the force at the nearest meshpoint, or by interpolating the force from the closest meshpoints.

The equation of motion of a particle in co-moving coordinates is written as:

$$\frac{d\vec{x_i}}{dt} = \frac{1}{a}\vec{v_i} \tag{20}$$

$$\frac{d\vec{v_i}}{dt} = -\frac{\dot{a}}{a}\vec{v_i} - \frac{1}{a}(\nabla\phi)_i \tag{21}$$

where the subscript in the last term in Eq. 19 means the gravitational acceleration is evaluated at position  $\vec{x_i}$ . One needs to solve the Poisson equation in order to find the gravitational potential. The Poisson equation is given by;

$$\nabla^2 \phi = \frac{4\pi G}{a} (\rho - \bar{\rho}) \tag{22}$$

where  $\rho$  is the local co-moving mass density of gas and particles (collisionless fluid), and  $\bar{\rho}$  is its global average value. Then the Poisson equation is solved



Figure 11: Visualization of NGP and CIC assignment scheme

in real space by a convolution of the density field with a Green function.

$$\nabla^2 \phi = \frac{4\pi G}{a} (\rho - \bar{\rho}) \quad \text{Poisson equation} \tag{23}$$

$$\phi(x,t) = \int \mathbb{G}(x-x')\rho(x',t)d^3x' \quad \text{in integral form}$$
(24)

$$\mathbb{G}(x - x') = \frac{G}{|x - x'|} \quad \text{Green function} \tag{25}$$

Here  $\mathbb{G}$  is the Green function for Newtonian geometry. In Fourier-space, the convolution becomes a simple multiplication:

$$\hat{\phi}(k) = \hat{g}(k).\hat{\rho}(k) \tag{26}$$

However, there is a problem in Eq. 14. When the distance between two particles i and j approaches zero, the divergence of  $F_{ij}$  predicts unphysical values for the mass distribution. This can be eliminated by replacing  $|x_j - x_i|$ by a softening kernel  $S(|x_j - x_i|)$ . Fundamentally, softening is a parameter to eliminate the artificial division by zero in the simulations.

$$F_{i} = \sum_{j=1, j \neq i}^{N} Gm_{j}S_{F}(|x_{j} - x_{i}|) \frac{x_{j} - x_{i}}{|x_{j} - x_{i}|}$$
(27)

Here,  $S_F(r)$ , where  $r = r_j - r_i$ , is the force softening kernel.

To be able to solve the Poisson equation, apart from the density value on the mesh the boundary conditions should be known as well. In Enzo periodic boundary conditions are used. Periodic boundary conditions mean that the grid is imagined to be one cell of an infinite lattice. After solving the Poisson equation, the gravitational force on the mesh is computed by finite differencing the mesh potential.



Figure 12: meshpoint scheme

The gravitational field on the mesh is calculated by taking the finite difference of the potential as:

$$g(x_1) = -\frac{\phi(x_{i+\frac{1}{2}}) - \phi(x_{i-\frac{1}{2}})}{\Delta x}$$
(28)

Then by reversing the interpolated force field back onto the particles we can compute the force on the particle.

#### 2.4 Relevant scales

In order to make a clear picture of the scales we are interested in in this research we explain the definitions of the most important scales that are used in the simulations.

*Jeans length*: The Jeans length is the critical radius at which a molecular cloud becomes gravitationally unstable and begins to collapse.

$$\lambda_j = \sqrt{\frac{15k_\beta T}{4\pi G\mu\rho}} \approx 0.062 \,\mathrm{kpc} \left(\frac{\mathrm{T}}{200 \,\mathrm{K}}\right)^{\frac{1}{2}} \left(\frac{\mathrm{n}}{10^4 \,\mathrm{cm}^{-3}}\right)^{-\frac{1}{2}}$$
(29)

where  $k_{\beta}$  is the Boltzmann constant, T is the temperature of the cloud, G is the gravitational constant,  $\mu$  is the mass per particle in the cloud,  $\rho$  is the mass density of the cloud, and  $\lambda_j$  is the radius of the cloud. At this critical radius the pressure of the cloud and its gravity are in equilibrium.

*Jeans Mass*: The maximum mass of a cloud that is in an equilibrium is given by the Jeans mass:

$$M_j = \left(\frac{5kT}{G\mu m_p}\right)^{3/2} \left(\frac{3}{4\pi\rho}\right)^{\frac{1}{2}}$$
(30)

If  $M_{cloud} > M_j$  then the cloud will collapse. The generalized Jeans mass to include external pressure is  $M_{j,p} \propto T^2 \rho^{\frac{-1}{2}}$ , for turbulence  $M_{j,t} \propto \Delta V^4 P^{\frac{-1}{2}}$ , and for magnetic flux support  $M_j \propto B^3 \rho^{-1}$ 

*Free fall time*: Free fall time is the time that a cloud would take to collapse under its gravity if there are no other forces present.

$$t_{ff} = \sqrt{\frac{3\pi}{32Gnm_H}} \approx 0.347 \,\mathrm{Myr} \left(\frac{\mathrm{n}}{10^4 \,\mathrm{cm}^{-3}}\right)^{-\frac{1}{2}}$$
 (31)

*Cooling time*: This is the time for a cloud to radiate all its energy.

$$n\frac{d}{dt}(\frac{3}{2}k_{\beta}T) = -\frac{3k_{\beta}(T-T_E)}{2t_T}$$
(32)

where  $t_T$  is the cooling time. The net input of energy per cubic centimeter, per second, equals the corresponding rate of increase of thermal energy, plus the work done by the gas, this gives the result for a monatomic gas

$$\frac{d}{dt}(\frac{3}{2}k_{\beta}T) - k_{\beta}T\frac{dn}{dt} = \sum_{\zeta,\eta}(\Gamma_{\zeta,\eta} - \Lambda_{\zeta,\eta}) = \Gamma - \Lambda$$
(33)

Here n is the total number of free particles per  $cm^3$  in the interstellar gas,  $\Gamma$  is the heating rate, and  $\Lambda$  is the cooling rate. For constant n,  $t_T$  equals the ratio of the excess of energy density to the net cooling rate  $\Gamma - \Lambda$ 

$$t_T = \frac{3}{2}nk_\beta \frac{(T - T_E)}{\Lambda - \Gamma} \tag{34}$$

*Recombination time*: Recombination occurred when the temperature of the universe decreased below  $10^4$  K, at this point neutral hydrogen formed from the primordial electron-proton plasma. Above this temperature Thompson scattering from electrons in the plasma prevented photons to propagate. This transition happened at redshift  $z_{rec} = 1089$ . The recombination time can be computed by

$$t_{rec} = \frac{1}{k_{rec}n_{H^+}} \tag{35}$$

where  $k_{rec}$  is the rate coefficient for radiative recombination, and  $n_{H^+}$  is the number density of  $H^+$ .

