

FIREbox: Simulating galaxies at high dynamic range in a cosmological volume

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ABSTRACT

We introduce a suite of cosmological volume simulations to study the evolution of galaxies at high numerical resolution as part of the *Feedback in Realistic Environments* project. FIREbox, the principal simulation of the present suite, provides a representative sample of galaxies (~ 1000 galaxies with $M_{\text{star}} > 10^8 M_{\odot}$ at $z = 0$) at a resolution ($\Delta x \sim 20$ pc, $m_b \sim 6 \times 10^4 M_{\odot}$) comparable to state-of-the-art galaxy zoom-in simulations. Furthermore, FIREbox captures the multiphase nature of the interstellar medium in a fully cosmological setting ($L = 22.1$ Mpc) thanks to its exceptionally high dynamic range ($\gtrsim 10^6$) and the inclusion of multi-channel stellar feedback. Here, we focus on validating the predictions of FIREbox by comparing to observational data. We find that, at a given stellar mass (for $M_{\text{star}} < 10^{10.5-11} M_{\odot}$), simulated galaxies have star formation rates, atomic and molecular gas masses, gas phase and stellar metallicities in broad agreement with observations. In addition, FIREbox shows that these galaxy scaling relations extend to the low mass regime ($M_{\text{star}} \sim 10^7 M_{\odot}$) and follow a (broken) power-law relationship. Also reproduced are the evolution of the cosmic H_I density and the H_I column density distribution at $z \sim 0 - 5$. At low z , FIREbox predicts a peak in the stellar-mass–halo-mass relation, but also a higher abundance of massive galaxies and a higher cosmic star formation rate density than observed, showing that stellar feedback alone is insufficient to reproduce the properties of massive galaxies at late times. Given its high resolution and sample size, FIREbox offers a baseline prediction of galaxy formation theory in a Λ CDM Universe while also highlighting modeling challenges to be addressed in next generation galaxy simulations.

Key words: galaxies: evolution – galaxies: ISM – galaxies: stellar content – galaxies: star formation – methods: numerical

1 INTRODUCTION

High-resolution galaxy surveys, e.g., with MUSE (Bacon et al. 2010; Emsellem et al. 2022), ALMA (Fomalont et al. 2015; Leroy et al. 2021a), and soon JWST (Gardner et al. 2006), ELT (Gilmozzi & Spyromilio 2007), and SKA (Hall 2007) are promising to transform our understanding of how galaxies form and evolve. These observational advances will benefit from matched theoretical studies that quantify how the relevant (astro-)physical processes operating on sub-kpc scales shape the properties of galaxies and their interstellar medium (Somerville & Davé 2015; Naab & Ostriker 2017). This goal of galaxy theory is best approached with numerical simulations

given the complexity, interconnectedness, and multi-scale nature of the involved physics (e.g., Vogelsberger et al. 2020).

In the past, two main approaches have been employed to simulate the evolution of galaxies in a proper cosmological context. Cosmological volume simulations provide large samples of galaxies with a broad range in properties residing in a variety of cosmological environments (e.g., Dubois et al. 2014; Vogelsberger et al. 2014; Schaye et al. 2015; Khandai et al. 2015; Dave et al. 2016; Pillepich et al. 2018a; Davé et al. 2019). Here, physical processes are usually modeled in a simplified, parametrized manner and at a comparably low numerical resolution, e.g., the scale heights of disk galaxies (~ 100 pc) are typically unresolved. Furthermore, by modeling the relevant physics, especially the effects of stellar feedback (Mayer et al. 2008; Scannapieco et al. 2012; Crain et al. 2015), on a sub-grid scale, the predictions of the simulations are highly susceptible to model degeneracies. The alternative option are cosmological zoom-in simulations

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which can reach higher numerical resolution thus enabling them to model baryonic processes in the interstellar medium (ISM) on a more physical basis (e.g., Guedes et al. 2011; Hopkins et al. 2014; Ceverino et al. 2014; Feldmann & Mayer 2015; Agertz & Kravtsov 2015; Wang et al. 2015; Wetzel et al. 2016; Bellovary et al. 2019). Primary drawbacks of the zoom-in approach are the resulting much smaller sample sizes and/or higher computational costs.

Combining the strengths of both approaches offers the prospect of providing large samples of highly-resolved, realistic galaxies that can then be compared with high-resolution observations to constrain galaxy theory. Recently, first efforts have been undertaken in this direction. These approaches differ in many aspects, e.g., in the implementation and calibration of the baryonic physics and in the numerical method of solving the underlying system of equations.

One general option is to run a large collection of high-resolution zoom-in simulations of individual galaxies (or small groups thereof) to increase samples sizes (e.g., Wang et al. 2015; Sawala et al. 2016; Feldmann et al. 2016; Grand et al. 2017; Hopkins et al. 2018; Kruijssen et al. 2019). While a powerful method, this approach also has a number of severe shortcomings, e.g., potential selection biases, limited large scale correlations, and the contamination of the refinement region, that limit its applicability. Instead, the approach of the NEWHORIZON zoom-in simulation (Dubois et al. 2021) is to resolve an ensemble of galaxies in a large refined patch of $\sim (16 \text{ cMpc})^3$. NEWHORIZON is run down to $z = 0.25$ with the adaptive mesh refinement code RAMSES (Teyssier 2002) and makes use of a heavily modified version of the physical model of the HORIZON-AGN simulation (Dubois et al. 2014; Volonteri et al. 2016; Kaviraj et al. 2017). High numerical resolution and the modeling of low temperature cooling enable NEWHORIZON to partly resolve the multiphase nature of the ISM.

An alternative approach is to increase the resolution of cosmological volume simulations and improve the employed physical modeling. One advantage of using cosmological volumes over large zoom-ins is that the former can be analyzed more straightforwardly given that the high-resolution region spans the entire cubic volume thus eliminating contamination artifacts.

The TNG50 simulation (Nelson et al. 2019b), run with the moving mesh code AREPO (Springel 2010), applies the IllustrisTNG physics model (Pillepich et al. 2018a) to a $(51.7 \text{ cMpc})^3$ cosmological box providing a sizable sample of galaxies at a mass resolution (baryonic particle mass $m_b \sim 9 \times 10^4 M_\odot$) similar to many zoom-ins. Originally calibrated for large volume simulations (Pillepich et al. 2018b; Nelson et al. 2019a), the physics model of TNG50 accounts for many baryonic processes in an idealized manner, e.g., the multiphase structure of the ISM is not directly resolved, star formation often takes place in low density gas ($n \geq 0.11 \text{ cm}^{-3}$), and galactic outflows are put in by hand and temporarily decoupled from the hydrodynamics.

The ROMULUS25 simulation (Tremmel et al. 2017), run with the smoothed particle hydrodynamics solver CHANGA (Menon et al. 2015), partly addresses some of these shortcomings by adopting a physics model used previously in a large number of high-resolution zoom-in simulations (e.g., Governato et al. 2007, 2010; Shen et al. 2010; Guedes et al. 2011) and by applying it, after re-tuning of some of the model parameters, to a $(25 \text{ cMpc})^3$ cosmological box with a mass resolution of $m_b \sim 2 \times 10^5 M_\odot$. Specifically, ROMULUS25 includes lower temperature gas cooling and a more physical driving of galactic outflows via localized supernova explosions. However, in this model the cooling time of gas heated by supernova feedback is artificially prolonged (Stinson et al. 2006). Furthermore, ROMULUS25 does not attempt to trace the dense, star forming (usually molecu-

lar) component of the ISM and thus does not properly model the distribution of star formation and stellar feedback in galaxies.

While these recent simulations undoubtedly demonstrate significant progress, a potential concern is the existence of model degeneracies given that their underlying physical models both differ starkly and, in the case of TNG50 and ROMULUS25, are calibrated to observational data. One particularly promising, but challenging, path towards increasing the predictive power of galaxy simulations is to aim for a full accounting of well understood physical processes with only a minimal number of (ideally zero) tunable parameters. Implementing this research direction requires a sufficiently high dynamic range to model the relevant physical processes in a fully cosmological context. For instance, identifying the sites of star formation requires a resolution better than a few tens of pc while cosmological accretion and gravitational tides involve scales of tens of Mpc. Furthermore, the adopted physical model should be sufficiently realistic and comprehensive, e.g., the different ISM phases should be reproduced and stellar feedback modeled with as few assumptions as possible. Finally, a sufficiently large (and preferably unbiased) sample of highly-resolved galaxies is needed to compare with observational data across cosmic history.

Fortunately, following this path has now become feasible given the increased computing capacity of supercomputers and algorithmic improvements in modeling galaxies numerically. Most critical, however, is the recent development of more accurate galaxy models that account for the relevant baryonic processes based on physical principles and that minimize the use of ad hoc parametrization (e.g., Hopkins et al. 2011; Agertz et al. 2013; Hopkins et al. 2014; Semenov et al. 2016; Kim & Ostriker 2017; Li et al. 2017; Hopkins et al. 2018; Marinacci et al. 2019; Kim et al. 2020; Hopkins et al. 2022). In particular, the detailed accounting of stellar feedback sources has shown to be paramount for producing galaxies in zoom-in simulations with more realistic properties, e.g., flatter rotation curves, lower stellar masses, and larger mass loading factors of galactic outflows (Guedes et al. 2011; Hopkins et al. 2014; Muratov et al. 2015; Applebaum et al. 2021).

As a first step on this challenging path, we have designed and run the FIREbox suite of cosmological volume simulations as part of the *Feedback in Realistic Environments* (FIRE) project¹ (Hopkins et al. 2014, 2018, 2022). The primary simulation (FIREbox) of this suite improves over current state-of-the-art in two important aspects. First, FIREbox evolves a cosmological volume of $(22.1 \text{ cMpc})^3$ down to $z = 0$ using a baryonic physics model without explicitly tuned sub-grid parameters. This model (FIRE-2, Hopkins et al. 2018) has been used previously in cosmological zoom-in simulations (e.g. Anglés-Alcázar et al. 2017b; Chan et al. 2018; Ma et al. 2018, 2019; Stern et al. 2021a; Pandya et al. 2021) but it has not yet been applied to cosmological volumes. Secondly, FIREbox achieves a dynamic range of $\sim 10^6$, which is about an order of magnitude higher than TNG50, NEWHORIZON, and ROMULUS25, see section 2.4. The corresponding high spatial resolution ($\sim 20 \text{ pc}$) coupled with the more accurate physical modeling and representative sample size makes FIREbox a unique data set to explore the internal structure of galaxies across cosmic time. FIREbox is thus well suited to both studying the properties of typical galaxies, e.g., the link between galaxy size and dark matter (DM) halo properties (Rohr et al. 2021) or the atomic gas scale heights of Milky-Way analogs (Gensior et al. in prep), to exploring rare galaxy populations, such as low mass, DM deficient galaxies (Moreno et al. 2022) or starburst galaxies

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(Cenci et al. in prep), and to quantifying the properties of the circumgalactic and intergalactic medium. Furthermore, it can be used as a training set for machine learning based emulators, e.g., to predict the distribution of atomic hydrogen on large scales (Bernardini et al. 2022).

We highlight the high dynamic range of the simulation in the bottom row of Fig. 1. FIREbox can model both structures on cosmological scales as well as hydrodynamical processes within the dense interstellar medium. Fig. 1 also visualizes the distribution of the various matter components in FIREbox. The top row shows the distribution of DM and star particles in the simulation volume at different redshifts, highlighting the formation and subsequent growth of large scale structure. This cosmic web consists of over-dense clusters of DM as well as filaments, sheets, and voids arranged in a complex pattern (e.g., Peebles 1980; Klypin & Shandarin 1983; Davis et al. 1985). Much of the DM in the cosmic web gravitationally collapses into virialized DM halos which then attract gas from their cosmic environments (middle row). Subsequently, stars and galaxies form at the halo centers (White & Rees 1978).

A particular feature of the physics-based approach that we follow in this paper is that we intentionally exclude feedback from active galactic nuclei (AGNs) given the large uncertainties involved in its physical modeling. The FIREbox simulation should thus be understood as providing baseline predictions in the absence of AGN feedback. Discrepancies between simulation predictions and observations can then be used to make inferences about the role of AGN feedback in galaxy theory. For instance, we will find that while AGN feedback may be necessary to create massive, quenched galaxies, it appears to have little impact otherwise on the global scaling relations of star-forming galaxies. We leave a detailed analysis of the role of AGN feedback to future work (see Wellons et al. 2022 for a first exploration of the effects of AGN feedback in a large suite of FIRE-2 zoom-in simulations).

