Impact of an accurate modelling of primordial chemistry in high-resolution studies

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ABSTRACT
The formation of the first stars in the Universe is regulated by a sensitive interplay of chemistry and cooling with the dynamics of a self-gravitating system. As the outcome of the collapse and the final stellar masses depend sensitively on the thermal evolution, it is necessary to accurately model the thermal evolution in high-resolution simulations. As previous investigations raised doubts regarding the convergence of the temperature at high resolution, we investigate the role of the numerical method employed to model the chemistry and the thermodynamics. Here we compare the standard implementation in the adaptive-mesh refinement code ENZO, employing a first-order backward differentiation formula (BDF), with the fifth-order accurate BDF solver DLSODES. While the standard implementation in ENZO shows a strong dependence on the employed resolution, the results obtained with DLSODES are considerably more robust, both with respect to the chemistry and thermodynamics, but also for dynamical quantities such as density, total energy or the accretion rate. We conclude that an accurate modelling of the chemistry and thermodynamics is central for primordial star formation.

Key words: astrochemistry – methods: numerical – stars: Population III – early Universe.

1 INTRODUCTION
According to the hierarchical paradigm of structure formation, the first stars are formed as a result of gravitational collapse in minihaloes of \(10^3\)–\(10^6\) \(M_\odot\) at \(z\) \(\sim\) 20–30 (Abel, Bryan & Norman 2002; Bromm & Larson 2004; Yoshida, Omukai & Hernquist 2008). The formation and masses of these stars are relevant due to their radiative, chemical and mechanical feedback on the environment (Ciardi & Ferrara 2005; Tornatore, Ferrara & Schneider 2007; Schleicher, Banerjee & Klessen 2008; Schneider et al. 2008).

While the first simulations pointed towards masses of more than 100 \(M_\odot\), more recent studies suggest efficient fragmentation in self-gravitating protostellar discs, implying that the stellar masses might be substantially reduced (Clark et al. 2011; Greif et al. 2011, 2012; Smith et al. 2011). Simulations including radiative feedback indeed suggest upper mass limits of the order of \(\sim 60 \ M_\odot\) (Hosokawa et al. 2011; Susa 2013).

As fragmentation in turbulent gas clouds depends sensitively on the thermodynamics of the gas (Li, Klessen & Mac Low 2003; Peters et al. 2012), an accurate modelling of chemistry and cooling is thus necessary. In a high-resolution study pursued with the adaptive-mesh refinement code ENZO, Turk et al. (2012) reported a strong dependence of the thermodynamics and chemistry on the resolution per Jeans length, which resulted in strong variations of physical quantities such as the radial velocities and the accretion rates. While local quantities like the detailed morphologies may indeed depend on the resolution in a turbulent self-gravitating system (Sur et al. 2010; Federrath et al. 2011; Latif et al. 2013b), radially averaged properties are typically expected to have only a minor resolution dependence. At the same time, Greif, Springel & Bromm (2013) reported only a weak resolution dependence in calculations of primordial star formation, employing the moving-mesh code AREPO (Springel 2010) and a high-order scheme for solving the chemistry and thermodynamics. Understanding the origin of this discrepancy is crucial, and in this Letter, we will demonstrate that this behaviour is closely related to the solver employed for solving the chemical network.

One of the most commonly used chemistry solvers in the context of primordial star formation is the first-order backward differentiation formula (BDF) scheme proposed by Anninos et al. (1997), which involves two central approximations aimed at reducing the computational time: (i) some of the species (e.g. \(\mathrm{H}^-\) and \(\mathrm{H}_2^+\)) are assumed to instantaneously reach the equilibrium due to their short reaction time-scales and are decoupled from the non-linear system; (ii) the thermal evolution, i.e. the cooling and the heating functions are evaluated outside the BDF scheme and are used to determine the maximum chemical time-step instead of being solved non-linearly within the BDF scheme. In the release of ENZO v2.2, we note that the second approximation was relaxed significantly by iterating
between the chemistry and cooling module on a time-step that is the minimum of the chemical and cooling time-step.

In Turk, Abel & O’Shea (2009) and Turk, Norman & Abel (2010) an improvement of the simple first-order BDF method has been presented. A TIGRESS second-order BDF solver based on a Gauss–Seidel technique including an Aitken extrapolation to accelerate convergence has been employed (Verwer 1994). All the rate equations have been solved without applying equilibrium criteria.

More sophisticated solvers have also been used in private and public versions of theFLASH code (Gray & Scannapieco 2010, 2013; Micic et al. 2012, 2013). The latter includes two higher order solvers compared to the standard BDF method: the semi-implicit multi-order Bader–Deuflhard solver (Bader & Deuflhard 1983) and the third-order Rosenbrock method (Rentrop & Kaps 1979) that while being more performant is not very well suited for a system with dimensions N > 10 (Press et al. 1992).