*Sound speed*: The speed with which a sound wave travels through a gas is called sound speed and is given by

$$v_s = \sqrt{\frac{\gamma P}{\rho}} \tag{36}$$

where  $\gamma$  is the heat capacity ratio, P is the ambient pressure, and  $\rho$  is the density.

### 3 Additional Physics

Once the gas has virialized in the potential wells of dark matter halos, additional cooling is required for the further collapse of the gas and to form stars. In this section we will discuss these cooling processes, and the formation and metal enrichment of the first stars. For this we follow the cooling of the primordial gas as explained in the papers of Spaans & Meijerink (2008); Meijerink & Spaans (2005), and for the star formation we use the algorithm from Cen & Ostriker (1992).

#### 3.1 Cooling

In the early history of the state-of-art cosmological simulation codes, the radiative cooling was implemented by means of an equilibrium cooling function. But in the presence of a shock or when photoionization becomes more important than collisional ionization, which is the case in the intergalactic medium, the ionization equilibrium breaks down. Therefore, Cen (1992) treated cooling by following the non-equilibrium abundances of free electrons and all atomic, ionic, and molecular species that are relevant to cooling. At first only the rate equations for electrons and all ionization states of hydrogen and helium were taken into account. Later on Haehnelt et al. (1996) added heavier elements (metals), and more recent work include  $H^-$ ,  $H_2^+$ , and  $H_2$  (Haiman et al. 1996; Abel et al. 1997; Anninos et al. 1997; Gnedin & Ostriker 1997).

The formation of a star depends on the ability of interstellar gas to cool and form dense molecular clouds. So the chemical composition and the metallicity of the interstellar gas is the key parameter to study. Although the primordial gas is complex, we can simplify the chemistry according to the contributions of the various elements to the cooling process (see Table 1).

Name	Metallicity $(Z)$	Mass $(M \odot)$	Formation
Pop III.1	0	$\lesssim 100$	$H_2$ cooling
Pop III.2	0	$\gtrsim 10$	HD and $H_2$ cooling
Pop II.5	$\lesssim Z_{crit}$	$\gtrsim 10$	metal line cooling
Pop II	$> Z_{crit}$	local IMF	metal enriched star formation

Table 1: Typical metallicity, mass values and dominant cooling mechanisms of the first stars.

The main coolants for primordial gas with temperatures  $T \geq 10^4 K$  are Lyman  $\alpha$  emission of neutral atomic hydrogen (HI 1216 Å), and helium (He II, 304 Å). Below this temperature, which is the case in the minihalos with temperatures  $T_{vir} \leq 10^4 K$ , the cooling process is dominated by molecular hydrogen ( $H_2$ ), where one can calculate  $T_{vir}$  as follows

$$T_{vir} = 1.98 \times 10^4 (\frac{\mu}{0.6}) (\frac{M}{10^8 h^{-1} M_{\odot}})^{\frac{2}{3}} (\frac{\Omega}{\Omega_z} \frac{\Delta}{18\pi^2})^{\frac{1}{3}} (\frac{1+z}{10}) K$$
(37)

where  $\mu$  is the mean molecular weight and  $\Delta$  is the collapse overdensity.

The importance of  $H_2$  cooling in primordial gas was first realized by Saslaw & Zipoy (1967); Peebles & Dicke (1968). In present day molecular clouds  $H_2$  formation occurs primarily on the surface of interstellar dust grains (Gould & Salpeter 1963; Cazaux & Tielens 2002; Cazaux & Spaans 2004). However, in the absence of dust  $H_2$  forms via the gas phase reactions listed below:

$$H + H \to H_2 + h\nu \tag{38}$$

The formation of  $H_2$  through the reaction above is not common because it is necessary to have an excited electronic state of hydrogen. This happens near the end of the re-ionization epoch (Latter & Black 1991; Rawlings et al. 1993).

$$H + H + H \to H_2 + H, \tag{39}$$

$$H + H + H_2 \to H_2 + H_2, \tag{40}$$

This is called three-body formation. In these reactions the rate coefficients are small therefore this pathway only becomes important at high densities  $(n \gtrsim 10^8 \text{ cm}^{-3}, \text{Palla et al. (1983)})$ . On the other hand the dominant reactions that lead to the formation of  $H_2$  at low densities are as follows

$$H + e^- \to H^- + h\nu \tag{41}$$

$$H^- + H \to H_2 + e^- \tag{42}$$

$$H^+ + H \to H_2^+ + h\nu, \tag{43}$$

$$H_2^+ + H \to H_2 + H^+ \tag{44}$$

For these two paths of  $H_2$  formation at low densities, the formation rate is directly proportional to the fractional ionization of the gas. The  $H^-$  in the first reaction forms much faster than  $H^+$  in the second reaction. Therefore the first reaction is more efficient in forming  $H_2$  at low densities.

One can calculate the  $H_2$  cooling rate for given  $H_2$  abundances, density and temperature of the gas. The first excited rotational state of  $H_2$  lies at  $\sim 500K$ . Figure 13 shows that the cooling rate of  $H_2$  falls of exponentially with decreasing temperatures, due to the large excitation energy of the first accessible excited state, and is essentially negligible below 100 K. It scales with density as  $\Lambda_{H_2} \propto n^2$  at low densities, where radiative de-excitation dominates, and as  $\Lambda_{H_2} \propto n$  at high densities, where collisional de-excitation dominates and the level populations approach their local thermodynamic equilibrium (LTE) values.