The outline of this paper is as follows. In section 2 we introduce our suite of cosmological volume simulations, including its set-up, the numerical modeling, and various aspects of our post-processing analysis. Subsequently, we focus on the primary simulation (FIREbox). We discuss basic properties of FIREbox galaxies, including various galaxy-scaling relations, in section 3. Subsequently, in section 4, we analyze the evolution of the cosmic star formation rate density, the cosmic gas density, and the column density distribution function of atomic and molecular hydrogen. We summarize our findings in section 5.

2 METHODOLOGY

2.1 Initial conditions

In contrast to previous FIRE simulations, the FIREbox suite does not use the zoom-in approach to study galaxy evolution but rather it simulates gas, stars, and dark matter in a cubic cosmological volume of $V = (15 \text{ cMpc } h^{-1})^3 \sim (22.1 \text{ cMpc})^3$ with periodic boundary conditions. Initial conditions for all simulations in the FIREbox suite were created with the MUlti-Scale Initial Conditions tool (MUSIC)² (Hahn & Abel 2011). Cosmological parameters were taken from Planck-2015 cosmic microwave background measurements combined with baryon acoustic oscillation data as well as supernova and cepheid observations, see (Planck Collaboration et al. 2015): $\Omega_m = 0.3089$, $\Omega_\Lambda = 1 - \Omega_m = 0.6911$, $\Omega_b = 0.0486$, $h = 0.6774$,

$\sigma_8 = 0.8159$, $n_s = 0.9667$. Transfer functions for baryons, cold DM, and total matter were calculated for the same cosmology via the Code for Anisotropies in the Microwave Background (CAMB)³ (Lewis et al. 2000) with $z_{\text{init}} = 120$ as starting redshift.

The specific initial conditions for the FIREbox suite were chosen by first running a suite of 27 low-resolution (128^3) dark-matter-only (DMO) N -body simulations of the chosen volume. Subsequently, one of the DMO boxes was selected and corresponding higher-resolution initial conditions with and without baryonic matter were created. The objective of this manual selection was to obtain a realization of the halo mass function that is close to average for most redshifts. In addition, the selection was weighted towards boxes that do not contain a halo of exceptionally high mass at $z = 0$ to avoid the associated higher computational cost and to reduce cosmic variance.

2.2 Gravity and baryonic physics

The selected cosmological volume was evolved down to $z = 0$ both with and without baryonic physics with the combined hydrodynamics and gravity solver GIZMO⁴ (Hopkins 2015). GIZMO calculates gravitational forces between particles with a heavily modified version of the tree gravity solver of GADGET-3 (Springel 2005; Springel et al. 2008) and it models hydrodynamical processes with the meshless-finite-mass (MFM) method (Hopkins 2015).

Baryonic processes, such as gas cooling and heating, star formation, and stellar feedback, are accounted for via the FIRE-2 physics model (Hopkins et al. 2018). Supermassive black holes and AGN feedback are not included, see below. We now briefly review the most important details of the FIRE-2 model.

The temperature of the gas is calculated over the $T \sim 10 - 10^{10}$ K range by modeling free-free, Compton, photo-electric, photo-ionization, metal-line, molecular, fine-structure, dust collisional, and cosmic ray heating (but not cosmic ray transport) and/or cooling processes both from local sources and from a redshift dependent, spatially uniform ultraviolet background (Faucher-Giguère et al. 2009). The simulations follows 15 species (H, He, C, N, O, Ne, Mg, Si, S, Ca, Fe, and 4 tracker species for r -process elements) and includes sub-grid metal diffusion from unresolved turbulence (Su et al. 2017; Escala et al. 2018). Each gas particle starts with a metallicity of 2×10^{-6} , i.e., about 10^{-4} solar. Metal ionization states are tabulated via CLOUDY (Ferland et al. 1998). Self-shielding from both local sources and the cosmic UV background is accounted for via a Sobolev-length approximation based on the density gradient calibrated on radiative transfer experiments (Gnedin et al. 2009; Faucher-Giguère et al. 2010; Rahmati et al. 2013).

Star formation takes place in self-gravitating, dense ($n \geq 300 \text{ cm}^{-3}$ for FIREbox, see Table 1), Jeans unstable, molecular (self-shielding) gas with a 100% efficiency per local free-fall time. The molecular-to-neutral gas ratio is calculated via an analytic model (Krumholz et al. 2008, 2009; McKee & Krumholz 2010) assuming photo-dissociation and two-phase equilibrium. This model requires as inputs the metallicity Z and the dust optical depth for Lyman-Werner photons τ , see Krumholz & Gnedin (2011). The metallicity is known for each particle and the dust optical depth is estimated via a local Sobolev-length approximation. Specifically, $\tau = 434.8 \text{ cm}^2 \text{ g}^{-1} \Sigma_{\text{gas}} [0.1 + Z/0.02]$ where Z is the metallicity and $\Sigma_{\text{gas}} = \rho [d + \rho / |\vec{\nabla} \rho|]$ is the gas mass surface density. Furthermore, d is the inter-particle separation

² www-n.oca.edu/ohahn/MUSIC

³ camb.info

⁴ <http://www.tapir.caltech.edu/~phopkins/Site/GIZMO.html>

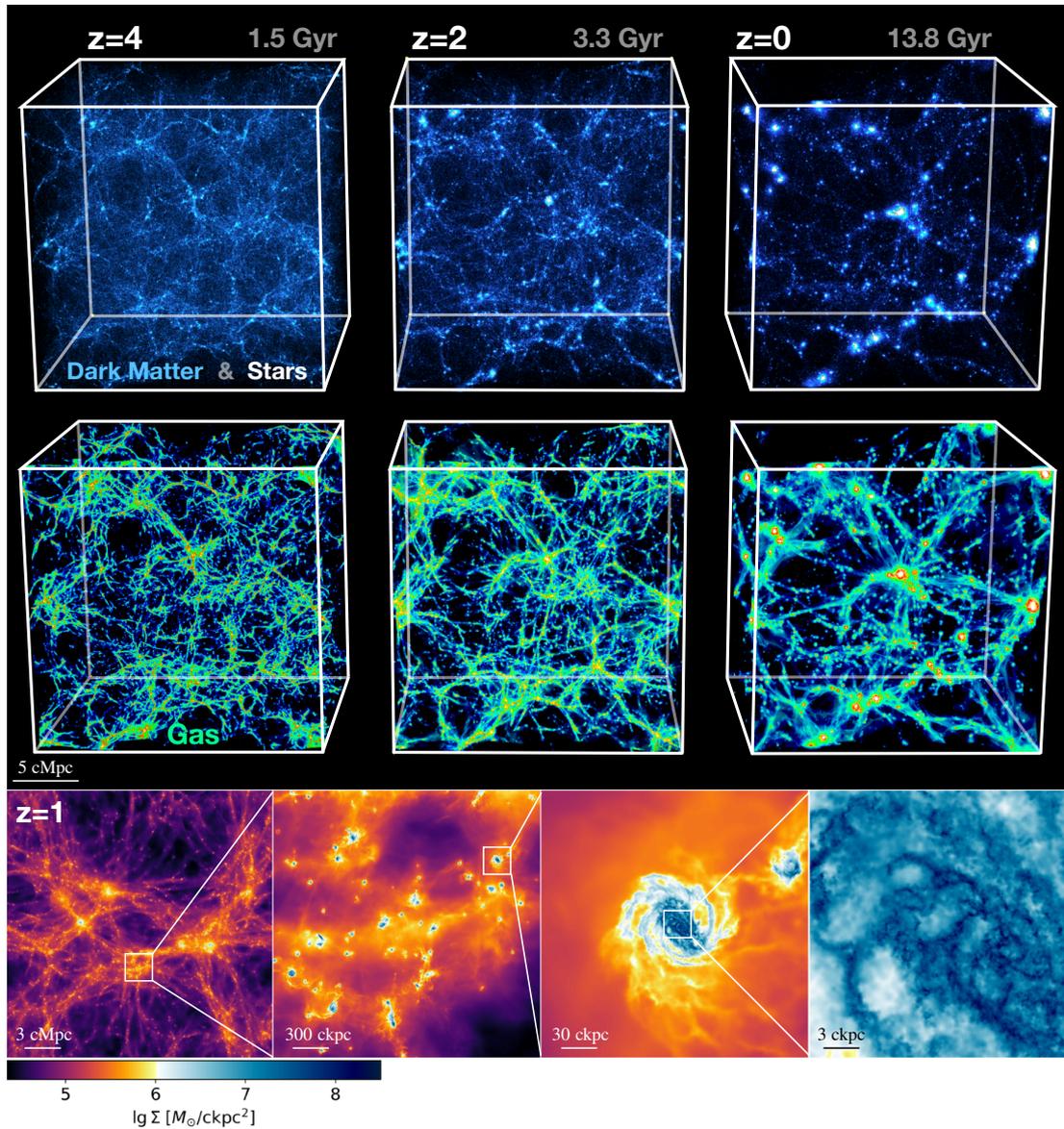


Figure 1. Visualization of the matter distribution in FIREbox. (Top row) Three-dimensional rendering of the dark matter (blue) and stars (white) in the simulation volume at $z = 4$, $z = 2$, and $z = 0$ (from left to right). Dark matter forms a cosmic web of filamentary structures, overdensities, and voids which evolves with redshift. Stars form at the centers of collapsed dark matter halos. (Middle row) Visualization of the gas distribution which mirrors the cosmic network of dark matter. (Bottom row) Column density maps of the gas projected along the ~ 22.1 cMpc depth of the box at $z = 1$. Starting from a view of the gas distribution on cosmological scales, the panels zoom into the interstellar medium of one of many simulated galaxies, illustrating the high dynamic range of FIREbox.

which is closely related to the kernel length of the given gas particle (Hopkins 2015; Hopkins et al. 2018).

Stellar feedback includes energy, momentum, mass, and metal injections from supernovae (type II and type Ia) and stellar winds (OB and AGB stars). Most feedback quantities are taken from tabulated stellar population models (STARBURST99; Leitherer et al. 1999) for a Kroupa (2001) initial stellar mass function (IMF). In addition, SN Ia rates are taken from Mannucci et al. (2006) and yields from Iwamoto et al. (1999). SN II yields are from Nomoto et al. (2006) and yields for OB/AGB stars follow Wiersma et al. (2009). Radiative feedback in the form of photo-ionization and photo-electric heating as well as radiation pressure is also included. Radiative transfer effects are accounted for in the Locally Extincted Background Radiation in Optically thin Networks (LEBRON) approximation (Hopkins et al. 2012, 2014, 2018; Hopkins & Grudić 2019).

As pointed out before, none of the current FIREbox runs include AGN feedback for the following main reason. The aspirational goal of FIREbox is to provide a robust prediction of galaxy theory based only on (more or less well) understood physical processes. In other words, FIREbox is designed as a baseline simulation to test how well our current model of galaxy formation works. While most likely an important piece of the puzzle, the role and impact of AGN feedback on galaxy formation is not yet physically understood and, furthermore, it cannot be modeled at present in a self-consistent and ab initio manner in a cosmological simulation. We thus made the deliberate choice to not include AGN feedback or other less well understood physical processes in our baseline simulation. Importantly, this strategy welcomes mismatches between the model predictions and observations as they may pin-point important areas in our current theoretical understanding that need improvement. This ansatz thus differs from the

Name	Comment	N	z_{final}	L (cMpc)	n_{SF} (cm^{-3})	m_{b} ($10^4 M_{\odot}$)	m_{DM} ($10^5 M_{\odot}$)	$\epsilon_{\text{gas,min}}$ (pc)	$d_{\text{gas,SF}}$ (pc)	ϵ_{star} (pc)	ϵ_{DM} (pc)
FB1024	FIREbox	2×1024^3	0	22.1	300	6.26	3.35	1.5	20.4	12	80
FB512	lower res. re-run	2×512^3	0	22.1	100	50.1	26.8	4	58.8	32	160
FB256	lower res. re-run	2×256^3	0	22.1	10	401	215	16	253	128	320
FB2048-DM	higher res. N -body	2048^3	0	22.1	-	-	0.50	-	-	-	40
FB1024-DM	N -body	1024^3	0	22.1	-	-	3.98	-	-	-	80
FB512-DM	lower res. N -body	512^3	0	22.1	-	-	31.8	-	-	-	160
FB256-DM	lower res. N -body	256^3	0	22.1	-	-	255	-	-	-	320

Table 1. The FIREbox simulation suite. A systematic name and a short description for each run are provided in the first two columns. Columns three to six list the number of particles at the start of each simulation, the redshift reached by each simulation, the box size, and density threshold for star formation. The final six columns provide the masses of baryonic (gas and star) particles, the masses of dark matter (DM) particles, the minimum gravitational softening length of gas particles, the inter-particle spacing of gas particles at the star formation threshold, and the gravitational softening lengths of star and DM particles. For comparison with the literature, the force resolution is stated in equivalent Plummer softening lengths. The corresponding spline softening lengths are larger by a factor of ~ 1.4 . For every hydrodynamical simulation, there is a corresponding dark-matter-only (DMO) N -body simulation with particle masses $m_{\text{DMO}} = m_{\text{b}} + m_{\text{DM}}$ and gravitational softening lengths $h_{\text{DMO}} = h_{\text{DM}}$. The main focus of the present work is the FB1024 cosmo-hydrodynamical simulation (FIREbox) listed in the top row.

more conventional approach of tweaking ad hoc prescriptions with many tunable parameters to obtain as good a match with observations as possible. In the future, FIREbox simulations with additional physics such as cosmic ray physics (Chan et al. 2019; Hopkins et al. 2020) and AGN feedback (Wellons et al. 2022) will allow us to explicitly study the differential impact of these potentially important physical processes by comparing with FIREbox.

