Simulating the enrichment of cosmological gas: incorporating a new chemical enrichment model in Simba

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Abstract. Large-scale, state-of-the-art cosmological simulations allow us to follow the evolution of various galaxies, and since these contain detailed knowledge of e.g. the metal content of the stars in each galaxy, it can then be compared to galaxies in the real Universe. In our work, we are improving the implementation of a stellar feedback model for the cosmological simulation Simba. This simulation is the merged product of GIZMO's public and Mufasa/Simba codes to create realistic large-scale environments. Specifically, we are improving the current instantaneous recycling of the metals model, with a more accurate cosmic chemical enrichment, called the Chem5 model. This will improve the stellar evolutionary tracks, allow the tracing of more individual elements, and treat each gas particle as an evolving particle rather than instantaneously giving away its metals. This will lead to a better understanding how the metallicities impact the gas and stellar metallicities in galaxies and the Circumgalactic medium.

1. Introduction

In modern large-scale structure cosmology, there is a drive to understand the formation and the evolution of galaxies, based on their environment. However, due to the extremely long time-scales over which these events occur, it can become very difficult to understand their evolutionary paths [1]. Therefore, trying to create an evolutionary track can be incomplete. There are two main methods used to get an idea about these evolutionary paths.

The first method is statistical observations. The idea behind this method is to get observational data from as many sources as possible [1]. These sources will need to have similar properties. For example, observing a certain mass galaxy with a certain star formation rate. Since their basic key properties are the same, it is assumed that their evolutionary track will be the same. If they are formed at different epochs in the cosmic age, they will be at different stages in their evolution. We can then use each object's evolution point to create an evolutionary track. However, this method can lead to gaps being formed in this track if there is a lack of observational data [1]. Therefore, trying to come to conclusions about their evolution can lead to a distorted view of how they form and evolve.

The second method is to use cosmological computer simulations [1, 2, 3]. By this we mean, create a simulated galaxy, by using physics laws. The basic idea is that you start with the initial conditions of the Universe (or a certain volume of it), namely those suggested by the Cosmic Microwave Background (CMB) radiation, and the computer simulation will evolve this mock

Universe, galaxy, stars, accounting for physics. It does this by evolving gas, stellar and dark matter particles through time, while determining how they interact with each other.

In this work we will be looking specifically at the second method. We are incorporating a new metal-enrichment model into one of these cosmological simulations to improve the metal production in certain events that will occur with these particles. This will enable us to better understand the star formation histories, since these simulations can enable a detailed data analysis of each particle's metal component and how it evolved.

1.1. Cosmological simulations

Before we can discuss this new model's functions and which simulation we will be using, we need to understand how these simulations work. The first step is the initial conditions, i.e. the CMB. Then we need physics models. These models include [1, 2]:

- Gravity $\sim$ Gravity solvers are needed, since they control the formation of large-scale objects, structure, halos and mergers. Fundamentally, these models need to be able to determine the force on each mass element from all others by solving Poisson's equation. After computing the gravitational forces on these particles the system evolves forward in discrete time-steps.
- Hydrodynamics $\sim$ Solving the equations of hydrodynamics is required for modelling gas particle interactions. This needs to be solved concurrently with the gravity solver. There are two main methods: Firstly, the Lagrangian method, for example the Smoothed Particle Hydrodynamics (SPH) and the Meshless Finite-Mass (MFM) solvers, where the particles themselves carry the information about the fluid, which is obtained via a kernel-weighted sum over neighbouring particles. Secondly, the Eulerian method is where you discretize the fluid onto grid cells and then compute the advection of properties across the cell boundaries.
- Thermal evolution $\sim$ Radiative cooling and photo-ionization heating of the gas particles via radiative processes found in baryons.
- Chemical evolution $\sim$ Tracking the enrichment of heavy elements in gas particles are required for the cooling calculations, as well as for predictions of galactic chemical evolution. Early models tracked only Type II supernovae (SN) enrichments due to its relation with the Oxygen abundance. Later models also track asymptotic giant branch (AGB) stars, since they are required to understand the abundances of Carbon (their ejecta dominate the present-day Carbon observations), while Type Ia SN models are required to produce Iron.
- Sub-grid/sub-resolution models $\sim$ These are processes which occur on scales smaller than the resolution of a single grid space and therefore, cannot be directly modelled. They are treated using heuristic models. For example, two of many different sub-grid models are [3]:
  - Star and black hole formation $\sim$ The accumulated gas particles due to gravity, must be able to create stars and black holes to be able to form galaxies.
  - Feedback processes $\sim$ These models are required to re-heat the cooling flow gas particles. The reason for this re-heating is due to the fact that cooling gas particles form stars, since it is observed that stars form in the dense, cold, molecular phase of the interstellar medium (ISM). So if the gas continues to cool it will form stars at an increasing rate. However, it is observed that at around $z \sim 2$, namely Cosmic High Noon, this star formation rate is at its highest and is quenched after this epoch [4]. It is, therefore, assumed that some feedback processes re-heat the gas. Feedback consist out of two general classes, preventive (stopping the gas from accreting into the ISM) and ejective (removing gas from the ISM after it has been accreted). Some feedback processes are: Photo-ionization suppression, star formation via stellar winds or supernovae, and Active Galactic Nuclei (AGB) feedback from black holes.

1.2. Observational confirmation

All of the aforementioned models will be used to evolve the initial conditions into a "Mock Universe". This simulated Universe's properties can then be compared to known global and structural properties to determine whether or not the simulation was successful in creating a "realistic approximation" of the Universe [2]. These observational tests include testing the global distribution functions, which refers to the comoving number density of galaxies as a function of global properties, such as luminosity or stellar mass. Some known distribution functions are the colour-luminosity function which tells us whether a galaxy is star forming (blue cloud - younger stellar populations) or are quiescent (red-sequence - older stellar populations).

Other observational tests include global scaling relations, such as the mass-metallicity relation (galaxies with a given mass has a lower gas-phase metallicity at high redshift) or structural scaling relations, such as the correlation of galaxies' stellar mass with their radial size. We can also test the simulated galaxy's demographics against known galaxy morphology.

Taking all of these into account there is an abundance of different global and structural property tests that we can use to determine whether the simulation succeeded. Other global and structural property tests are further discussed in-depth in [1, 2, 3].