Hydrogen deuteride, HD, is an important important coolant below 200 K in the primordial gas. The first excited rotational state of HD lies at a temperature of ~ 150 K. If there is enough HD, the gas can cool down to the temperature of the cosmic microwave background (CMB) (Nakamura & Umemura 2002; Nagakura & Omukai 2005; Vasiliev & Shchekinov 2006; Johnson & Bromm 2006; Yoshida et al. 2007). Although the primordial deuterium abundance is small relative to hydrogen  $\left(\frac{n_D}{n_H} = 4 \times 10^{-5}\right)$ , chemical fractionation leads to an enhancement of the ratio,  $\frac{n_{HD}}{n_{H_2}} \approx 10^{-3}$  (Puy et al. 1993; Galli & Palla 1998; Stancil et al. 1998).

Molecular hydrogen does not have a permanent electric dipole moment while the HD molecule has and that makes HD a better coolant than  $H_2$ . The dominant reactions that lead to HD formation are listed below.

$$H_2 + D^+ \to HD + H^+ \tag{45}$$

and

$$D + H_2 \to HD + H \tag{46}$$

Here the first reaction is endothermic (absorbs energy) by 462 K. Therefore, at low temperatures the HD cooling rate per molecule is greater than that of  $H_2$  (Glover 2007). The efficiency of HD cooling depends on whether the gas is ionized or not. In Pop III star formation calculations, the fractional ionization is small and the temperature of the gas is not low enough for chemical



Figure 13: A comparison of various parametrizations of the  $H_2$  cooling function, plotted in units of erg cm<sup>3</sup> s<sup>-1</sup>. Rates are computed assuming that  $n >> n_{H_2}$ , and that the ortho-to-para ratio is 3:1. The lower set of lines corresponds to a gas density  $n = 10^6$  cm<sup>3</sup>; the upper set corresponds to n =100 cm<sup>3</sup>. Solid line Le Bourlot et al. (1999); dashed line Galli & Palla (1998); dotted line Lepp & Shull (1983); dash-dotted line Hollenbach & McKee (1979).

fractionation to become efficient. Therefore we can neglect the effect of HD cooling. On the other hand, in an initially ionized gas HD will form in high abundances (Shapiro & Kang 1987). In their work Nagakura & Omukai (2005) found that the gas would re-collapse and form significant amounts of HD due to the presence of free electrons, and Johnson & Bromm (2006) showed that when primordial gas is significantly ionized the cooling from HD is sufficient to lower the temperature to the level of the CMB and therefore this can give rise to Pop III.2 stars (see Figure 14).



Figure 14: Effect of HD cooling on to the star formation mass.

In the paper of McGreer & Bryan (2008) it has been discussed that the minimum temperature which can be reached by  $H_2$  cooling occurs at a density of  $n \sim 10^3 - 10^4$  cm<sup>-3</sup> while in the case of HD cooling the minimum temperature is reached at a density of  $n \sim 10^4 - 10^5$  cm<sup>-3</sup>. This shift in the density can be explained under the assumption that the gas is driven to LTE. The gravitational energy (adiabatic compression) input per unit volume can be estimated as

$$n(\frac{GM(r)}{r})t_{dyn}^{-1} \propto n^{\frac{3}{2}}$$

$$\tag{47}$$

We can estimate the cooling function approximately as

$$\Lambda = \begin{cases} n^2 T^{\alpha} & n < n_{cr} \\ n T^{\alpha} & n > n_{cr} \end{cases}$$

If we equate these two equations then we can obtain the relation between density and temperature. One can see that the temperature reaches a minimum at the critical density, where it transitions from  $T \sim n^{-0.5}$  to  $T \sim n^{0.5}$ .

When the primordial gas is enriched by metals as a result of SNe of Pop III stars then one has to take into account the cooling from the fine-structure lines of metals. Many atoms have fine-structure lines. The relative motion of any orbiting electron and a charged nucleus creates a torque on the magnetic moment associated with the intrinsic spin of the electron. Because the electrons of H and He atoms are described by single-particle wavefunctions without any associated orbital angular momentum (l=0), and the electric ground states of these atoms do not have internal torque there is no fine-structure splitting in these atoms. On the other hand, atoms like C,O, Si, Fe,... have fine-structure lines which cause cooling in the metal enriched primordial gas.



Figure 15: Fine-structure splitting of the electronic ground states of O I and C II.

The energy difference between the  ${}^{6}P_{1}$  and  ${}^{6}P_{2}$  levels of [O I]  $63\mu m$  is  $2 \times 10^{-2}$ 

eV corresponding to a temperature of 230 K. By using a number density of oxygen relative to hydrogen of  $4 \times 10^{-4}$  and noting that the degeneracy of each J-state is 2J+1, one can evaluate subcritical volumetric cooling rate of [O I] as follows

$$\Lambda_{OI} = 2 \times 10^{-10} \left(\frac{n_H}{10^3 cm^{-3}}\right)^2 exp\left(-\frac{230K}{T_g}\right) \,\text{eV}\,\text{cm}^{-3}\,\text{s}^{-1}$$
(48)

For carbon, the energy difference between the  ${}^{2}P_{3/2}$  and  ${}^{2}P_{1/2}$  levels of [C II]  $158\mu m$  is  $7.93 \times 10^{-3} eV$ , corresponding to a temperature of 92 K. The subcritical volumetric cooling rate of [C II] can be computed as follows

$$\Lambda_{CII} = 3 \times 10^{-9} \left(\frac{n_H}{10^3 cm^{-3}}\right)^2 exp\left(-\frac{92K}{T_g}\right) \,\text{eV}\,\text{cm}^{-3}\,\text{s}^{-1} \tag{49}$$

Metal enriched primordial gas cools more efficiently by fine-structure lines of [C II] (157.74  $\mu m$ ), [O I] (63.18  $\mu m$ , 145.5  $\mu m$ ), [Si II] (34.8  $\mu m$ ), and [Fe II] (25.99  $\mu m$ , 35.35  $\mu m$ ) than by HD or H<sub>2</sub> emission. The cooling rate of the metals depends on their ionization state. These atoms will be excited to higher levels by collisions, which will eventually de-excite through photon emission, and carry the energy out of the region (see table 2).

coolant	density $(cm^{-3})$	Temperature $(K)$				
Н	$\gtrsim 10^8$	$> 10^4$				
$H_2$	$10^3 - 10^4$	$\gtrsim 200$				
HD	$10^4 - 10^6$	$\lesssim 200$				
C II	$10^{3}$	92				
ΟΙ	$10^{5}$	230				

Table 2: Relevant temperature and density values for coolant components

All the data that are used in our calculations are taken from Hollenbach & McKee (1989) (see Appendix A), except for  $Si^+$  (Dufton & Kingston 1994),  $C^+$  (Sampson et al. 1994), and  $O^+$  (McLaughlin & Bell 1993).