2.3 Numerical resolution

In all runs, gravity is softened with a cubic spline kernel. The force resolution of gas particles is adaptive and set to the gas inter-particle spacing $h = (m_{\text{b}}/\rho_{\text{b}})^{1/3}$ subject to a lower limit ($\epsilon_{\text{gas,min}}$). This lower limit is chosen such that the highest gravitationally-resolved gas density $n^{\text{max}} = m_{\text{b}}/(\epsilon_{\text{gas,min}})^3/m_{\text{H}}$ exceeds the star formation threshold density n_{SF} by a factor of ~ 1000 , see Hopkins et al. (2018). The force softenings of star and dark matter (DM) particles are non-adaptive. The softening length of star particles was chosen to be similar to the softening length of gas particles at the star formation threshold. Newly formed star particles have thus a similar softening length as the gas particles that spawned them. The Plummer equivalent softening length of DM particles is set to $\sim 20 \text{ pc} (m_{\text{DM}}/5000M_{\odot})^{1/3}$ to avoid over-softening of the central DM halo profile while also minimizing N -body relaxation due to particle scattering (Hopkins et al. 2018). The value of $\epsilon_{\text{gas,min}}$ and the softening lengths of star and DM particles are kept fixed in physical (comoving) coordinates at $z \leq 9$ ($z \geq 9$).

FIREbox (or FB1024), the primary simulation discussed in this paper, contains 1024^3 gas and 1024^3 DM particles at the starting redshift with masses $m_{\text{b}} = 6.3 \times 10^4 M_{\odot}$ and $m_{\text{DM}} = 3.3 \times 10^5 M_{\odot}$, respectively. A new star particle inherits the mass of the gas particle from which it was created. However, as a result of supernova explosions and stellar winds, star particles lower their mass over time to $\sim 0.5m_{\text{b}}$. The mass resolution in FIREbox is $\approx 8 \times$ lower than FIRE zooms of Milky-Way analogs (e.g., Wetzel et al. 2016; Hopkins et al. 2018). The minimum gas softening length (Plummer equivalent) is $\epsilon_{\text{gas,min}} = 1.5 \text{ pc}$. A more representative measure of the spatial resolution of hydrodynamical processes in the ISM is the inter-particle spacing of gas particles eligible for star formation ($\lesssim 20 \text{ pc}$ in FIREbox). Star particles (DM particles) have a Plummer equivalent softening length of $\epsilon_{\text{star}} = 12 \text{ pc}$ ($\epsilon_{\text{DM}} = 80 \text{ pc}$). Mass

and force resolution of the FB512 (FB256) runs are correspondingly lower, see Table 1.

2.4 Comparison with state-of-the-art galaxy formation simulations

Fig. 2 compares the hydrodynamic mass and spatial resolution of FIREbox with a compilation of cosmological galaxy formation simulations of intermediate-to-high mass galaxies reaching $z < 2$. Zoom-in simulations that specifically target very low mass galaxies (e.g., Fitts et al. 2017; Revaz & Jablonka 2018; Wheeler et al. 2019; Munshi et al. 2019) can reach a higher numerical resolution and are not included in this comparison. While not an exhaustive list, the compilation is representative of the current state-of-the-art and includes a range of hydrodynamics solvers, such adaptive mesh refinement (AMR), smoothed particle hydrodynamics (SPH), moving mesh hydrodynamics, and mesh-less hydrodynamics as well as both zoom-in runs and large-volume simulations. Specifically, the compilation includes cosmological volume simulations from the Illustris (Vogelsberger et al. 2014; Genel et al. 2014), IllustrisTNG (Pillepich et al. 2018a; Nelson et al. 2019b), OWLS (Schaye et al. 2010), EAGLE (Schaye et al. 2015), MUFASA (Dave et al. 2016), SIMBA (Dávě et al. 2019), MassiveBlack-II (Khandai et al. 2015), Romulus (Tremmel et al. 2017), and Horizon-AGN (Dubois et al. 2014) projects, representative zoom-in simulations from the FIRE project (Hopkins et al. 2014, 2018), such as Latte (Wetzel et al. 2016) and Massive-FIRE (Feldmann et al. 2016, 2017; Anglés-Alcázar et al. 2017b), as well as runs by Agertz & Kravtsov (2015) and zoom-in simulations from the Apostle (Sawala et al. 2016), Argo (Feldmann & Mayer 2015), Auriga (Grand et al. 2017, 2021), DC Justice League (Bellovary et al. 2019; Applebaum et al. 2021), Eris (Guedes et al. 2011), NewHorizon (Dubois et al. 2021), NIHAO (Wang et al. 2015), and VELA (Ceverino et al. 2014) projects.

Given the intrinsic ambiguity in defining mass and spatial resolution across such a variety of models, we adopt the following operational definitions. For particle-based hydrodynamics codes, the mass resolution is defined as the typical gas particle mass in the simulation. Adopting a more physics-based definition, e.g., using the minimal resolved Jeans mass, would favor even more simulations, such as FIREbox, that directly model the multiphase ISM (shown by filled symbols) compared with simulations that do not (empty symbols), i.e., those that prevent gas from cooling to low

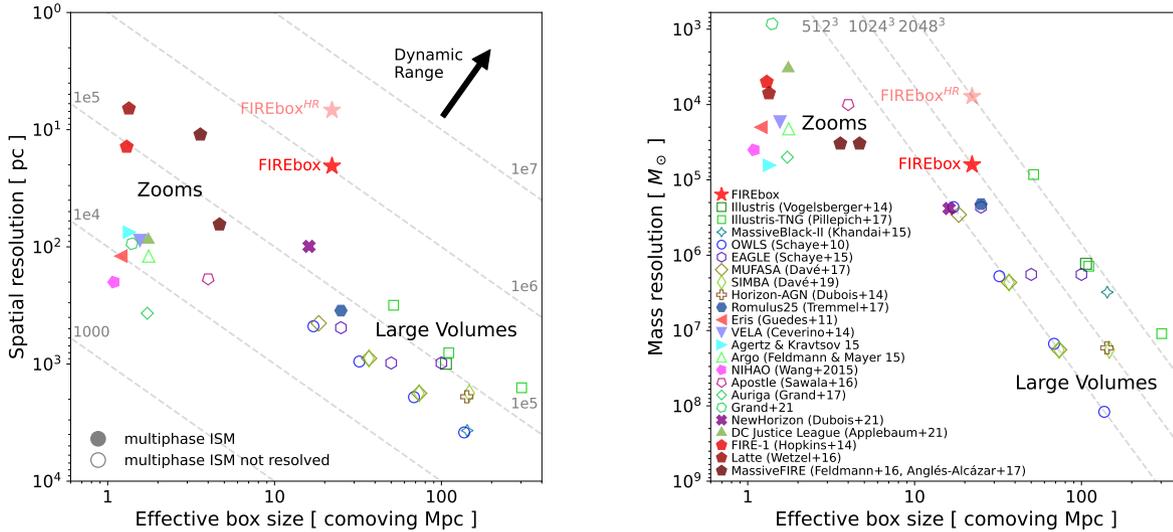


Figure 2. Hydrodynamic resolution and size of FIREbox compared with a representative selection of state-of-the-art cosmological galaxy formation simulations (see legend and text). In each panel, FIREbox is shown as a bright red star. A faint red star shows the properties of a future, higher resolution and higher redshift follow-up simulation (FIREbox^{HR}). The present work focuses only on FIREbox. Filled (empty) symbols indicate simulations that do (do not) resolve the multiphase structure of the ISM, see text. (Left) Spatial resolution vs effective box size. The spatial resolution is defined as the larger of the inter-particle distance at the star formation threshold density and the gravitational softening length of gas particles (see text). The effective box size equals the comoving box length for cosmological volume simulations. For zoom-in simulations, the effective box size is set to 5 times the comoving virial radius of the largest halo in the zoom-in region at the final snapshot. Not shown are zoom-in simulations that do not resolve at least one Milky-Way mass halo or that have a baryonic mass resolution worse than $10^5 M_{\odot}$. Diagonal dashed lines show the resolved dynamic range of the simulation, i.e., the ratio between the effective box size and the spatial resolution. (Right) Baryonic mass resolution vs effective box size. Diagonal dashed lines show the approximate number of gas particles in the simulation volume. FIREbox is a cosmological volume simulation with a resolution comparable to state-of-the-art zoom-ins and the first cosmological galaxy formation simulation run to $z = 0$ with a dynamic range of more than one million. As such, FIREbox is able to resolve the multiphase structure of gas in and around galaxies in a fully cosmological context and across cosmic history.

temperatures ($T < 1000$ K) and/or use an effective equation of state to model the cold ISM. The spatial resolution is set to the larger of the gas inter-particle spacing d_{SF} at the star formation threshold, $d_{\text{SF}} = 74 \text{ pc} (m_{\text{b},4}/n_{\text{SF},0})^{1/3}$ with $m_{\text{b},4} = m_{\text{b}}/(10^4 M_{\odot})$ and $n_{\text{SF},0} = n_{\text{SF}}/\text{cm}^{-3}$, and the minimum spline gravitational softening length of gas particles. We note that while dynamical processes may be resolved on scales smaller than d_{SF} , those scales are affected by the physics of sink particle formation. For grid-based methods, we adopt $m_{\text{b}} = \Omega_{\text{b}}/(\Omega_{\text{m}} - \Omega_{\text{b}})m_{\text{DM}}$ as hydrodynamic mass resolution, while the spatial resolution is defined as the larger of d_{SF} and the minimum cell size.

The figure also shows the effective box size of the simulations. The effective box size equals the comoving box length for cosmological volume simulations. For zoom-ins, it is set to 5 times the comoving virial radius of the most massive halo in the highest resolution region at the final simulation redshift (not all shown simulations reach $z = 0$) to approximately reproduce the typical extent of the zoom-in region uncontaminated by low-resolution dark matter particles. Only the largest simulation is considered when calculating the effective box size for simulations suites consisting of multiple independent runs of similar resolution, such as Apostle, Auriga, or MassiveFIRE. Zoom-in simulations that do not resolve at least one Milky-Way mass halo or that have a baryonic mass resolution worse than $10^5 M_{\odot}$ are not included in the figure. The ratio between the effective box size and the spatial resolution of a simulation defines its dynamic range.

FIREbox opens a new frontier in studying the evolution of galaxies with hydrodynamical simulations given its unique combination

of high numerical resolution (comparable to state-of-the-art zoom-ins) and accurate physical modeling in a cosmological volume of $(22.1 \text{ cMpc})^3$. Specifically, FIREbox is able to both directly resolve the thermodynamic state of the ISM (by enabling self-consistent cooling down to $\sim 10 - 20$ K) and to accurately account for multiple stellar feedback channels tied to stellar population synthesis models (see section 2.2). The underlying FIRE-2 physics model has been employed previously in zoom-in simulations to study the multiphase nature of the ISM, e.g., the overall properties of massive giant molecular clouds (Benincasa et al. 2020; Guszejnov et al. 2020) and the vertical pressure profiles and scale heights of galactic disks (Gurvich et al. 2020). With FIREbox, we can study galaxies and their ISM with larger, representative samples from a contiguous cosmological volume enabling a proper statistical analysis and a study of cosmological environments. While the dynamic range of FIREbox ($\gtrsim 10^6$) already exceeds significantly those of contemporary galaxy formation simulations, future follow-up simulations (FIREbox^{HR}) combined with dedicated zoom-ins promise to further extend this frontier towards larger samples of better resolved galaxies.