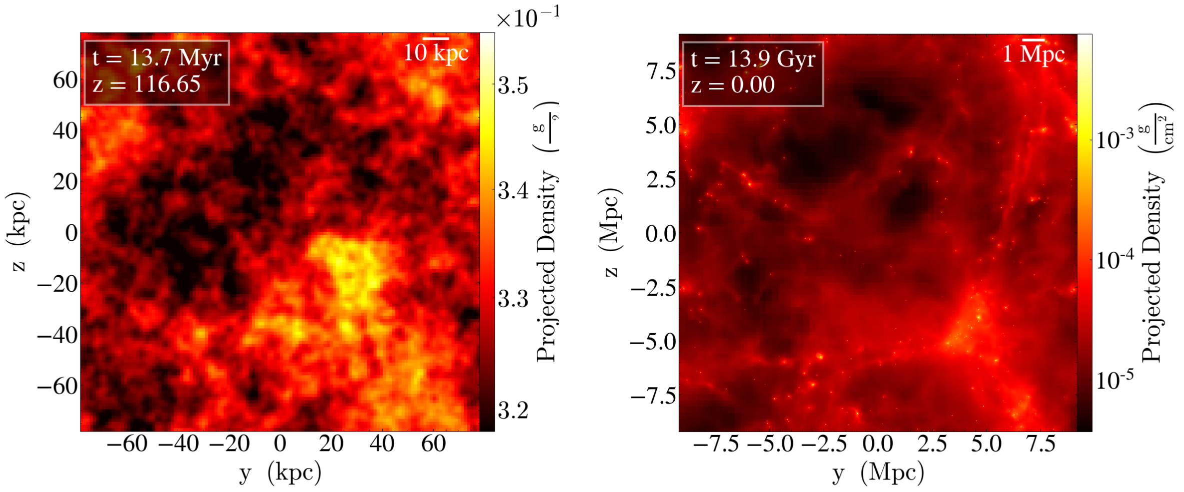
2. The Simba simulation

2.1. GIZMO-Simba

From the description above, it follows that there is a lot of preparational work to create this type of simulations. Therefore, we will not be creating a new simulation from scratch, but rather improve on a current simulation. There exist a lot of different cosmological simulations, each trying a different approach to solving this problem. According to [1], these simulations can be separated into four different categories: 1) Zoomed simulation/dark matter-only e.g. Aquarius simulation, 2) Zoomed simulations/dark matter + baryons e.g. FIRE simulation, 3) Large volume/dark-matter only e.g. Millennium simulation, and lastly 4) Large Volume/dark matter + baryons e.g. Simba simulation. In this categorization it comes down to whether only gravity models are needed for dark matter halos, or whether hydrodynamics are also needed for the baryonic particle interactions. A simulation best suited to the problem should be chosen. This will also determine which known global and structural observational tests can be used to test the simulation.

Since we want to look at how a new metals production model improves the current simulation, we would firstly need baryons. Secondly, we want to see whether it improves our current statistics, therefore the 4th category. Specifically, we will be using the Simba simulation developed by [5]. There are other simulations in this category e.g. EAGLE, Illustris, Romulus25, that we also could have used. The Simba simulation is the successor of the Mufasa simulation [6] and gives updated sub-resolution star formation and feedback models. The Simba simulation consists out of 2 different components, namely GIZMO (a cosmological gravity plus hydrodynamics MFM solver [7]) and Simba. GIZMO is based on the simulation "GAlaxies with Dark matter and Gas intEracT 3" or GADGET3 [8] and it evolves dark matter and gas elements together. In essence this is the backbone of Simba, since it controls the large-scale structure formation and particle interactions.

The second component, namely Simba itself controls the sub-grid/resolution models as discussed in section 1.1. Therefore, Simba will control the star and black hole formation (just two of many different processes) and the way they interact with their environments. Even though chemical/thermal evolution is part of the hydrodynamics part of the simulations, they are also controlled via Simba, since for example a SN occurs, metals and energy are produced on this sub-resolution scale and then distributed through the entire system. In figure 1, we show a small volume example run based on the default parameter values for the Simba simulation.



(*a*) (*b*)

Figure 1. GIZMO-Simba simulation [5] at 2 different epochs ($z \sim 116, 0$) displaying the large-scale evolution of a 12.5 Mpc volume box size and a resolution of 128^3 particles. *(a)* Contains mostly diffused cooling gas left over from the Big Bang. *(b)* At present day these gas particles are accumulated through gravity to form the large-scale structure, called the "Cosmic Web".

2.2. Chem5 metals model

From figure 1, it is clear that the large-scale structure component of the simulation do in fact represent a realistic idea of the large-scale evolution. So we do not want to change this part of the simulation, rather improve the small details in the metals production. You may ask why the metal production? The answer comes down to the fact that the chemical enrichment evolution of the gas particles influences the formation of stars and how they evolve, since it mediates how efficiently gas cools by impacting the stellar metallicities in galaxies and the Circumgalactic medium, and therefore influencing the following generation of stars being formed [9]. Therefore, we need to be able to accurately simulate the metal production to create more realistic galaxies.

However, due to the computationally expensive nature of these simulations, assumptions are made [5]. For example, in Simba only 11 elements (H, He, C, N, O, Ne, Mg, Si, S, Ca, Fe) are tracked from SN Ia/II and AGB stars. This still results in a somewhat "realistic" galaxy formation, since more that 90% of the Universe's metal mass come from these 11 elements and they are the most important elements in star formation and feedback systems. Furthermore, Simba uses an instantaneous recycling of the distributed metals approximation. Therefore, we would want to add more elements into the system to obtain knowledge about how the less abundant elements influence the star formation histories, while also wanting to remove the instantaneous recycling of the distributed metals approximation.