CMB photons, for z > 10 can be an excitation source (radiative pumping) of atomic and molecular levels. This allows the CMB temperature to act as a thermodynamic floor, below which gas cannot cool, provided that collisional de-excitation dominates the removal of population from the excited state. Furthermore, gas-dust cooling can be impacted as well, in the sense that dust grains will be heated to at least the CMB temperature. We also include ion-molecule chemistry. The most important ones are CO, H<sub>2</sub>O, OH, HCN, HNC, HCO<sup>+</sup>. These are relevant for cooling below 10<sup>3</sup> K.

#### **3.2** Star formation

We use the star formation criteria of Cen & Ostriker (1992) to create stars in Enzo. Whenever these criteria in a grid cell are met, Enzo converts that gas particle into a star particle. The criteria that we use are as follows:

- Baryonic density: This criterion checks whether the baryonic density of a cell exceeds the mean density in the Universe by a certain factor, that is called threshold value in Enzo, and defined by the user. The default value in Enzo is 100.
- Jeans Mass: It is the Jeans mass criterion that checks whether the mass density of the gas in a cell exceeds the local Jeans mass.
- Convergent flow: The gas that forms a star should be in a collapsing region. Therefore it is required that the gas particles are part of a converging flow. When the divergence of the velocity field, ∇.v, is negative, the criterion is satisfied, and it is assumed that the gas particle is part of a collapsing flow.
- Cooling time: The cooling time, t<sub>cool</sub>, of the gas to collapse should be less than the dynamical time which is given by:

$$t_{dyn} = \sqrt{\frac{3\pi}{32G\rho_{tot}}} \tag{50}$$

When all these criteria are met in a cell then the gas is converted into a star particle. The star particle that has formed does not represent a single star. It is a cluster of stars with a mass of:

$$m_* = \epsilon \frac{\Delta t}{t_{dyn}} \rho_{gas} \Delta x^3 \tag{51}$$

where  $\epsilon$  is the star formation efficiency,  $\Delta t$  is the size of the time step,  $t_{dyn}$  is the dynamical time, and  $\rho_{gas}$  is the baryon density.

Apart from the criteria listed above there is an additional condition. In Enzo one can define the minimum mass value of a star particle. This is a computational issue and can be decided by the user to be used or not. By adding this condition, small star particles are not taken into account in the simulation, which saves computational time.

#### 4 Simulations

In our research we perform several cosmological runs for two different sets of initial conditions. In the first set of runs we follow the pre-collapse of minihalos for different metallicities by using the chemical network of Spaans & Meijerink (2008), initialized at redshift z=70, for a cosmological co-moving box size of  $0.25h^{-1}$  Mpc. In the second set, we turn on the star formation flag, and use the same chemical network but initialize the simulation at z=99 and for a cosmological co-moving box size of  $1 h^{-1}Mpc$ .

First we run a low resolution, pure N-body simulation to identify the volume of a pre-collapsing minihalo with a mass of  $10^6 M_{\odot}$ . Hence we focus on dwarf like galaxies. Then by using the HOP analysis tool we get the coordinates of the minihalo and use it for higher resolution runs where we zoom in on the minihalo. HOP is a new Group finding algorithm for N-body simulations written by Eisenstein & Hut (1998). It divides the set of particles into equivalence classes such that each particle is a member of only one group. It starts by assigning an estimate of the local density to each particle. Then it calculates the density around each particle by using  $N_{dens}$  nearest neighbors. Afterward it searches for the densest of each particle's  $N_{hop}$  nearest neighbors and repeats this stepfor the densest neighbor. When a particle has no denser neighbors anymore, the particle with the highest density is reached. All particles in a path that leads to the same maximum density particle constitute a single group. Then the code compiles the densest boundary pairs between each pair of groups. Every particle is assigned to a group; since we are interested in the high density regions, we simply remove particles below a given overdensity threshold (160).

We start with  $128^3$  grid cells on the top grid and two nested subgrids, each refining by a factor of 2, for an effective topgrid resolution of  $512^3$ . For the cosmological parameters we use the following values:  $\Omega_M = 0.279$ ,  $\Omega_{\Lambda} = 0.7208$ ,  $\Omega_B = 0.0462$ , and Hubble constant, h=0.7, in units of 100 km s<sup>-1</sup> Mpc<sup>-1</sup>. The power spectrum of initial density fluctuations is given by Eisenstein & Hu (1999), with  $\sigma_8 = 0.9$  and n = 1. For the runs with star formation we use baryonic density and cooling time criteria to form stars.

The metallicities that we consider are assumed to be the result of preenrichment by earlier star formation, i.e, chemical feedback. For  $Z_i 10^{-3} Z_{\odot}$ , there is little contribution from metal lines to the overall cooling.

The code is ran in parallel on 16 processors of the supercomputer at the Centre for High Performance Computing and Visualization (HPC/V), University of Groningen, Netherlands. Each processor has two dual-core 2.6 Ghz Opteron processors (4 cores in total), and 4 Gigabytes of internal memory.

#### 4.1 Metallicity



Figure 16: Temperature (T) vs number density (n) at redshift 13 for metallicities  $10^{-3}$  (red),  $10^{-2}$  (green),  $10^{-1}$  (blue)  $Z_{\odot}$ .



Figure 17: Temperature (T) vs number density (n) at redshift 10 for metallicities  $10^{-3}$  (red),  $10^{-2}$  (green),  $10^{-1}$  (blue)  $Z_{\odot}$ .

Here we present the output of our simulations for the star formation off case and for metallicities  $10^{-3}$ ,  $10^{-2}$ ,  $10^{-1} Z_{\odot}$ . Every plot shows the gas properties



Figure 18: Temperature (T) vs number density (n) at redshift 7 for metallicities  $10^{-3}$  (red),  $10^{-2}$  (green),  $10^{-1}$  (blue)  $Z_{\odot}$ .