2.5 Simulation output

The properties of gas, star, and dark matter particles are saved as Gadget HDF5 files in (semi-)regular intervals for subsequent analysis. All FIREbox runs, except FB2048-DM, use 1201 save-points that are approximately equally spread in cosmic time between $z_{\text{init}} = 120$ and $z_{\text{final}} = 0$, resulting in a close to 11 Myr average save-point

intervals. For FB2048-DM, fewer save-points are used at $z < 2$ to mitigate its high storage footprint. Furthermore, three out of every four save-points are stored at reduced resolution (‘snapshots’) to reduce the overall storage cost of the simulation suite, see below. In addition, all save-points (both snapshots and regular snapshots) are stored in gzip compressed format.

A save-point is stored either as a level 0 snapshot, a level 1 snapshot, or a level 2 ‘snapshot’. Level 0 snapshots are compressed in a loss-less manner but are otherwise identical to the original HDF5 output files. The compression can reduce the file size by up to a factor of 2. Level 1 snapshots are identical to level 0 snapshots except that the abundances of individual elements (but not the total metallicity) are stored at reduced precision (1 byte) in hydrodynamical simulations. Level 2 snapshots differ significantly from snapshots. Densities, electron abundances, neutral hydrogen abundances, helium abundances, total metallicities, internal energies, softening lengths, and velocities of gas particles are stored at reduced resolution (typically as a half-precision float and after a log transform for non-negative fields). Additionally, the individual abundances of elements heavier than Helium are dropped. Gas particle masses and coordinates are kept at full resolution, however. In addition, star particles keep the same information as for level 1 snapshots. Dark matter particles are down-sampled randomly by a factor 8 with the help of a scrambled Xorshift generator (Marsaglia 2003; Vigna 2016) such that the same particles are removed (or kept) in all snapshots.

2.6 Halo and galaxy catalogs

We identify dark matter halos and catalog their various properties, including halo positions, masses, radii, and whether or not a given halo is a sub-halo or a main halo, with the help of the AMIGA Halo finder (AHF; Gill et al. 2004; Knollmann & Knebe 2009). We include only halos with at least 100 particles in our subsequent analysis. Halo masses (M_{halo}) and radii (R_{vir}) are calculated based on the virial overdensity definition (Bryan & Norman 1998). Growth histories for individual halos are constructed with the AHF MergerTree tool by linking halos in subsequent snapshots via the identification numbers of their DM particles.

In the context of this paper, ‘sub-halos’ are DM halos that reside within another DM halo identified by AHF. All other DM halos are ‘main halos’. Galaxies in sub-halos are called satellite galaxies, while the primary galaxy of a main halo is called its central galaxy.

With the help of the AHF particle files, we identify both the direct host halo (which can be a sub-halo or a main halo) for each particle as well as the main halo containing the particle. Subsequently, we use this information to calculate a variety of particle based properties, e.g., stellar masses, star formation rates (SFRs), and gas masses in various three-dimensional spherical apertures, and store them in HDF5 files for subsequent analysis. Halo properties are measured within a sphere of radius R_{vir} , while a smaller radius R_g (see below) is used to measure galaxy properties. For sub-halos, R_{vir} , as reported by AHF and used below, refers to the smaller of the virial and the tidal radius.

The total radius R_g and the stellar half mass radius R_{half} of galaxies are defined using two different approaches based on the cumulative spherical stellar mass profile $M_{\text{star}}(< R)$ and the virial radius. The first approach follows Hopkins et al. (2018). Starting from an initial choice for R_g of $0.15 R_{\text{vir}}$, the half mass radius is computed as $M_{\text{star}}(< R_{\text{half}}) = 0.5 M_{\text{star}}(< R_g)$ and the total radius is updated as $R_g = 3 \times R_{\text{half}}$. The latter steps are repeated until the relative change in R_g between one iteration and the next is less than 10^{-5} . The second

approach sets $R_g = 0.1 R_{\text{vir}}$ and subsequently calculates R_{half} from the stellar mass profile within R_g . Unless stated otherwise, stellar masses, SFRs, and other properties of galaxies refer to integrated properties within R_g computed as in the first method.

2.7 Gas fractions and temperatures

The mass m_{gas} of each gas particle can be divided into the mass of ionized (m_{HII}), atomic (m_{HI}), and molecular hydrogen (m_{H_2}) as well as the mass in Helium and in the various metals. The total hydrogen mass of a gas particle is $m_{\text{H}} = m_{\text{HI}} + m_{\text{H}_2} + m_{\text{HII}} = X m_{\text{gas}}$, where the hydrogen mass fraction X can vary from particle to particle. The neutral hydrogen fraction $f_{\text{HI}+\text{H}_2} = (m_{\text{HI}} + m_{\text{H}_2})/m_{\text{H}}$ of each particle is calculated during the run-time of the simulation as described in Hopkins et al. (2018) and is provided in the simulation snapshots. At the level of individual gas particles, $f_{\text{HI}+\text{H}_2}$ is also the neutral gas fraction ($m_{\text{atm}} + m_{\text{mol}}/m_{\text{gas}}$ provided we define atomic and molecular gas masses of particles as $m_{\text{atm}} = m_{\text{HI}}/X$ and $m_{\text{mol}} = m_{\text{H}_2}/X$. The molecular gas fraction $f_{\text{H}_2} = m_{\text{H}_2}/m_{\text{H}} = m_{\text{mol}}/m_{\text{gas}}$ of each particle, which is also calculated at run-time, is not part of the simulation output, however. We thus recalculate it based on the snapshot data. Specifically, we first calculate the molecular-to-neutral gas ratio $f_{\text{H}_2}/f_{\text{HI}+\text{H}_2}$ based on its dust optical depth and metallicity following the same approach (Krumholz & Gnedin 2011) as for the run-time calculation described above, see section 2.2. Given the various assumptions entering this approach, the resulting estimate of the molecular-to-neutral gas ratio should be understood as an approximation that may be highly inaccurate under certain conditions, e.g., at metallicities below $0.01 Z_{\odot}$. We then convert the molecular-to-neutral gas ratio to the molecular gas fraction by multiplying the former with $f_{\text{HI}+\text{H}_2}$. The atomic gas fraction of a particle $f_{\text{HI}} = m_{\text{HI}}/m_{\text{H}} = m_{\text{atm}}/m_{\text{gas}}$ is calculated as $f_{\text{HI}+\text{H}_2} - f_{\text{H}_2}$.

Gas temperatures are re-calculated from the internal energy per unit mass ϵ , electron abundance $f_e = n_e/n_{\text{H}}$, Helium abundance Y , metallicity Z , all of which are provided in the simulation output and from the molecular gas fraction f_{H_2} calculated as described above. The gas temperature is given as $T = \epsilon(\gamma - 1)\mu/k_{\text{B}}$ with the mean molecular weight $\mu = m_{\text{H}}/[X(1 - 0.5 f_{\text{H}_2}) + Y/4 + f_e X + Z/16]$ and with $X = 1 - Y - Z$. FIREbox employs a floor in specific internal energy that amounts to a temperature floor of ~ 10 K in atomic gas and ~ 18 K in molecular gas.

3 PROPERTIES OF FIREbox GALAXIES

In this section, we analyze basic properties of FIREbox galaxies. Our main focus lies in comparing our simulation predictions to available observational data. We will demonstrate that many basic galaxy scaling relations predicted by the simulation, e.g., the relations between galaxy stellar mass and their star formation rates, gas content, and metallicity, agree reasonably well with observations. Other properties, such as the stellar mass functions (SMF) and the galaxy stellar mass – halo mass relation (SHMR) are not reproduced as well. Here, the predictions of FIREbox are more in line with recent stellar mass estimates based on non-parametric panchromatic spectral energy distribution (SED) modeling.

Throughout this section, a Chabrier (2003) IMF is adopted for all observational data. Specifically, we lower stellar masses and SFRs by 0.25 dex when converting from Salpeter (1955) IMF to Chabrier (2003) IMF (see, e.g., Lee et al. 2006; Gallazzi et al. 2008; Herrmann et al. 2016). We ignore the small shift between a Chabrier (2003) IMF and the Kroupa (2001) IMF adopted by FIREbox. These conversions

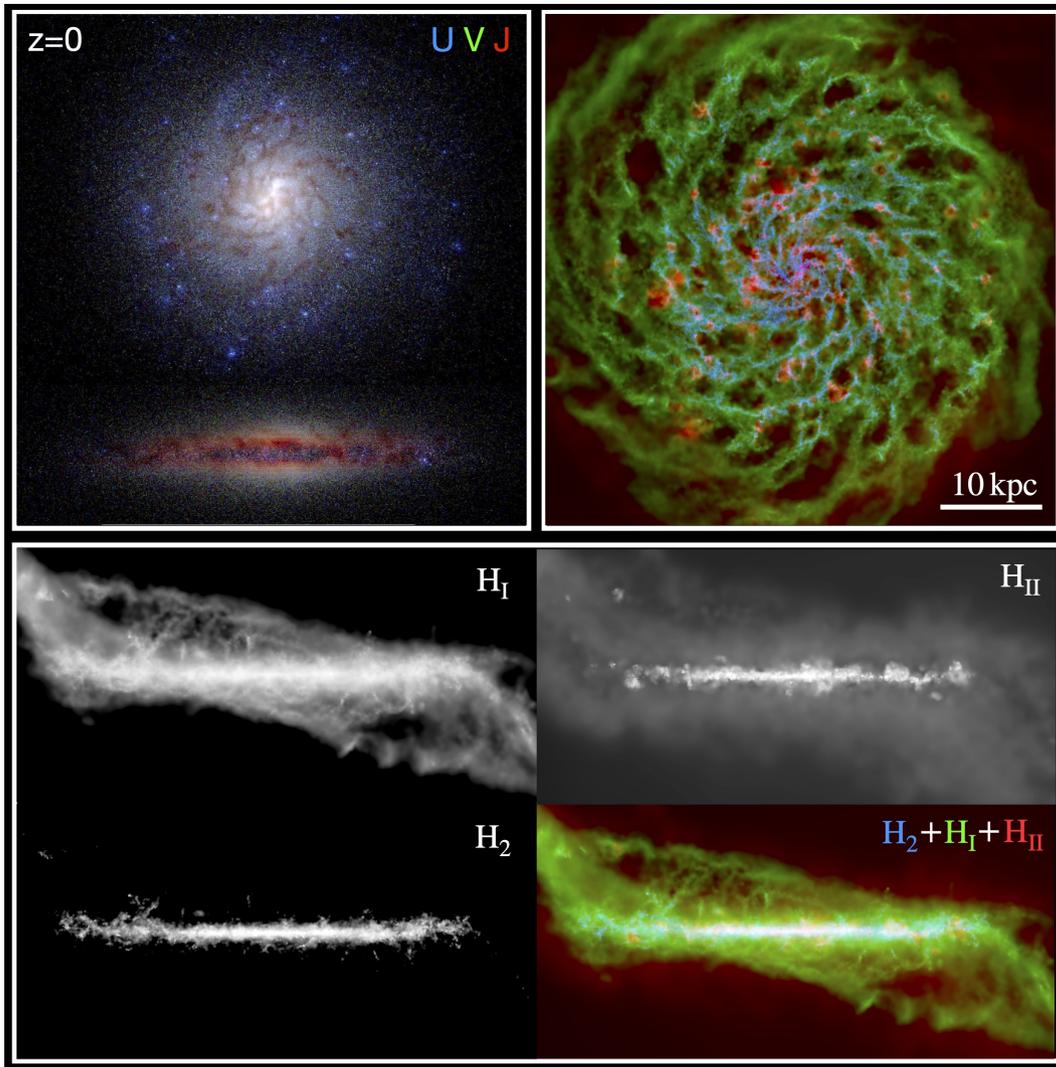


Figure 3. Visualization of the multiphase structure of baryons in a Milky Way like galaxy at $z = 0$ in FIREbox. (Top left) Color composite image in U (blue), V (green), and J (red) broad-bands, created with the radiative transfer code SKIRT (Baes et al. 2011; Camps & Baes 2015), showing the stellar and dust components of the depicted galaxy in a face-on and edge-on view. This galaxy has an overall disk morphology. (Top right) Face-on, color composite image of the galaxy’s molecular (H_2 , blue), atomic (H_I , green), and ionized (H_{II} , red) hydrogen content. (Bottom) Edge-on view of the atomic, ionized, molecular, and combined hydrogen content (see legend). The neutral interstellar medium (ISM) resides in an extended, but thin gas disk with a complex internal structure (see text). The neutral ISM is embedded in a thick, but comparably smooth, disk of ionized gas. Ionized gas is also present in regions of various sizes within the plane of the ISM disk. The locations of these ionized regions often coincide with those of young stellar clusters shown in blue in the UVJ image. The H_I and H_{II} disks are strongly warped at large radii. All images have the same physical scale (50 kpc from left to right), see legend, and show quantities on a logarithmic stretch. The center of the galaxy is shifted vertically in the top left panel. Many of the shown features, e.g., some of the H_2 spiral arms and H_{II} bubbles, are less than 100 parsecs across.

are simple but approximate as the proper conversion factor generally varies with the observable in question.