This is where the Chem5 model comes in to play. The Chem5 model was developed by [10] and continued improvements since [11], and it is a self-consistent 3D Chemodynamical model. This model can track 32 elements (H, He, Li, Be, B, C, N, O, F, Ne, Na, Mg, Al, Si, P, S, Cl, Ar, K, Ca, Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Ga, Ge), meaning that we can obtain a much more detailed description on how the metals influence the formation and evolution of the stars. This model also does not use the instantaneous recycling approximation method, rather treating each star particle as evolving stellar population which eject thermal energy, gas mass and heavy elements from stellar winds, SN Ia, SN II and Hypernovae (HNe) (previously not taken into account) as a function of time [10]. Other physical processes that it takes into account are radiative cooling, star formation, and photometric evolution.

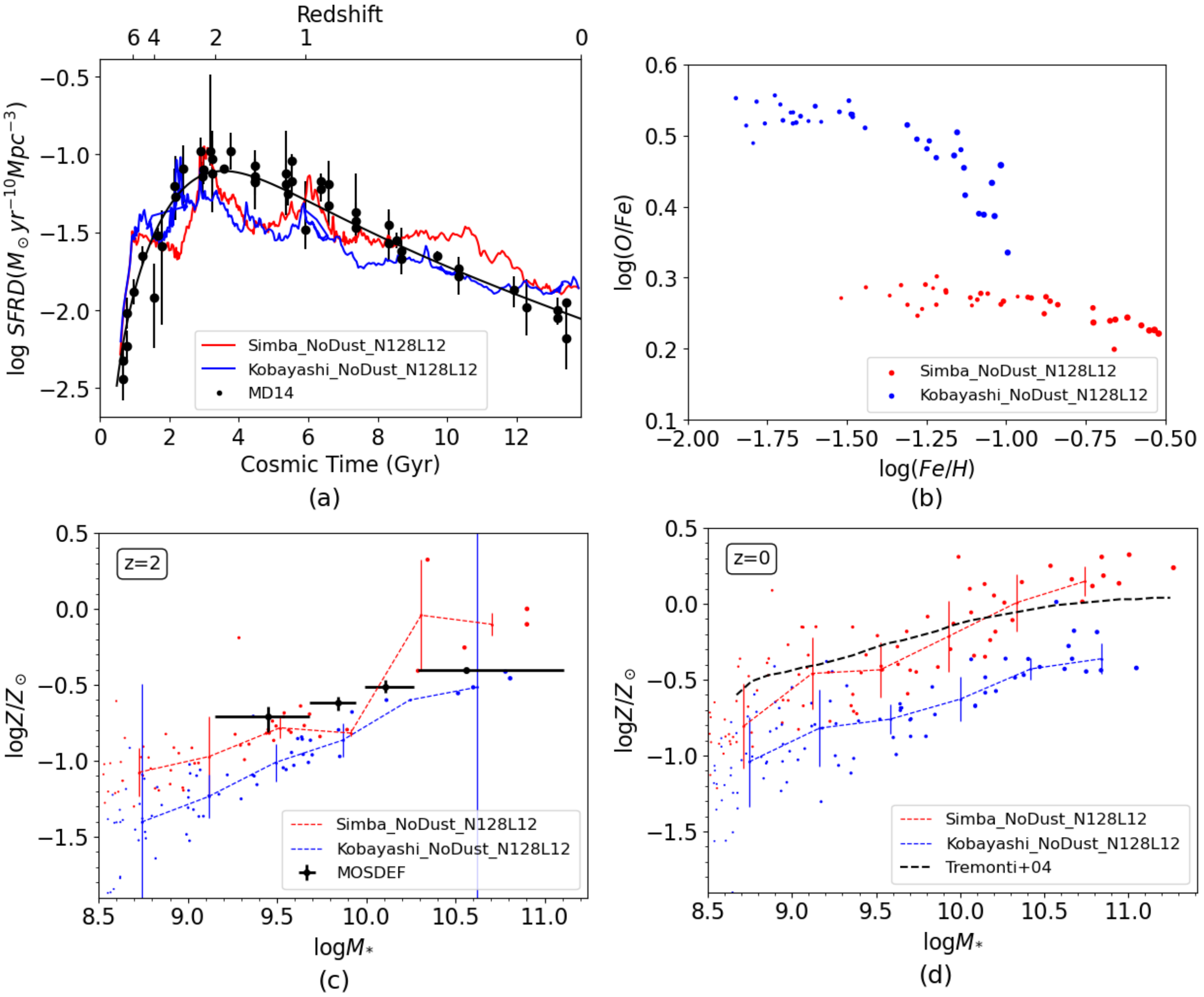


Figure 2. In *(a)*, we show the star formation rate over the Cosmic Time. We compare both the resultant simulations for the Simba instantaneous model (*red*) and the Chem5 model (*blue*) against observations from [4]. In *(b)*, we show the chemical abundance ratio's for the galaxies in the samples. In *(c)* and *(d)*, we show the mass-metallicity relation evolution from these simulated galaxies and compare it to the observation made by [12] as part of the MOSDEF survey and [13]. It should be noted that all three these tests were done without the dust models.

2.3. Simba simulation with the new metal production model

For this work, we incorporated this new metals model into the Simba simulation without disrupting the current set-up. We had to create the program in such a way that the user can still use the old instantaneous model if they do not have a need for accuracy in the chemical enrichment of the gas particles and therefore helping with the computationally expensive nature of these simulations. We had to take into account that events can happen across different computer nodes, therefore just looping through all neighbouring particles that will receive the distributed metals, will lead to the same "event" needing to be calculated more than once, leading to the ejected energy/mass/metals being erroneously subtracted more than once. At this stage we are also not yet including the dust models from the Simba simulation, since it requires information about the metallicity structure. We will incorporate this after the integration phase. We present three early integration phase test plots to show the state of the integration in figure 2. This is once again for the 12.5 Mpc volume box size and a particle resolution of 128^3. We also compare it to some well known observations, as well as against the original Simba simulation.