Figure 19: Temperature (T) vs number density (n) at redshift 5 for metallicities  $10^{-3}$  (red),  $10^{-2}$  (green),  $10^{-1}$  (blue)  $Z_{\odot}$ .

of a minihalo. We plot the number density against the temperature for rings in the minihalo with increasing radius at a certain redshift (z = 13,10,7,5) and metallicity. Plots are ordered in such a way that the metallicities are combined for a specific redshift in one figure, the metallicity increases where from top to bottom.



Figure 20: Density distribution of a collapsing minihalo at redshift 16 for metallicities  $10^{-3}$  (left) and  $10^{-1}$  (right)  $Z_{\odot}$ .



Figure 21: Density distribution of a collapsing minihalo at redshift 5 for metallicities  $10^{-3} Z_{\odot}$  (left) and  $10^{-1}$  (right)  $Z_{\odot}$ .



Figure 22: Temperature (T) vs number density (n) at redshift 7 for metallicities  $10^{-3}$  (red)  $10^{-2}$  (green),  $10^{-1}$  (blue)  $Z_{\odot}$ .



Figure 23: Comparison of star formation on (top) and off (bottom) cases at redshift 7 for a metallicity  $10^{-3} Z_{\odot}$ .

In the simulations with star formation on we produce low-mass stars for the first time at redshift 8. Here we show the gas properties of a minihalo that has a star in it in the same way as the previous section, but for redshift 7.



Figure 24: Comparison of star formation on (top) and off (bottom) cases at redshift 7 for a metallicity  $10^{-2} Z_{\odot}$ .



Figure 25: Comparison of star formation on (top) and off (bottom) cases at redshift 7 for a metallicity  $10^{-1} Z_{\odot}$ .

In addition, we present plots that combine star formation on and off cases for a specific metallicity and a redshift to be able to show the multi-phase ISM structure clearly.



Figure 26: Density distribution of a collapsing minihalo for star formation on case at redshift 7 for metallicities  $10^{-3}$  (left) and  $10^{-1}$  (right)  $Z_{\odot}$ .

## 5 Results

In Figures 16 to 19 we clearly see that the minihalo with higher initial metallicity has lower temperatures at any specific redshift. Even though this effect is not significant between metallicities of  $10^{-3}$  and  $10^{-2} Z_{\odot}$ , there is a big difference between these metallicities and a metallicity of  $10^{-1} Z_{\odot}$ . This leads us to think that there is a transition region between metallicities  $10^{-3}$  and  $10^{-1} Z_{\odot}$ , as far as a multi-phase ISM is concerned. Because we did not take into account any feedback effects from the first stars we cannot say for sure when this transition occurs. This transition might cause the difference between the distinct formation modes of early star formation, Pop III, Pop II.5, and Pop II. To be able to determine the exact transition region we should incorporate more detailed chemical, mechanical and radiative feedback effects into the code.

In the case of star formation on we again see that the highest metallicity minihalo cools to lower temperature than the metal poor cases. When we compare star formation on and off cases for a specific redshift and metallicity we see that the temperature is much higher in the star formation on case. We also see that high densities are lacking in the star formation on case, due to the formation of HII regions. This is because we are plotting the gas properties and in the simulation with star formation algorithm, the highest density gas particles have turned into star particles. In the star formation on case the highest temperatures are reached at higher densities than the star formation off case.

### 6 Summary & Future Work

In the last two decades, cosmological simulations have become an important tool to understand structure formation and the evolution of the Universe. Cosmological simulations incorporate gravity, gas dynamics, chemistry, and radiative transfer. One of the biggest questions that remained unanswered is how, when, and under which conditions the first structures are formed in the early Universe. According to the CDM model of hierarchical structure formation, the first stars formed in dark matter halos of mass  $\sim 10^6 M_{\odot}$ . In this research we consider the pre-enrichment of minihalos, and work on the impact of metallicity on pre-collapsing minihalos and the formation of the first stars in the early Universe by using the Cosmological N-body Hydrodynamical simulation code Enzo.

To be able to study the collapse of minihalos and the formation of the first stars, it is crucial to implement cooling processes properly. For this purpose we implement the chemical network from Spaans & Meijerink (2008) which includes the cooling processes of H<sub>2</sub>, HD, metal fine structure lines and molecules like CO. We run simulations for metallicities,  $Z = 10^{-3}$ ,  $10^{-2}$ ,  $10^{-1}Z_{\odot}$  for star formation on and off cases. In our simulations we see that in the high metallicity case minihalos collapse and evolve faster than in the low metallicity case.

Our main goal is to understand the nature of the first stars, their feedback effects, and the impact of metallicity on the formation and evolution of Pop II.5 stars. To do this, in the near future we are going to modify the chemical network of Enzo by implementing the photon dominated region (PDR, Tielens & Hollenbach 1985), and X-ray dominated region (XDR, Maloney et al. 1996) codes of Spaans & Meijerink (2008) and add grain surface chemistry. The transition region between the fully ionized and fully molecular zones is known as the PDR. PDRs are formed by the far-ultraviolet radiation (FUV, 6.0 < E < 13.6 keV) from starbursts. Grains can absorb relatively low-energy light that filters through the H II regions and therefore they are the dominant opacity source throughout the PDR. On the other hand, XDRs are formed by hard X-ray radiation (E > 1 keV) from black hole environments (AGN). In PDRs and XDRs, the chemical structure and thermal balance are completely determined by the radiation field. Later on we will include mechanical (SNe) feedback effects. Also, we need to increase the resolution  $(1024^3)$  of our simulations to be able to resolve fragmentation. For that we need a supercomputer that has at least 64Gb RAM in one processor.