3.1 The multiphase interstellar medium

One of the main goals of the FIREbox project is to study the distribution of the various gas phases in and around galaxies at high spatial resolution. As such, it aims to provide a theoretical counterpart to the large number of observational efforts currently being undertaken to map the gas content of galaxies on sub-galactic (few hundreds of parsecs or better) scales, such as THINGS (Walter et al. 2008), LITTLE THINGS (Hunter et al. 2012), HI-MaNGA (Masters et al. 2019), ALMAQuest (Lin et al. 2020), PHANGS-ALMA (Leroy et al. 2021a), and PHANGS-MUSE (Emsellem et al. 2022).

We illustrate the ability of FIREbox to model and spatially resolve the multiphase ISM in Fig. 3. Here, we show gas maps as well as color-composite images of stellar light for a FIREbox galaxy at $z = 0$. The halo mass of this chosen galaxy ($1.3 \times 10^{12} M_\odot$) matches the estimated halo mass of the Milky Way (MW, Bland-Hawthorn & Gerhard 2016). Overall, this galaxy is a fairly typical example of a MW analog in FIREbox. We will discuss the properties of MW analogs in FIREbox more generally in section 3.4.

According to Fig. 3, this galaxy has a well-defined disk morphology. Face-on and edge-on images in U, V, and J broad-band filters, created with the help of the Monte Carlo radiative transfer code

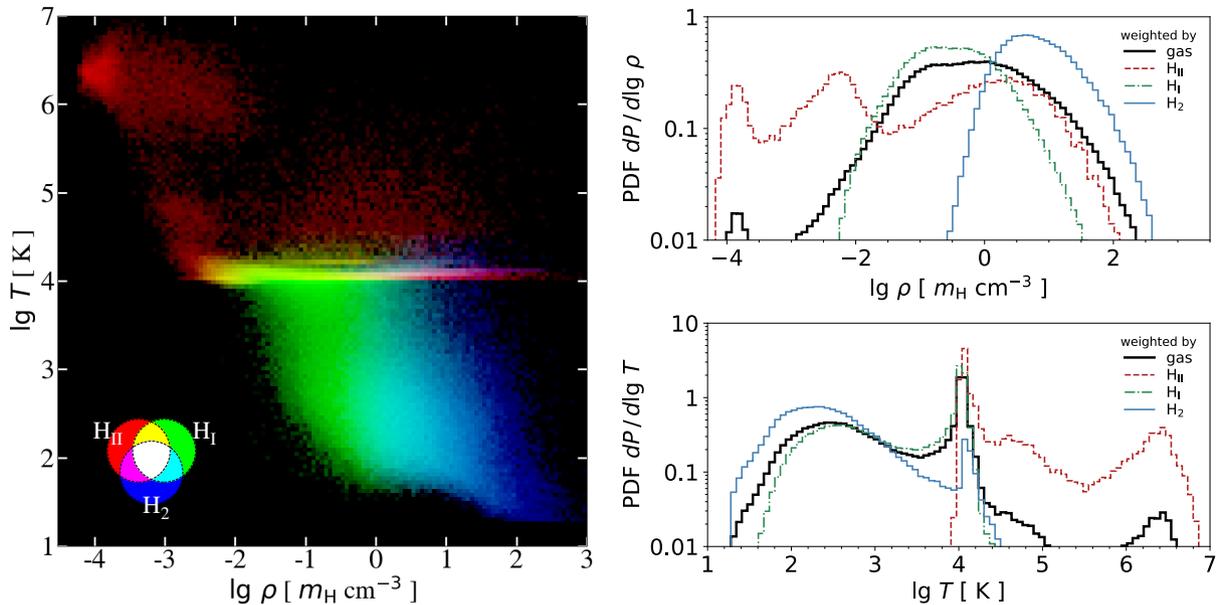


Figure 4. Thermal properties of the interstellar medium (ISM) of a Milky Way like galaxy at $z = 0$ in FIREbox. (Left) Phase diagram of hydrogen gas within a $0.1R_{\text{vir}} \sim 29$ kpc radius of the center of the galaxy. Densities (ρ) and temperatures (T) vary over many orders of magnitude ($\sim 10^{-4} - 10^3 m_H \text{ cm}^{-3}$ and $10 - 10^7$ K) highlighting the computational challenge for galaxy formation simulations. The phase diagram is color-coded according to the hydrogen phase, see legend. The hydrogen phase is not uniquely determined by gas density and temperature alone. (Top right) Fraction of gas within $0.1R_{\text{vir}}$ having density ρ per unit $\lg \rho$. (Bottom right) Fraction of gas within $0.1R_{\text{vir}}$ having temperature T per unit $\lg T$. In both right hand panels, particle number fractions are weighted by gas mass (thick black solid line), ionized hydrogen mass (red dashed line), atomic hydrogen mass (green dot-dashed line), and molecular hydrogen mass (blue solid line). The small fraction of molecular gas with temperatures near 10^4 K is an artifact of the approximate treatment of separating neutral gas into atomic and molecular components, see section 2.2. Neutral hydrogen consists of a combination of cold ($\sim 100 - 1000$ K) and warm ($\sim 10^4$ K) gas, while ionized gas consists of a hot, dilute ($\sim 10^{-4} m_H \text{ cm}^{-3}$) phase filling most of the volume (the diffuse hot halo), a warm / hot, low density ($\sim 10^{-3} - 10^{-2} m_H \text{ cm}^{-3}$) phase which forms a disk layer around the neutral ISM disk (see Fig. 3), and warm ionized, relatively dense gas located in the plane of the ISM disk.

SKIRT⁵ (Baes et al. 2011; Camps & Baes 2015), show young clusters of stars, patchy lanes of dust, and an underlying stellar disk that extends out to about 15-18 kpc. Face-on gas maps of the molecular, atomic, and ionized components of the ISM reveal a complex and intricate structure. Neutral hydrogen forms a relatively thin, but flocculent, disk with much of the molecular component residing in the inner, denser regions of the gas disk. Significant amounts of H_I gas can be found at large distances (> 25 kpc) from the galaxy center, i.e., far beyond the extent of the stellar disk, see also Trapp et al. (2022).

The vertical scale heights of the H_I and H_2 disks at $R \sim 8$ kpc for this simulated galaxy are approximately 200 ± 50 pc and 130 ± 70 pc when measured by fitting the vertical density profile in annulus sectors with a Gaussian (Gensior et al in prep). These scale heights are comparable (within a factor of 2-3) with estimates for the Milky Way (Bacchini et al. 2019b), M33 (Combes et al. 2012), and nearby star forming galaxies (Bacchini et al. 2019a). The H_I disk remains thin and regular out to about 20 kpc and shows warping at larger radii.

Most of the ionized gas surrounding this galaxy is part of a diffuse, hot circum-galactic medium filling much of the volume of the DM halo. However, ionized gas can also be found in a puffed-up disk layer surrounding the neutral ISM, possibly a rotating cooling flow that replenishes the disk with gas (Hafen et al. 2022), as well as in a thin disk within the plane of the neutral gas disk, often near the locations of young star clusters.

Fig. 4 explores further the thermal properties and phase structure

of the gas in the selected MW analog. The gas within $0.1R_{\text{vir}} \sim 29$ kpc varies broadly in density and temperature ($\sim 10^{-4} - 10^3 m_H \text{ cm}^{-3}$ and $10 - 10^7$ K) and consists of ionized, atomic, and molecular phases. In this example galaxy, most of the hydrogen gas within $0.1R_{\text{vir}}$ is atomic (70%). Molecular and ionized hydrogen contribute at the 22% and 8% level, respectively. When split by temperature, gas with $T < 6000$ K is predominantly neutral, while gas with $T > 15000$ K is predominantly ionized. The ionized gas is made up of 3 sub-components: a hot, dilute ($\sim 10^{-4} m_H \text{ cm}^{-3}$) phase filling most of the volume (the diffuse hot halo), a warm / hot, low density ($\sim 10^{-3} - 10^{-2} m_H \text{ cm}^{-3}$) phase which forms a smooth disk layer around the neutral ISM disk, and a warm ionized phase of relatively dense gas near the center plane of the ISM disk.

3.2 The star forming sequence

SFRs and stellar masses of star forming galaxies are tightly correlated with a redshift dependent normalization (Brinchmann et al. 2004; Noeske et al. 2007; Elbaz et al. 2007). This empirical relation, the star forming “main sequence”, links the star formation history of a galaxy (via its stellar mass) to its current star formation activity making it an important empirical constraint for theoretical models. The precise functional form of the star forming sequence is still somewhat uncertain given that it has been measured with a variety of different observational techniques and for galaxy samples subject to different selection effects (Speagle et al. 2014; Davies et al. 2016). However, advances in recent years, e.g., access to multi-band (UV to FIR) photometry (e.g., Schreiber et al. 2015; Davies et al. 2016) and improved modeling techniques (Chevallard & Charlot 2016; Leja

⁵ <http://www.skirt.ugent.be>.

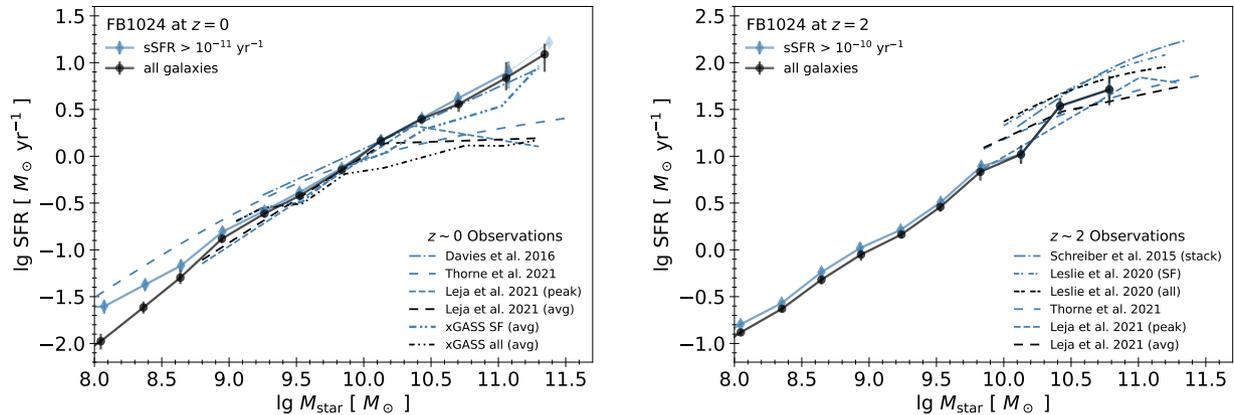


Figure 5. Star forming sequence in FIREbox and in observations at $z = 0$ (left) and $z = 2$ (right). Symbols show the logarithm of the average SFR in bins of stellar mass for all galaxies (black circles) and for star forming galaxies (blue diamonds) in FIREbox. The latter population of galaxies is defined as having specific SFRs exceeding 10^{-11} yr^{-1} at $z = 0$ and 10^{-10} yr^{-1} at $z = 2$. SFRs are averaged over the past 20 Myr. Error bars refer to 16-84% percentiles in each bin obtained via bootstrapping. Double dot-dashed lines show the star forming sequence for a representative sample of $z \sim 0$ galaxies from the xGASS survey (Catinella et al. 2018) with updated stellar masses as presented in Feldmann (2020). Dashed and dot-dashed lines show results of recent observational studies (Schreiber et al. 2015; Davies et al. 2016; Leslie et al. 2020; Thorne et al. 2020; Leja et al. 2021), see legend. Stellar masses by Leslie et al. (2020) are shifted by 0.2 dex to account for the known systematics of their stellar mass catalog. FIREbox predicts average SFRs of star forming galaxies in good agreement with observations but underestimates the presence of massive, quiescent galaxies at low z .

et al. 2017; Johnson et al. 2021), have resulted in more robust determinations of stellar masses and SFRs across cosmic history (e.g., Thorne et al. 2020; Leja et al. 2021). In principle, accurate measurements of different star formation tracers even allow constraints on the short-timescale variability of SFRs (Sparre et al. 2017; Flores Velázquez et al. 2021).