The hydrodynamics code ZEUS-MP (Glover & Mac Low 2007a,b; Glover et al. 2010), and cosmological codes GADGET (Jappsen et al. 2007; Clark et al. 2011) and AREPO (Springel 2010; Greif et al. 2011, 2012) employ the VODE class solvers (Brown, Byrne & Hindmarsh 1989), both in their FORTRAN (VODE) and C (CVODE) versions, which belong to the well-established ODEPACK/SUNDIALS package 1 (Hindmarsh et al. 2005) that allows us to solve stiff ordinary differential equation (ODE) systems more efficiently.

While VODE fits astrophysical problems as well, it can be inefficient when the system is represented by a sparse Jacobian. In that case, the DLSODES solver (Hindmarsh 1983), which has the capability of handling sparse matrices, is more efficient. In astrophysical applications, chemical networks frequently consist of a sparse or a very sparse Jacobian matrix (a Jacobian primarily populated with zeros). The performance of DLSODES has been already discussed in Nejad (2005), and the efficiency of the two solvers has been compared for a larger network (Wakelam & Herbst 2008) in previous studies (Grassi et al. 2012, 2013).

In this Letter, we will demonstrate the importance of choosing accurate chemistry solvers like DLSODES, and show how the latter leads to converged radially averaged profiles for physical quantities like the radial velocity or the accretion rate. The structure of this Letter is as follows. In Section 2, we describe the initial setup and our new implementation of the chemistry in the version 2.2 of cosmological code ENZO. Results for various resolutions of 16, 32, 64 and 128 cells per Jeans length are presented in Section 3. We compare our main results with earlier studies (Turk et al. 2012) and present our conclusions in Section 4.

2 NUMERICAL METHODS

The simulations are performed with the publicly available version 2.2 of the ENZO code. They are started from cosmological initial conditions generated from Gaussian random fields. Our simulations start at redshift z = 99 with a top grid resolution of 128 3 cells. Two initial nested levels of refinement are subsequently added each with a grid resolution of 128 3 cells. Our simulation box has a cosmological size of 0.3 Mpc h−1 and is centred on the most massive minihalo. In total, we initialize 5767 168 particles to compute the evolution of the dark matter dynamics and have a final dark matter resolution of 70 M⊙. The parameters for creating the initial conditions and the distribution of baryonic and dark matter components are taken from the Wilkinson Microwave Anisotropy Probe 7 yr data (Jarosik et al. 2011). We further allow additional 27 levels of refinement in the central 18 kpc region of the halo during the course of simulation. It gives us a total effective resolution of 0.9 au in comoving units. The resolution criteria used in these simulations are based on the Jeans length, the gas overdensity and the particle mass resolution. We stop the simulations once they reach the maximum refinement level. A split hydro solver with a third-order piece-wise parabolic method for hydrodynamical calculations is employed. The dark matter N-body dynamics is solved using the particle-mesh technique, and a multigrid Poisson solver is employed for the self-gravity computations.

2.1 Chemical package

In our new implementation, we adopt the scheme included in the new chemical package KROME, which will be presented in a forthcoming paper. It consists of a new chemical framework which includes accurate solvers, heating and cooling functions, rate equations routines and reduction techniques for chemical networks (see Grassi et al. 2012, 2013) that allows its applicability in a number of different astrophysical environments. All physical and computational ingredients to solve for the chemical and thermodynamical evolution come from the package and are included in ENZO through a call to the KROME routine.

The temperature is evolved alongside the rate equations and is updated at each internal solver’s time-step leading to a more accurate solution. The solver we decided to employ in the package is the DLSODES aimed at dealing with sparse Jacobian networks as the one employed in the present calculations (sparsity ~ 62 per cent).

2.2 Chemistry

We follow the non-equilibrium evolution of nine species: H, H+, H−, H2, H2+, He, He+, He2+ and e−. In total, 20 kinetic reactions have been included, the same as available with ENZO code (Turk et al. 2012). The formation of H2 is very sensitive to the choice of three-body reaction as pointed out by Turk et al. (2011b). Here we adopt the three-body rates of Abel et al. (2002) for all of our runs, both in the standard ENZO and in our KROME implementation.

The system of coupled ODEs that take into account the reactions which form and destroy the ith species is self-consistently solved within cosmological simulations. Heating and cooling include H2 formation heating/cooling due to the 3B reactions (4.48 eV per molecule) as described in Omukai (2000), H2 cooling as reported by Glover & Abel (2008), bremsstrahlung, H and He collisional ionization, excitation and recombination cooling as given by Cen (1992). The temperature change due to the heating and cooling is calculated as

$$\frac{dT}{dt} = \frac{\nu - 1}{k_B \sum_n n_i} (\Gamma - \Lambda) \text{ K s}^{-1}.$$  

which is integrated simultaneously with the chemical rate equation both in KROME and ENZO 2.2.