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## Appendix A

$ \begin{array}{c c c c c c c c c c c c c c c c c c c $		$E_{ij}$							
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Species (0, 1, 2) <sup>a</sup>	к (К) <sup>ь</sup>	λ° (Å)	$n_{\rm cr}^{e^{-d}}$ (cm <sup>-3</sup> )	$n_{\rm cr}^{\rm H d}$ (cm <sup>-3</sup> )	$A_{ij}^{e}$ (s <sup>-1</sup> )	$\gamma^e_{ij}(T_4 < 1)^{\rm f}$	$\gamma^e_{ij}(1 < T_4 < 20)^i$	$(cm^{-2})^{N_{\tau}^{8}}$
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$C_1({}^{3}P, {}^{1}D, {}^{1}S)$	1.5(4)	9823 9850	$1.1(4)T_4^{-0.58}$	$3.0(8)T_4^{-0.02}$	3.4(-4)	$2.7(-8)T_4^{0.57}$	$2.7(-8)T_4^{-0.13}$	5.4(25)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		3.1(4) 1.7(4)	4622 8727	$2.9(7)T_4^{-0.57}$	2.5(11)	2.6(-3) 0.5	$1.3(-8)T_4^{0.57}$ $1.2(-8)T_4^{0.57}$	1.3(-8) 1.2(-8)	1.4(26) 1.8(23)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$C II ({}^{2}P, {}^{4}P)$	6.2(4)	2326	$1.6(8)T_4^{0.50}$	3.6(12)	3.6	$2.3(-8)T_4^{-0.50}$		1.3(23)
$ \begin{array}{c} \begin{array}{c} 9,120 \\ 2,4(4) & 3675 \\ 2,4(4) & 6135 \\ 2,4(4) & 6135 \\ 2,4(4) & 6135 \\ 2,4(4) & 6135 \\ 2,4(4) & 6135 \\ 2,4(4) & 6135 \\ 2,4(4) & 6135 \\ 2,4(4) & 6135 \\ 2,4(4) & 6135 \\ 2,4(4) & 6135 \\ 2,4(4) & 136 \ \mum \\ 2,4(4) & 7(3)T_{4}^{0,43} & 1.4(9)T_{4}^{0,00} & 1.5(-3) \\ 1,5(-3) & 1.5(-7) \\ 1,1(-7)T_{4}^{2,57} & 2.0(-7)T_{4}^{0,11} & 2.1(25) \\ 1,0(-7)T_{4}^{2,57} & 1.0(-7)T_{4}^{2,57} & 1.$	Cl II $({}^{3}P, {}^{1}D, {}^{1}S)$	1.7(4)	8580	$1.9(6)T_4^{0.49}$	$1.3(11)T_4^{-0.01}$	0.13	$6.7(-8)T_4^{-0.50}$	•••	2.7(26)
$ \begin{split} & \operatorname{Fe}_1(^3D_4, ^5F_9, ^5F_4), \ldots, & 99(3) & 1.44 \ \mum & 79(3) \mathbb{T}_{0}^{-0.43} & 1.49(7) \mathbb{T}_{0}^{0.09} & 2.0(-3) & 1.2(-7) \mathbb{T}_{2}^{-0.73} & 2.0(-7) \mathbb{T}_{2}^{-0.13} & 2.1(25) \\ & 64(2) & 22.3 \ \mum & \ldots & 3.6(-3) & 1.5(-7) & \ldots & 3.2(24) \\ & 64(2) & 22.3 \ \mum & \ldots & 3.6(-3) & 1.5(-7) & \ldots & 3.2(24) \\ & 53(3) & 4.12 \ \mum & 1.4(4) \mathbb{T}_{2}^{-5.0} & 1.6(8) \mathbb{T}_{4}^{-0.11} & 2.8(-4) & 2.2(-8) \mathbb{T}_{4}^{-0.05} & \ldots & 3.2(24) \\ & 53(3) & 4.12 \ \mum & 1.4(4) \mathbb{T}_{2}^{-5.0} & 1.6(8) \mathbb{T}_{4}^{-0.11} & 2.8(-4) & 2.2(-8) \mathbb{T}_{4}^{-0.05} & \ldots & 3.2(24) \\ & 53(3) & 4.12 \ \mum & 4.8(7) \mathbb{T}_{4}^{-0.16} & 3.8(-8) \mathbb{T}_{4}^{-0.16} & \ldots & 3.2(24) \\ & 51(2 \ 1.79 \ \mum & \ldots & \ldots & 61(-3) & 3.8(-8) \mathbb{T}_{4}^{-0.06} & \ldots & 3.2(24) \\ & 5.2(-8) \mathbb{T}_{4}^{-0.06} & \ldots & 1.7(25) \\ & 8.0(3) \ 1.6(4 \ \mum & \ldots & \ldots & 1.9(-3) & 2.5(-8) \mathbb{T}_{4}^{-0.06} & \ldots & 1.7(25) \\ & 8.0(3) \ 1.6(4 \ \mum & \ldots & \ldots & 1.9(-3) & 2.5(-8) \mathbb{T}_{4}^{-0.06} & \ldots & 1.7(25) \\ & 8.0(-9) \mathbb{T}_{4}^{-5.7} & 8.0(-9) \mathbb{T}_{4}^{-0.13} & 2.7(28) \\ & 1.4(4) \ 1.64 \ \mum & \ldots & \ldots & 1.9(-3) & 2.5(-8) \mathbb{T}_{4}^{-0.06} & \ldots & 1.2(26) \\ & 1.4(4) \ 1.64 \ \mum & \ldots & \ldots & 1.9(-3) & 2.5(-8) \mathbb{T}_{4}^{-0.06} & \ldots & 1.2(26) \\ & 1.4(4) \ 1.64 \ 1.64 \ 1.9(7) \mathbb{T}_{4}^{-0.73} & 2.6(11) \ 5.0(-3) \ 4.5(-9) \mathbb{T}_{4}^{-5.7} & 8.0(-9) \mathbb{T}_{4}^{-0.13} & 2.7(28) \\ & 1.4(4) \ 1.64 \ 1.9(7) \mathbb{T}_{4}^{-0.73} & 2.6(11) \ 5.0(-3) \ 4.5(-9) \mathbb{T}_{4}^{-5.7} & 3.4(-8) \ 4.2(-8) \mathbb{T}_{4}^{-0.06} & \ldots & 1.2(26) \\ & 1.4(4) \ 1.64 \ 1.9(7) \mathbb{T}_{4}^{-5.9} & \dots & 1.1(-5) \ 8.0(-9) \mathbb{T}_{4}^{-5.7} & 3.4(-8) \ 8.3(-9) \mathbb{T}_{4}^{-0.13} & 3.2(2-8) \ 1.1(-5) \ 8.0(-9) \mathbb{T}_{4}^{-5.7} & 3.4(-8) \ 8.3(-9) \mathbb{T}_{4}^{-0.13} & 3.2(-9) \mathbb{T}_{4}^{-0.13} & 3.2(-8) \ 1.1(-5) \ 8.0(-9) \mathbb{T}_{4}^{-0.13} & 3.2(-8) \ 1.1(-5) \ 8.0(-9) \mathbb{T}_{4}^{-0.13} & 3.2(-8) \ 1.1(-5) \ 8.0(-9) \mathbb{T}_{4}^{-0.13} & 1.2(-8) \ 1.1(-5) \ 8.0(-9) \mathbb{T}_{4}^{-0.13} & 1.2(-8) \ 1.1(-7) \mathbb{T}_{4}^{-0.90} & \ldots & 1.2(-8) \ 1.1(-7) \mathbb{T}_{4}^$		4.1(4) 2.4(4)	3675 6153	3.7(7)T <sub>4</sub> <sup>0.50</sup>	1.8(12)	1.3 2.3	$3.5(-8)T_4^{-0.50}$ $6.4(-8)T_4^{-0.50}$		4.6(26) 9.3(25)
$ \begin{split} & \operatorname{Fe} \operatorname{II} (^{4}D_{9/2}, ^{4}F_{9/2}, ^{4}D_{7/2}) \dots & \begin{array}{c} 2.7(3) \\ 3.5(3) \\ 4.12 \\ 1.79 \\ \mu m \end{array} & \begin{array}{c} 1.4(5)T_{4}^{-5.0} \\ 2.9(9) \\ 1.0(-4) \\ \\ 6.1(-3) \\ 3.8(-8)T_{4}^{-0.50} \\ \\ 3.8(-8)T_{4$	Fe $I({}^{5}D_{4}, {}^{5}F_{5}, {}^{5}F_{4})$	9.9(3) 1.1(4) 6.4(2)	1.44 μm 1.36 μm 22.3 μm	$7.9(3)T_4^{-0.43}$ 2.6(4) $T_4^{-0.16}$	$\begin{array}{c} 1.4(9)T_4^{-0.09} \\ 6.6(9) \\ \dots \end{array}$	2.0(-3) 1.5(-3) 3.6(-3)	$2.0(-7)T_4^{0.57}$ $1.0(-7)T_4^{0.57}$ 1.5(-7)	$2.0(-7)T_4^{-0.13}$ 1.0(-7)	2.1(25) 2.1(25) 4.4(21)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Fe II $({}^{6}D_{9/2}, {}^{4}F_{9/2}, {}^{4}F_{7/2}) \dots$	2.7(3) 3.5(3) 8.1(2)	5.34 μm 4.12 μm 17.9 μm	$\begin{array}{c} 1.0(4)T_4^{0.50} \\ 1.4(5)T_4^{0.50} \\ \dots \end{array}$	$\frac{1.6(8)T_4^{-0.11}}{2.9(9)}$	2.8(-4) 1.0(-4) 6.1(-3)	$2.2(-8)T_{4}^{-0.50}$ $7.1(-9)T_{4}^{-0.50}$ $3.8(-8)T_{4}^{-0.50}$		3.5(24) 2.6(25) 5.3(21)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Fe II $({}^{6}D_{9/2}, {}^{4}F_{9/2}, {}^{4}D_{7/2})$	2.7(3) 1.1(4) 8.6(3)	5.34 μm 1.26 μm 1.64 μm	$\begin{array}{c} 6.7(3)T_4^{0.40} \\ 9.7(4)T_4^{0.50} \\ \dots \end{array}$	$\frac{1.6(8)T_4^{-0.11}}{3.7(9)}$	2.8(-4) 5.6(-3) 1.9(-3)	$2.2(-8)T_{4}^{-0.50}$ $5.2(-8)T_{4}^{-0.50}$ $2.5(-8)T_{4}^{-0.50}$	•••	3.5(24) 1.7(25) 2.2(25)
$ \begin{array}{c} 4.1(4) & 3466 \\ 1.4(4) & 1.04 \ \mu m \\$	N I $({}^{4}S, {}^{2}D, {}^{2}P)$	2.8(4)	5198 5201	$2.0(3)T_4^{-0.73}$	$2.0(7)T_4^{-0.06}$	1.1(-5)	$8.0(-9)T_4^{0.57}$	$8.0(-9)T_4^{-0.13}$	2.7(28)
$ \begin{split} & \operatorname{N} \mathfrak{u} \left({}^3P_1 D_1 {}^1S \right) \dots \dots \\ & 2.2(4)  6548 \\ & 6583 \\ & 4.7(4)  3063 \\ & 1.8(7) T_2^{0.50} \\ & 1.5(4)  5755 \\ & \dots \\ & 1.1 \\ & 3.4(-2) \\ & 2.8(-8) T_4^{-0.50} \\ & \dots \\ & 1.1 \\ & 3.4(-8) T_4^{-0.50} \\ & \dots \\ & 1.1 \\ & 3.4(-8) T_4^{-0.50} \\ & \dots \\ & 1.1 \\ & 3.4(-8) T_4^{-0.50} \\ & \dots \\ & 1.1 \\ & 3.4(-8) T_4^{-0.50} \\ & \dots \\ & 1.1 \\ & 3.4(-8) T_4^{-0.50} \\ & \dots \\ & 9.7(2) \\ & 1.8(3) \\ & 11.4 \\ \mu m \\ & \dots \\ & 7.0(4) T_2^{-0.10} \\ & 7.0(9) \\ & 3.2(-8) \\ & 3.2(-8) \\ & 3.4(-8) T_4^{-0.50} \\ & \dots \\ & 1.4(23) \\ & 9.7(2) \\ & 1.48 \\ \mu m \\ & \dots \\ & 7.0(-3) \\ & 9.7(2) \\ & 1.48 \\ \mu m \\ & \dots \\ & 0.7 \\ & 0.7 \\ & 0.7 \\ & 0.7 \\ & 0.9 \\ & 0.7(2) \\ & 1.48 \\ \mu m \\ & \dots \\ & 0.7 \\ & 0.7 \\ & 0.7 \\ & 0.7 \\ & 0.9 \\ & 0.7(2) \\ & 1.48 \\ \mu m \\ & \dots \\ & 0.7 \\ & 0.7 \\ & 0.7 \\ & 0.7 \\ & 0.9 \\ & 0.7(2) \\ & 1.48 \\ \mu m \\ & \dots \\ & 0.7 \\ & 0.7 \\ & 0.7 \\ & 0.9 \\ & 