Fig. 5 compares the star forming sequence in FIREbox with the observed one in today’s Universe ($z = 0$) and at Cosmic Noon ($z = 2$). Specifically, we plot the logarithm of the average SFR in bins of stellar mass both for galaxies in FIREbox (“all”) as well as for those galaxies that are actually star forming (“SF”). The latter are defined to exceed a specific star formation rate (sSFR) of 10^{-11} yr^{-1} at $z = 0$ and 10^{-10} yr^{-1} at $z = 2$. These limits approximately remove “quiescent” galaxies, i.e., galaxies with SFRs that are an order of magnitude or more below the star forming sequence at the considered redshifts. SFRs in FIREbox are averaged over the past 20 Myr. We find only minimal changes (< 0.05 dex) for the slope and normalization of the star forming sequence of $M_{\text{star}} > 10^9 M_{\odot}$ galaxies when we adopt a 5 Myr or 100 Myr averaging time instead.

We compare these theoretical predictions with fits to observational data reported in recent studies (Schreiber et al. 2015; Davies et al. 2016; Leslie et al. 2020; Thorne et al. 2020; Leja et al. 2021). We also analyze a representative sample of low redshift galaxies from the xGASS survey (Catinella et al. 2018) with updated stellar masses as presented in Feldmann (2020). SFRs smaller than their measurement uncertainties are set to their measurement uncertainty. We refer to Feldmann (2020) for a more systematic, parametric approach that simultaneously constrains the slope of the star forming sequence and the corresponding atomic and molecular gas sequences.

When we look at the main sequence of star forming galaxies in FIREbox, we find generally good agreement with observational data at both $z = 0$ and $z = 2$. Being able to reproduce the slope and normalization of the star forming sequence is a significant achievement of the FIRE-2 model given that the simulation is not tuned to reproduce this (or any other) relation. Our finding also agrees qualitatively with a similar result for galaxies in FIRE-2 zoom-in simulations at $z = 0$ (Gandhi et al. 2022).

The star forming sequence in FIREbox at $z = 0$ and $z = 2$ is well described by a linear function (in log-log space) over a broad range in stellar mass, i.e.,

$$y = A + \alpha_1(x - 10), \quad (1)$$

where $y = \lg \langle \text{SFR} / (M_{\odot} \text{ yr}^{-1}) \rangle$ is the logarithm of the average SFR of galaxies and $x = \lg (M_{\text{star}} / M_{\odot})$ is the logarithm of the stellar mass. Fit results are listed in Table 2.

Focusing on $z = 0$ galaxies with $\text{sSFR} > 10^{-11} \text{ yr}^{-1}$ and $M_{\text{star}} = 10^9 - 10^{11} M_{\odot}$, we obtain a slope of $\alpha_1 = 0.85$ and a normalization of $A = 0.03$. Excluding satellite galaxies reduces the slope slightly to 0.80. Either slope is somewhat steeper than the analogously calculated slope of ~ 0.68 for star forming galaxies with $M_{\text{star}} = 10^9 - 10^{11} M_{\odot}$ in the xGASS sample. The normalization of star forming sequence in xGASS is very similar, however, differing by only about 0.1 at the $M_{\text{star}} = 10^{10} M_{\odot}$ pivot mass.

Both the normalization and the slope of the star forming sequence depend on redshift. The normalization of the star forming sequence increases by about one order of magnitude when going from $z = 0$ to $z = 2$ while the slope steepens, becoming near linear (~ 0.94) at $z = 2$ (or 0.95 if satellites are excluded). A linear slope would imply a mass-independent star formation timescale $M_{\text{star}}/\text{SFR}$ (Schreiber et al. 2015) and could help explain the invariant shape of the stellar mass function of star forming galaxies (Peng et al. 2010). Furthermore, as discussed in Feldmann (2020), the slope of the star forming sequence is naturally linked to the evolution of gas masses in galaxies and it becomes linear if the gas mass histories of galaxies have all the same shape. A sufficient but not necessary condition for the latter scenario is that galaxies are close to ‘equilibrium’ (Bouché et al. 2010; Davé et al. 2012), i.e., the masses of their ISM evolve only mildly with redshift as frequently seen in models across broad redshift and mass ranges (Finlator & Davé 2008). A non-linear slope (as found at low z) may instead suggest ‘downsizing’ of the gas mass, i.e., more massive galaxies reach their maximum gas masses at earlier times and subsequently have faster declining gas masses at late times. We plan to analyze the link between gas masses and star formation rates in more detail in future work.

Selection	Mass	A	α_1	x_b	α_2	Δ
Star forming sequence at $z = 0$						
sSFR $> 10^{-11} \text{ yr}^{-1}$	9 – 11	0.03	0.85	-	-	-
all galaxies	9 – 11	0.01	0.84	-	-	-
Star forming sequence at $z = 2$						
sSFR $> 10^{-10} \text{ yr}^{-1}$	8 – 11	1.00	0.94	-	-	-
all galaxies	8 – 11	0.98	0.97	-	-	-
Atomic hydrogen sequence at $z = 0$						
within 30 kpc	7 – 11.5	8.86	0.85	8.55	0.37	0.21
within $0.1 R_{\text{vir}}$	7 – 11.5	8.41	1.15	8.10	0.41	0.39
Molecular hydrogen sequence at $z = 0$						
within 10 kpc	7 – 11.5	8.68	1.59	9.82	0.26	0.39
within $0.1 R_{\text{vir}}$	7 – 11.5	8.52	1.59	9.65	0.56	0.30
Gas-phase oxygen abundance at $z = 0$						
within 3 kpc	6.5 – 11.5	9.29	0.58	10.28	0.19	0.07
within $0.1 R_{\text{vir}}$	6.5 – 11.5	9.15	0.57	10.21	-0.18	0.18
Stellar iron abundance at $z = 0$						
within 3 kpc	6.5 – 11.5	7.39	0.53	10.05	0.13	0.23
within $0.1 R_{\text{vir}}$	6.5 – 11.5	7.37	0.51	10.28	0.01	0.37

Table 2. Parameters of galaxy scaling relations in FIREbox. The first column refers to the selected galaxy population or 3-dimensional aperture, see sections 3.2, 3.3, and 3.5. The second column provides the stellar mass range over which the fit was performed. In each case we fit $\lg(Q)$ as a function of $\lg M_{\text{star}}$, where (Q) is the average SFR, atomic hydrogen mass, molecular hydrogen mass, gas-phase oxygen abundance, or stellar iron abundance for all considered galaxies in the given stellar mass bin. The star forming sequence is well fit by a linear function (equation 1) over the quoted mass regime with normalization A (column 3) and slope α_1 (column 4). Similarly, the gas and metallicity sequences are well fit by a broken linear function (equation 2) over the quoted mass regime with the parameters listed in columns 3-7.

At $z = 2$, a single power-law describes the star forming sequence well both for the “all” and the “SF” sample down to $M_{\text{star}} = 10^8 M_{\odot}$. In contrast, at $z = 0$ we observe a steepening of the slope for the “all” sample below $M_{\text{star}} = 10^9 M_{\odot}$. The difference between the $z = 0$ “all” and “SF” samples at low masses is a consequence of a significant number of low mass, central galaxies with very low or vanishing sSFR in FIREbox.

An important difference with observational data is the low fraction of massive, quiescent galaxies in FIREbox, see Fig. 6. Consequently, the average SFR (at fixed stellar mass) of all galaxies in FIREbox is very similar to the average SFR of star forming galaxies alone (except at the lowest masses). While the quiescent fraction is indeed low at early cosmic times, e.g., $\sim 70\% - 80\%$ of galaxies with $M_{\text{star}} \sim 10^{11} M_{\odot}$ are star forming at $z = 2$ (Behroozi et al. 2019), massive galaxies ($M_{\text{star}} \sim 10^{11} M_{\odot}$) are usually ($\sim 65\%$) quiescent in today’s Universe (Muzzin et al. 2013; Moustakas et al. 2013; Behroozi et al. 2019; Leja et al. 2021).

Fig. 6 shows the quiescent fraction in FIREbox both for central galaxies, satellites, and the full sample. Here, a galaxy is defined as quiescent at $z = 0$ if its sSFR averaged over the last 100 Myr is below a threshold of either $10^{-10.5} \text{ yr}^{-1}$ or 10^{-11} yr^{-1} . We also include the data from Leja et al. (2021) for the case of a 100 Myr SFR averaging time and a sSFR-based cut of $10^{-10.5} \text{ yr}^{-1}$ to separate quiescent and star forming galaxies. Additionally, we plot the predictions of an em-

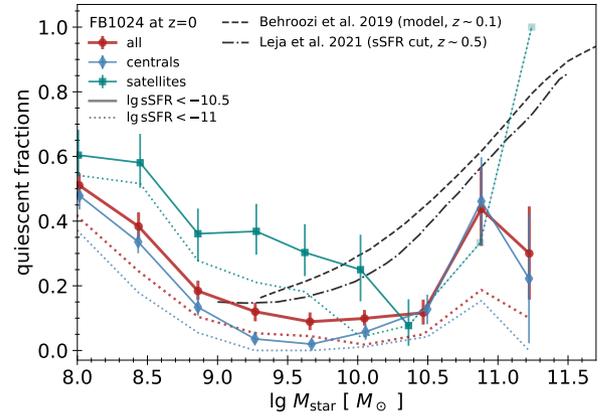


Figure 6. The fraction of quiescent galaxies in FIREbox at $z = 0$. Symbols and solid lines show the fraction of galaxies (red circles), central galaxies (blue diamonds), and satellite galaxies (green squares) with specific SFRs below $10^{-10.5} \text{ yr}^{-1}$. Dotted lines are the corresponding results for a specific SFR threshold of 10^{-11} yr^{-1} . Error bars refer to 16-84% percentiles in each bin obtained via bootstrapping. Light shaded symbols without error bars refer to bins containing less than 4 galaxies. Dot-dashed and dashed lines are observational and empirical estimates of the quiescent fraction by Leja et al. (2021) and Behroozi et al. (2019). SFRs of FIREbox galaxies are averaged over the last 100 Myr as in Leja et al. (2021). At $M_{\text{star}} \lesssim 10^{10} M_{\odot}$, satellite galaxies have a higher quiescent fraction than central (or all) galaxies, presumably as a result of environmental effects (e.g., Simha et al. 2009; Feldmann et al. 2011; Peng et al. 2012; Wetzel et al. 2013; Samuel et al. 2022). FIREbox generally underpredicts the quiescent fraction among massive galaxies when compared with observations. The difference is most severe at the highest masses $M_{\text{star}} > 10^{11} M_{\odot}$ but a significant difference is also seen in galaxies of intermediate mass $M_{\text{star}} \sim 10^{9.5-10.5} M_{\odot}$. Lowering the threshold from $10^{-10.5} \text{ yr}^{-1}$ to 10^{-11} yr^{-1} reduces the quiescent fraction significantly which shows that most quiescent, massive galaxies in FIREbox are not fully quenched.

pirical model by Behroozi et al. (2019) based on low z observational data (Bauer et al. 2013; Muzzin et al. 2013).

In FIREbox, 10-20% of moderately low mass galaxies ($M_{\text{star}} \sim 10^9 M_{\odot}$) are quiescent in agreement with observational data. However, FIREbox significantly underpredicts the quiescent fraction in more massive galaxies. For instance, 30% of $M_{\text{star}} \sim 10^{11.2} M_{\odot}$ galaxies are quiescent in FIREbox (for a $10^{-10.5} \text{ yr}^{-1}$ sSFR cut), compared with 70-80% in observations (Muzzin et al. 2013; Leja et al. 2021). Hence, stellar feedback alone (at least if modeled as in FIRE-2) is not sufficient to reproduce the observed fraction of massive, quiescent galaxies at $z \sim 0$. Evidently though, some massive, quiescent central galaxies can form even without additional feedback sources. However, these quiescent galaxies should be seen as an extension of the star forming sequence towards low SFRs and not as truly passively evolving (‘quenched’) galaxies, given that the majority of them have sSFR between $10^{-10.5} \text{ yr}^{-1}$ and 10^{-11} yr^{-1} . Perhaps they are related to the observed transition galaxies (Fang et al. 2018). We conclude that alternative forms of feedback, such as cosmic ray feedback (e.g., Booth et al. 2013; Salem & Bryan 2014; Chan et al. 2019; Hopkins et al. 2020) and AGN feedback (e.g., Springel et al. 2004; Croton et al. 2006; Vogelsberger et al. 2013; Wellons et al. 2022) are needed to reproduce observational data. Indeed, recent cosmological simulations with AGN feedback reproduce well the observed quiescent fraction at $z = 0$ (e.g., Furlong et al. 2015; Donnari et al. 2019).