In figure 2, the star formation rates between simulations are similar, with the chem5 function obtaining a slightly more favourable comparison to the data. We also see in the abundance ratio graph that only the chem5 function obtained the know platau of 0.5 and the "*bend*" close to -1 [11]. This is an improvement over Simba. But the Chem5 model still struggles with the total metallicity values, being under the observations and Simba in the mass-metallicity relation. Therefore, the integration phase is not yet complete.

3. Conclusions and future work

In this work, we introduced different ways to determine the evolutionary paths of celestial objects, such as galaxies, namely statistical observations and computer simulations. We then had a more in-depth look into how to create these computer simulations. We also discussed the Simba simulation and how we can use it for the research that we want to achieve. We briefly discussed the new Chem5 model and how it improves on the simplified nature of the current instantaneous recycling of the metals model in the Simba simulations. We then showed some integration phase plots, namely the star formation rate graph and the mass-metallicity relation plot. Both were compared to the Simba simulation and to observations.

For future work, we can see from figure 2, that some improvements are still necessary, but we are in a position to start incorporating the Chem5 model to work concurrently with the dust models and hopefully this will improve some of these results. We do have at least one improvement over Simba already, with the top R. H. S. panel obtaining [O/Fe] $\sim$ 0.5, which is much closer to the observed values than Simba, but the "*bend*" that it obtained at [Fe/H] $\sim$ -1.3 is yet not correct and it should be closer to -1.

For future science applications, we can e.g. study the less abundant elements, look at the mass-metallicity relation's evolution for these new elements, or we can also track the metallicity of the intragroup and intracluster gas more accurately due to the larger element sample, which can give us clues into their formation history. We can also look at the detailed chemical abundances (e.g. alpha-enhancements) in the galaxies to better understand the star formation timescales. We will use papers like [5] to test improvements over Simba.

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