0.7(2) \\ & 1.48 \\ & \mu m \\ & \dots \\ & 0.7 \\ $		4.1(4) 1.4(4)	3466 1.04 μm	$1.9(7)T_4^{-0.57}$	2.6(11)	5.0(-3) 7.9(-2)	$4.5(-9)T_4^{0.57}$ $2.3(-8)T_4^{0.57}$	4.5(-9) 2.3(-8)	1.2(26) 7.4(23)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	N II $({}^{3}P, {}^{1}D, {}^{1}S)$	2.2(4)	6548 6583	$7.8(4)T_4^{0.50}$	$4.0(9)T_4^{-0.01}$	4.1(-3)	$5.2(-8)T_4^{-0.50}$	•••	4.6(25)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		4.7(4) 1.5(4)	3063 5755	$1.8(7)T_4^{0.50}$	5.7(11)	3.4(-2) 1.1	$\frac{2.8(-8)T_4^{-0.50}}{3.4(-8)T_4^{-0.50}}$		1.2(26) 9.4(23)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Ni $I({}^{3}F_{4}, {}^{3}D_{3}, {}^{3}D_{2})$	2.9(2) 1.3(3) 9.7(2)	48.8 μm 11.4 μm 14.8 μm	$6.0(-4)T_4^{-0.47}$ $7.0(4)T_4^{-0.10}$	$4.9(1)T_4^{-0.11}$ 7.0(9)	8.0(-11) 3.2(-8) 7.0(-3)	$7.0(-8)T_4^{0.57}$ $3.4(-8)T_4^{0.57}$ 9.3(-8)	$7.0(-8)T_4^{-0.13}$ 3.4(-8)	3.2(29) 8.7(28) 1.4(23)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Ni II $({}^{2}D_{5/2}, {}^{4}F_{9/2}, {}^{4}F_{7/2}) \dots$	1.2(4) 1.3(4) 1.3(3)	1.19 μm 1.07 μm 10.7 μm	$2.9(1)T_4^{0.36}$ $1.2(5)T_4^{0.50}$	$3.2(6)T_4^{-0.15}$ 1.4(10)	7.5(-6) 1.4(-3) 2.7(-2)	$\frac{1.1(-7)T_4^{-0.50}}{1.1(-7)T_4^{-0.50}}$ $\frac{1.1(-7)T_4^{-0.50}}{1.1(-7)T_4^{-0.50}}$		1.5(29) 2.6(27) 8.8(22)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$O_1({}^{3}P, {}^{1}D, {}^{1}S)$	2.3(4)	6300 6363	$1.3(6)T_4^{-0.58}$	$6.6(9)T_4^{-0.01}$	6.7(-3)	$5.1(-9)T_4^{0.57}$	$5.1(-9)T_4^{0.17}$	9.3(24)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		4.9(4) 2.6(4)	2972 5577	$1.8(8)T_4^{-0.57}$	6.9(11)	6.7(-2) 1.3	$2.5(-9)T_4^{0.57} \\ 5.2(-9)T_4^{0.57}$	$\begin{array}{c} 2.5(-9)T_4^{0.13} \\ 5.2(-9)T_4^{0.15} \end{array}$	1.1(25) 1.5(23)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	O II $({}^{4}S, {}^{2}D_{5/2}, {}^{2}D_{3/2})$	3.9(4) 3.9(4) 3.0(1)	3729 3726 508 μm	$\begin{array}{c} 1.4(3)T_4^{0.50} \\ 4.7(3)T_4^{0.50} \\ \dots \end{array}$	2.5(7) 9.0(7)	5.1(-5) 1.7(-4) 1.3(-7)	$\begin{array}{c} 1.3(-8)T_4^{-0.50}\\ 1.3(-8)T_4^{-0.50}\\ 2.5(-8)T_4^{-0.50} \end{array}$		2.0(27) 7.1(26) 5.6(20)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$S_{I}({}^{3}P, {}^{1}D, {}^{1}S)$	1.3(4)	1.08 μm 1.13 μm	$7.0(5)T_4^{-0.01}$	$3.5(10)T_4^{-0.01}$	3.6(-2)	$5.1(-8)T_4^{0.57}$	$5.1(-8)T_4^{-0.13}$	(3.4(23)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		3.2(4) 1.9(4)	4589 7725	$4.5(7)T_4^{-0.57}$	1.1(12) 	0.36 1.8	$2.5(-8)T_4^{0.57} 2.3(-8)T_4^{0.57}$	2.5(-8) 2.3(-8)	5.8(23) 4.0(22)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$S \amalg ({}^{4}S, {}^{2}D_{3/2}, {}^{2}D_{5/2}) \ldots$	2.1(4) 2.1(4) 4.5(1)	6731 6717 318 μm	$\frac{1.1(4)T_4^{0.50}}{3.6(3)T_4^{0.50}}$	7.2(8) 2.4(8)	1.8(-3) 4.7(-4) 3.3(-7)	$4.9(-8)T_4^{-0.50}$ $4.9(-8)T_4^{-0.50}$ $8.0(-8)T_4^{-0.50}$	···· ····	1.2(25) 3.1(25) 4.1(20)
Si $\pi(^{2}P, ^{4}P)$ 6.2(4) 2240 1.0(11) $T_{4}^{0.50}$ 6.8(15) 6.4(3) 6.5(-8) $T_{4}^{-0.50}$ 1.5(21)	Si $({}^{3}P, {}^{1}D, {}^{1}S)$	9.1(3) 2.2(4) 1.3(4)	1.62 μm 6527 1.1 μm	$5.7(5)T_{4}^{-0.58}$ 1.4(7) $T_{4}^{-0.57}$	$3.4(10)T_4^{-0.02}$ 4.0(11)	3.6(-2) 3.7(-2) 0.8	$\begin{array}{c} 6.2(-8)T_4^{0.57}\\ 3.0(-8)T_4^{0.57}\\ 2.8(-8)T_4^{0.57} \end{array}$	$6.2(-8)T_4^{-0.13}3.0(-8)2.8(-8)$	1.5(24) 1.1(26) 5.9(23)
	Si II ( <sup>2</sup> P, <sup>4</sup> P)	6.2(4)	2240	$1.0(11)T_4^{0.50}$	6.8(15)	6.4(3)	$6.5(-8)T_4^{-0.50}$		1.5(21)