At low stellar masses ($10^8 M_{\odot} < M_{\text{star}} < 10^9 M_{\odot}$), the quies-

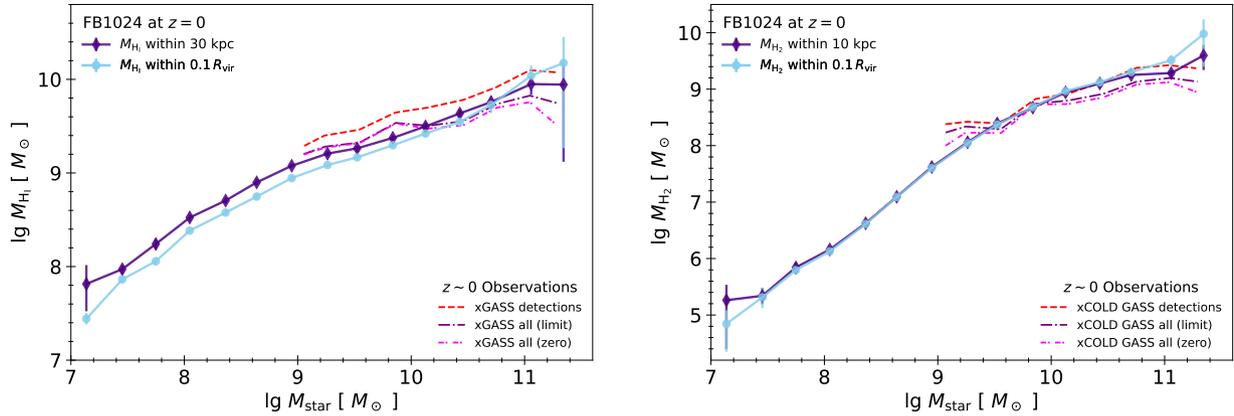


Figure 7. Relationship between the mass of atomic hydrogen (M_{HI} , left) or molecular hydrogen (M_{H_2} , right) and galaxy stellar mass at $z = 0$ in FIREbox and in observations. Symbols and solid lines show the logarithm of the average H_1 or H_2 mass in bins of stellar mass for central galaxies in FIREbox within a fixed physical radius (purple diamonds) and within $0.1 R_{\text{vir}}$ (light blue circles). Error bars refer to 16–84% percentiles of the average gas mass obtained via bootstrapping. Red dashed lines show analogously computed results for galaxies with detected gas masses ($5 - \sigma$ in H_1 , $3 - \sigma$ in H_2) from xGASS (Catinella et al. 2018) and xCOLD GASS (Saintonge et al. 2017) with updated stellar masses as presented in Feldmann (2020). Purple (Magenta) dot-dashed lines show corresponding xGASS and xCOLD GASS results when including non-detections by setting the gas mass to the detection limit (to zero). FIREbox predicts average atomic and molecular gas masses in good agreement with these observations. A broken-linear dependence captures well the scaling of M_{HI} and M_{H_2} with stellar mass, see Table 2.

cent fraction increases with decreasing mass. For instance, FIREbox predicts that for our chosen 100 Myr averaging time of star formation, 40–50% of all $M_{\text{star}} \sim 10^8 M_{\odot}$ galaxies are quiescent (the number reduces slightly to 35–45% if only central galaxies are considered), see also Feldmann (2017). The quiescent fraction is higher among satellite galaxies than centrals (for $M_{\text{star}} < 10^{10} M_{\odot}$), likely as a result of environmental quenching processes (e.g., Simha et al. 2009; Feldmann et al. 2011; Peng et al. 2012; Wetzel et al. 2013; Samuel et al. 2022). The high quiescent fraction at low stellar masses ($M_{\text{star}} < 10^9 M_{\odot}$), especially among centrals, may be in tensions with observations (Geha et al. 2012). We find that the averaging time of the SFR has a significant impact on the quiescent fraction at the low mass end. For a 10^{-11} yr^{-1} sSFR threshold, increasing the averaging time to 500 Myr reduces the quiescent fraction of centrals with $M_{\text{star}} = 10^{8.5} M_{\odot}$ from 16% to 4.8% (and from 37% to 12% for $M_{\text{star}} = 10^8 M_{\odot}$ centrals). In contrast, reducing the averaging time to 20 Myr, increases the quiescent fraction to 26% at $M_{\text{star}} = 10^{8.5} M_{\odot}$ and to 60% at $M_{\text{star}} = 10^8 M_{\odot}$. The dependence of the quiescent fraction on the averaging time is likely a consequence of the bursty nature of star formation in low mass FIRE galaxies (Sparre et al. 2017; Flores Velázquez et al. 2021). Numerical resolution may also play a role here, resulting in excessive burstiness at low stellar masses (Hopkins et al. 2018; Samuel et al. 2022).

3.3 The gas content of galaxies

Atomic and molecular gas masses of galaxies are correlated with their stellar masses (e.g., Catinella et al. 2010; Saintonge et al. 2011). Inferring the shape of these gas sequences is challenging because of a variety of measurement systematics and selection effects. The availability of ‘representative’ (in terms of H_1 and H_2 content), purely stellar mass selected galaxy samples (Saintonge et al. 2017; Catinella et al. 2018) substantially simplifies this challenges but biases may still arise from incorrect modeling assumptions and from the treatment of non-detections (e.g., Feldmann 2020).

We compare the gas content of FIREbox galaxies at $z = 0$ with observational data from xGASS (Catinella et al. 2018) and xCOLD

GASS (Saintonge et al. 2017) in Fig. 7. Specifically, we compare the average atomic and molecular hydrogen masses (M_{HI} and M_{H_2}) in bins of stellar mass. We lowered the molecular gas masses reported in (Saintonge et al. 2017) by a factor of 1.36 to exclude the contribution from Helium and metals. The gas masses of simulated galaxies are measured in 3-dimensional spheres of fixed physical radius⁶ r : 10 kpc for H_2 and 30 kpc for H_1 .

Gas masses (M_{HI} or M_{H_2}) are not detected in a significant fraction of the galaxies in xGASS and xCOLD GASS. This raises a subtle issue for the comparison with FIREbox. Instead of attempting a full forward modeling, we consider three basic possibilities of dealing with undetected sources. First, we include all galaxies in the observational catalog but assume that undetected sources have gas masses that correspond to their detection limit (‘all-limit’). Our second analysis is similar to the first but we assign undetected sources a gas mass of zero (‘all-zero’). The average gas mass calculated via these two

⁶ The precise values of these radii are somewhat arbitrary but we chose them for the following reasons. Low mass galaxies ($M_{\text{star}} < 10^{10} M_{\odot}$) in xGASS and xCOLD GASS are at redshifts $z = 0.01 - 0.02$, while the redshift range of more massive galaxies is $z = 0.025 - 0.5$. The 3.1–3.5 arcminute half power beamwidth of the Arecibo telescope at the relevant frequencies translates into an aperture radius of 21–41 kpc at $z = 0.01 - 0.02$ and a radius of 51–100 kpc at $z = 0.025 - 0.05$. A 30 kpc fixed radius is thus a sensible choice for galaxies with $M_{\text{star}} < 10^{10} M_{\odot}$, while for more massive galaxies we could adopt a larger radius. However, we find that even including all the atomic hydrogen in the virial radius of a $M_{\text{star}} = 10^{11} M_{\odot}$ galaxy ($R_{\text{vir}} \sim 280$ kpc) would increase the average H_1 mass by only 0.3 dex (and by significantly less in galaxies of lower stellar mass) compared to the 30 kpc fixed radius. The IRAM telescope has a beam width of 22 arcseconds at the frequency of the CO (1–0) line, which corresponds to aperture radii of 2.3–4.6 kpc for $z = 0.01 - 0.02$ and 5.7–11.1 kpc for $z = 0.025 - 0.05$. Adopting a fixed radius of 3 kpc instead of 10 kpc has only a small impact on the inferred H_2 mass of low mass FIREbox galaxies but misses a large fraction of the molecular gas mass in massive galaxies, e.g., M_{H_2} is lowered by 0.6 dex on average for a $M_{\text{star}} = 10^{11} M_{\odot}$ galaxy. Furthermore, the reported CO line luminosities in xCOLD GASS are aperture corrected to include contributions at larger radii belonging to the ISM.

approaches brackets the true value. Finally, we also calculate average gas masses for only the detected sources (‘detections’).

According to Fig. 7, the atomic and molecular hydrogen masses of FIREbox galaxies agree well (to usually better than 0.2 dex over the $M_{\text{star}} = 10^9 - 10^{11} M_{\odot}$ mass range) with those of galaxies (‘all-limit’ or ‘all-zero’) in xGASS and xCOLD GASS. The figure also shows the average atomic and molecular hydrogen masses of FIREbox galaxies within 10% of the virial radius. The latter masses differ usually only by a small amount (0.2 dex) from the average gas masses calculated in the chosen fixed physical radii.

FIREbox offers a prediction of how the atomic and molecular gas sequences scale towards low stellar masses. We find that a broken-linear scaling (in log-log space) captures the general behavior quite well over a broad range in stellar masses ($M_{\text{star}} = 10^7 - 10^{11.5} M_{\odot}$). Specifically, we adopt the following fitting function:

$$y = A + \alpha_1(x - x_b) + (\alpha_2 - \alpha_1) \left[\ln \left(1 + e^{\frac{x-x_b}{\Delta}} \right) - \ln 2 \right] \Delta, \quad (2)$$

where $y = \lg(M_{\text{H}_1}/M_{\odot})$ ($y = \lg(M_{\text{H}_2}/M_{\odot})$) is the logarithm of the average atomic (molecular) hydrogen mass in galaxies of a given stellar mass with $x = \lg(M_{\text{star}}/M_{\odot})$. This function has 5 fit parameters: an overall amplitude (A), a break stellar mass (x_b), a slope at low stellar masses (α_1), a slope at high stellar masses (α_2), and a parameter determining the smoothness of the transition from the low mass to the high mass regime (Δ). For $x \ll x_b$, $y \propto \alpha_1 x$, while for $x \gg x_b$, $y \propto \alpha_2 x$. The fit parameters are listed in Table 2.

Both gas sequences have a steeper slope at low stellar masses than at high stellar masses. For atomic hydrogen, we find a low mass slope near 1 (0.85 for $r = 30$ kpc, 1.15 for $r = 0.1 R_{\text{vir}}$), while for molecular hydrogen the slope is super-linear (1.6 for both $r = 10$ kpc and $r = 0.1 R_{\text{vir}}$). We speculate that the steeper slope in low mass galaxies is a consequence of stellar feedback and the UV background more strongly regulating their gas content (see e.g., van de Voort et al. 2016; Fitts et al. 2017; Hafen et al. 2019; Pandya et al. 2020). Furthermore, since lower mass galaxies tend to have lower ISM metallicities (e.g., Tremonti et al. 2004; Finlator & Davé 2008) and lower dust-to-metal ratios (e.g., Rémy-Ruyer et al. 2014; Feldmann 2015), a smaller fraction of the neutral ISM is in molecular form (e.g., Krumholz et al. 2008; Gnedin & Kravtsov 2011) thus explaining the steeper slope of the molecular gas sequence compared with the atomic gas sequence. At the high mass end, slopes are sub-linear (0.4 for atomic hydrogen and 0.3-0.6 for molecular hydrogen) qualitatively consistent with the decline of the atomic and molecular gas to stellar mass ratios with increasing stellar mass found observationally (e.g., Saintonge et al. 2017; Catinella et al. 2018) and in models (e.g., Davé et al. 2020). The break stellar mass between the two regimes is $10^{8.1-8.6} M_{\odot}$ for H_1 and $10^{9.6-9.8} M_{\odot}$ for H_2 . We find that galaxies with a stellar mass near the break stellar mass of the atomic (molecular) hydrogen sequence have an atomic (molecular) hydrogen content of $M_{\text{H}_1} \sim 10^{8.4-8.9} M_{\odot}$ ($M_{\text{H}_2} \sim 10^{8.5-8.7} M_{\odot}$).

3.4 The gas content of Milky Way analogs – where are the “missing” baryons?

The Milky Way (MW) is a particularly useful object of comparison for FIREbox given the abundance of measurements of the various mass components in the Galaxy and its halo. To this end, we selected all 23 FIREbox main halos with virial masses between $7.5 \times 10^{11} M_{\odot}$ and $2.5 \times 10^{12} M_{\odot}$ at $z = 0$. One system, a late stage, galaxy major merger, was excluded from the analysis below. The average halo mass of this sample is $1.3 \times 10^{12} M_{\odot}$ matching the current consensus estimate of the virial mass of the Milky Way (Bland-

Hawthorn & Gerhard 2016). The average virial radius of the sample is 279 kpc.