3 RESULTS

In all, we have carried out eight simulations to study the thermal evolution of minihaloes which are potential sites for the formation of the first stars. We compare our new implementation with the one employed in ENZO 2.2. The Jeans resolutions of 16, 32, 64 and 128 cells (hereafter called J16, J32, J64 and J128 for standard runs, and
KJ16, KJ32, KJ64 and KJ128 for KROME were mandated throughout the evolution of the simulations. The abundances of various chemical species for different Jeans resolutions are shown in Fig. 1 both for KROME and ENZO 2.2. On a qualitative level, the results from both solvers approximately follow our expectations. In particular, the electron density shows a characteristic power-law decrease towards high densities, while the H$_2$ abundance grows significantly at densities of $\sim 100$ cm$^{-3}$ and again at densities of $\sim 10^{10}$ cm$^{-3}$ due to the three-body reactions. However, the results obtained with the ENZO 2.2 implementation show a significant amount of variation, while the KROME results are close to each other and show a considerably improved convergent behaviour. We note that the J64 and J128 runs in the ENZO 2.2 implementation were stopped earlier due to non-convergence in the chemical solver while our results reached higher densities. For the sake of clarity, the final results are plotted for the same peak density allowing a more consistent comparison between the different runs.

The dynamical quantities for the same peak density are shown in Fig. 2. The density profiles follow an almost isothermal behaviour and are similar for various runs. Larger differences are present in the ENZO 2.2 runs, in particular at densities above $10^6$ cm$^{-3}$ due to the discrepancies in the H$_2$ and electron abundances. The KROME results, on the other hand, are almost identical. Consequently, the total energy and accretion rates are similar for different resolutions, but relatively large variations are found for the ENZO 2.2 runs. Overall, better convergence is found for the radial velocity in KROME, even though we note a small deviation in the J128 run, where the radial velocity is slightly higher. The rotational velocities are about 1 km s$^{-1}$ for all runs at radii larger than 0.1 pc. The variations in the centre may arise due to the differences in the morphologies, as we always expect some fluctuations in turbulent self-gravitating systems.

Fig. 3 shows the density distribution, temperature and the H$_2$ abundance for our highest resolution run (i.e. KJ128). It is noted that the H$_2$ abundance largely follows the density, and also the temperature reflects the underlying density field. Due to the large density range shown here, the density distribution shows only minor deviations from spherical symmetry, as the global collapse dynamics are dominating the evolution. Clear deviations from spherical symmetry and signs of rotation can however be recognized in the temperature, as the overall contrast between high-density and low-density regions is now decreased. Similar features can be seen in the H$_2$ abundance, which is however increasing towards the central core.

We focused here on ENZO 2.2 for illustrative purposes, but note that we performed additional tests with ENZO versions 2.0, 2.1, 2.2 and 3.0 (still in development). Their overall behaviour is quite similar, implying a temperature drop above some critical resolution. ENZO 3.0 appears to be slightly more stable up to a resolution of 64 cells per Jeans length, but shows a similar behaviour at higher resolution.

4 DISCUSSION AND CONCLUSIONS

Overall, our results suggest significant improvements in the convergence behaviour when the high-order DLSODES solver implemented in the KROME package is employed for the ENZO simulations. We then relate the non-convergent behaviour reported by Turk et al. (2012) to the first-order BDF method. In addition, our results agree with the findings by Greif et al. (2013), who also employed a higher order accurate method for the chemistry. We thus conclude that an accurate modelling of the chemistry is crucial for high-resolution studies of primordial star formation.

We expect the latter to be particularly relevant in situations of strong cooling, i.e. where the temperature changes significantly with density. This effect can be further enhanced in the presence of metals or dust (Omukai et al. 2005; Schneider et al. 2006; Dopcke et al. 2013) and also in situations where H$_2$ cooling is initially suppressed by photodissociating backgrounds, but becomes relevant at higher densities (e.g. Shang, Bryan & Haiman 2010; Schleicher, Spaans & Glover 2010; Latif, Schleicher & Spaans 2012).

As previous studies pointed towards a need of high resolutions per Jeans length for an accurate modelling of turbulence and turbulent fragmentation (Sur et al. 2010; Federrath et al. 2011; Turk et al. 2012; Latif et al. 2013a,b), we here highlight the importance of using high-order BDF methods such as DLSODES for modelling the chemical evolution. The package KROME will be published in a companion paper, including a general framework to construct

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Figure 1. Chemical species mass fraction for different resolutions. Both original ENZO (marked as J) and our new implementation (marked as KJ) results are shown. From the top-left to bottom-right panels: molecular hydrogen, atomic hydrogen, electron and H$^+$ fractions.
Figure 2. Spherically averaged radial profiles of the eight simulations taken at roughly the same peak density. Upper left shows the total density in g cm$^{-3}$, upper right shows the temperature in K, middle left shows the accretion rate in M$_{\odot}$ yr$^{-1}$, middle right shows the radial velocity in km s$^{-1}$, bottom left shows the total energy density in erg g$^{-1}$ and bottom right shows the rotational velocity in km s$^{-1}$. Note that radial and rotational velocities have been evaluated subtracting the bulk velocity (for details, see Latif et al. 2013a).

Figure 3. The slices for the density (left-hand columns), temperature (middle columns) and molecular hydrogen mass fraction (right-hand columns) for the KJ128 run are shown at fields of view of 0.1 and 2000 au from the top to bottom.

chemical networks, specific examples and code interfaces, and will be released for the public use.

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