The MW contains about $8 \times 10^9 M_{\odot}$ of atomic hydrogen (Kalberla & Dedes 2008; McMillan 2017; Cautun et al. 2020) and $\sim (1 \pm 0.3) \times 10^9$ of molecular hydrogen (Heyer & Dame 2015; McMillan 2017). Both mass estimates are subject to large modeling uncertainties and are reported here without contributions from metals and Helium. While they only account for the gas in the MW disk and center, the neutral hydrogen mass in MW satellites is relatively low. The Large Magellanic Cloud (Small Magellanic Cloud) contributes about $5 \times 10^8 M_{\odot}$ in atomic hydrogen (Kim et al. 1999) ($4 \times 10^8 M_{\odot}$, Stanimirovic et al. 1999) and $\sim 5 \times 10^7 M_{\odot}$ in H_2 (Fukui et al. 1999) with some additional neutral gas in the Magellanic bridge, stream, and leading arm (e.g., Nidever et al. 2010; Besla et al. 2012). In comparison, FIREbox predicts an average atomic hydrogen mass of $6.37^{+1.27}_{-1.05} \times 10^9 M_{\odot}$ and a molecular hydrogen mass of $1.79^{+0.22}_{-0.27} \times 10^9 M_{\odot}$ within 10% of R_{vir} , both in reasonable agreement with observations. Here, sub- and superscripts refer to 16th and 84th percentiles of the averages obtained via bootstrapping. For the mass of neutral hydrogen FIREbox predicts $8.16^{+1.54}_{-1.36} \times 10^9 M_{\odot}$ which can be compared with the observed value of $\sim 9 \times 10^9 M_{\odot}$.

The mass of the warm-hot and hot gaseous halo (corona) around the Milky-Way has been constrained to $2.5 \pm 1 \times 10^{10} M_{\odot}$ via a variety of independent observables (Bland-Hawthorn & Gerhard 2016), including X-ray emission (Miller & Bregman 2015), pulsar dispersion measures from the Large Magellanic Cloud (LMC) (Anderson & Bregman 2010), H_{α} emission from the Magellanic H_1 stream (Bland-Hawthorn & Gerhard 2016), and ram-pressure effects on the LMC gas disk (Salem et al. 2015). A more recent estimate by Bregman et al. (2018) based on a combined analysis of a variety of observational data is $2.8 \pm 0.5 \times 10^{10} M_{\odot}$ of hot gas within 250 kpc of the MW. FIREbox predicts an average mass of gas with $T > 2 \times 10^5$ K of $3.24^{+0.64}_{-0.62} \times 10^{10} M_{\odot}$ within the virial radii of MW-like halos ($3.18^{+0.64}_{-0.60} \times 10^{10} M_{\odot}$ within $0.1 - 1 \times R_{\text{vir}}$), in good agreement with the observational estimates. These gas masses include contributions from Helium and metals. This warm-hot and hot gas amounts to 58% of the total gas mass in such halos and it exceeds the 35% fraction of cooler gas ($M_{\text{gas}}(T < 2 \times 10^4 \text{K}) = 1.9 \times 10^{10} M_{\odot}$). Gas at intermediate temperatures ($2 \times 10^4 \leq T/\text{K} \leq 2 \times 10^5$) contributes only about 7%, as expected from the high cooling rate in this temperature range.

Numerical models predict that hot halos around galaxies are strongly affected by galactic winds driven by feedback (e.g., van de Voort et al. 2016; Hafen et al. 2019; Stern et al. 2021b; Vijayan & Li 2021). Observations with future X-ray telescopes may be able to measure the diffuse halo gas in L_* galaxies out to moderate redshifts (Kaastra et al. 2013; Simionescu et al. 2021) thus potentially providing a sensitive probe of the physics of feedback processes. We plan to study the formation and evolution of hot halos in FIREbox galaxies in future work.

The observed baryonic content of the Milky Way halo falls short of the amount expected from the universal baryon fraction (McGaugh et al. 2010). Current observational estimates provide a baryon fraction (M_b/M_{halo}) of only 7% (Bland-Hawthorn & Gerhard 2016), i.e., less than half of $\Omega_b/\Omega_m = 15.7\%$. Whether significant amounts of halo baryons have evaded detection so far or whether they are truly ‘missing’ from the halo is still debated. In FIREbox, the baryon fraction of MW-like halos at $z = 0$ is $11.6^{+0.5}_{-0.4}\%$, i.e., only about 25% of the cosmic baryons are missing from MW halos, i.e., reside outside the halo either because they were removed at some point or never accreted in the first place.

The remaining “extra” baryons, compared with observations, are distributed among various matter components. First, a significant amount ($\sim 7 \times 10^9 M_\odot$) of ionized gas in MW-like halos in FIREbox has temperatures below 2×10^5 K, i.e., it is not in a hot phase. Interestingly, estimates based on modeling of the O_{VI} absorption line of L^* galaxies predict an even larger average mass of warm ionized gas (Werk et al. 2014). Secondly, the hot gas mass (see discussion above) and the galaxy stellar mass in FIREbox are slightly higher than empirical estimates. The average stellar mass of the centrals in our sample of MW analogs is $5.73^{+0.57}_{-0.53} \times 10^{10} M_\odot$ for $R_g = 3 R_{\text{half}}$ ($7.64^{+0.81}_{-0.63} \times 10^{10} M_\odot$ for $R_g = 0.1 R_{\text{vir}}$) compared with empirically determined stellar mass of $\sim 5 \times 10^{10} M_\odot$ (Flynn et al. 2006; Cautun et al. 2020) for the MW. Finally, halos of MW analogs in FIREbox harbor a significant amount of stars in a smooth extragalactic component ($2.4^{+0.3}_{-0.3} \times 10^{10} M_\odot$ for a galaxy size of $R_g = 3 R_{\text{half}}$, $5.6^{+0.8}_{-1.0} \times 10^9 M_\odot$ for $R_g = 0.1 R_{\text{vir}}$) and in satellite galaxies ($\sim 9 \times 10^9 M_\odot$). This extra-galactic stellar component exceeds current observational estimates of the ‘stellar halo’ of the MW ($\sim 1.4 \times 10^9 M_\odot$ Deason et al. 2019; Mackereth & Bovy 2020). However, the latter estimates involve various modeling and selection steps that will need to be properly taken into account, e.g., via forward modeling of our simulated galaxies, to allow for a direct, quantitative comparison.

3.5 Mass-metallicity relation

The metallicity of the ISM is set by a complex network of processes including metal injections from supernovae (Woosley & Weaver 1995; Nomoto et al. 2006), star formation, galactic outflows that remove metals from galaxies, and inflows of comparably metal-poor gas from the cosmic environment (Sánchez Almeida et al. 2014; Muratov et al. 2015, 2017). The observation of a correlation between ISM metallicity and the stellar mass of galaxies, the mass–metallicity relation (MZR, Tremonti et al. 2004), may thus provide insights into the role these processes play in galaxy evolution. Various physical mechanisms have been proposed to explain the MZR including the ejection of metal-rich gas from low mass halos by supernova feedback (Dekel & Silk 1986; Dekel & Woo 2003), inefficient star formation (due to feedback in the ISM) in low mass galaxies (Brooks et al. 2006), and the potential under-abundance of massive stars in low mass galaxies as a result of clustered star formation (Köppen et al. 2007).

In the equilibrium model of galaxy formation (Larson 1972; Finlator & Davé 2008; Davé et al. 2012; Feldmann 2013; Lilly et al. 2013; Dekel & Mandelker 2014), the ISM metallicity is set by the present balance of metal enrichment, removal, and dilution processes with any memory of the past enrichment level erased over a few gas depletion times. In this model, the star formation activity in a galaxy adjust such that stellar feedback driven outflows roughly balance any gas inflows resulting in gas and metal masses in the ISM that are approximately constant in time. Low mass galaxies tend to have large mass loading factors (Muratov et al. 2015; Anglés-Alcázar et al. 2017a; Pandya et al. 2021), and thus require only small SFRs to achieve this balance, resulting in low equilibrium metallicities (Finlator & Davé 2008). The self-regulatory feature of this model also helps to explain why the MZR has such a small scatter. Furthermore, by allowing for evolving ISM masses, this model naturally introduces a dependence of the ISM metallicity on SFR at fixed stellar mass (Lilly et al. 2013) as potentially observed (Mannucci et al. 2010; Sanders et al. 2021).

While the metallicity of the ISM is expected to quickly reach equilibrium values under most circumstances, the metallicity in the photosphere of stars is determined to a large degree by the metallicity

of the molecular clouds they formed from. The stellar metallicity of galaxies thus reflects both the past ISM metallicity, the star formation history, and the accretion of stars in galaxy mergers. In addition, it may hold clues to the nature and time scale of galaxy quenching (Peng et al. 2015). Similar to ISM metallicities, the stellar metallicities of observed galaxies are found to correlate with their stellar masses (Gallazzi et al. 2005).

We compare the gas phase and stellar metallicities of FIREbox with observational data in Fig. 8. Observed oxygen abundances are reproduced in the figure as originally reported (Tremonti et al. 2004; Lee et al. 2006; Sánchez et al. 2019). Kirby et al. (2013) assumed a Solar iron abundance of 7.52 (consistent with Asplund et al. 2009) and we use this value to convert their results from relative to absolute abundances. Gallazzi et al. (2005) measured stellar metallicities (relative to Solar) via stellar absorption indices based primarily on magnesium and iron lines. We equate their reported metallicities with iron abundances relative to Solar and convert to absolute values using again a Solar iron abundance of 7.52. To aid the comparison with observations, we measure metallicities in FIREbox in a 3-dimensional aperture radius of 3 kpc to match approximately the 1.5 arcsecond radius of SDSS fibers at the median redshift ($z \sim 0.1$) of the samples of Tremonti et al. (2004) and Gallazzi et al. (2005). However, since this radius is too small to include gas in the outskirts of larger galaxies, we also provide a more scale-invariant aperture choice of $0.1 R_{\text{vir}}$. To account for oxygen depletion inside HII regions, we reduce the oxygen abundance predicted by the simulation by 0.12 dex (Peimbert & Peimbert 2010). This quantitative comparison likely suffers from additional systematic uncertainties related to, e.g., the observational metallicity calibration as well as the metal yields and supernova rates adopted by the simulation (Hopkins et al. 2018), all of which are beyond the scope of this paper.

To highlight the general trend between metallicity and stellar mass, we aggregate the metallicities of FIREbox galaxies in 0.3 dex wide bins of stellar mass. Specifically, we show in Fig. 8 the quantities $12 + \lg(\langle \text{O}/\text{H} \rangle)$ (top left panel) and $12 + \lg(\langle \text{Fe}/\text{H} \rangle)$ (top right panel), where $\langle \text{O}/\text{H} \rangle$ ($\langle \text{Fe}/\text{H} \rangle$) represents the average ratio between the number of oxygen and hydrogen nuclei in the gas phase (the average ratio between the number of stellar iron nuclei and stellar hydrogen nuclei) of FIREbox galaxies in 0.3 dex wide bins of stellar mass. In the bottom panels we show the corresponding scatter defined as half the difference between the 84 and 16 percentile of $12 + \lg(\text{O}/\text{H})$ or $12 + \lg(\text{Fe}/\text{H})$ for the galaxies in the given stellar mass bin.

FIREbox broadly reproduces the observed MZR at $z = 0$ over ~ 5 orders of magnitude in stellar mass (Tremonti et al. 2004; Lee et al. 2006; Sánchez et al. 2019), similar to previous results of FIRE-1 zoom-in simulations (Ma et al. 2016). The match is not perfect, however, as FIREbox possibly slightly overpredicts (underpredicts) the oxygen abundance in galaxies with $M_{\text{star}} > 10^{10} M_\odot$ (with $M_{\text{star}} < 10^{7.5} M_\odot$). We caution that this comparison is plagued by calibration systematics which can exceed 0.2 dex (Kewley & Dopita 2002; Kewley & Ellison 2008; Sánchez et al. 2019). As a specific example, we show the MZR reported by Sánchez et al. (2019) for two different metallicity calibrations; one based on [NII], [SII] and H α emission lines (Dopita et al. 2016), the other one using [OII], [OIII], and H β (Pagel et al. 1979; Tremonti et al. 2004).

Matching simultaneously both the observed MZR and the star forming sequence of low mass galaxies ($M_{\text{star}} \lesssim 10^9 M_\odot$) has been pointed out as a major challenge for galaxy formation models (Somerville & Davé 2015). The reasonable match between FIREbox and the observational data shown in Fig. 5 and Fig. 8 suggests

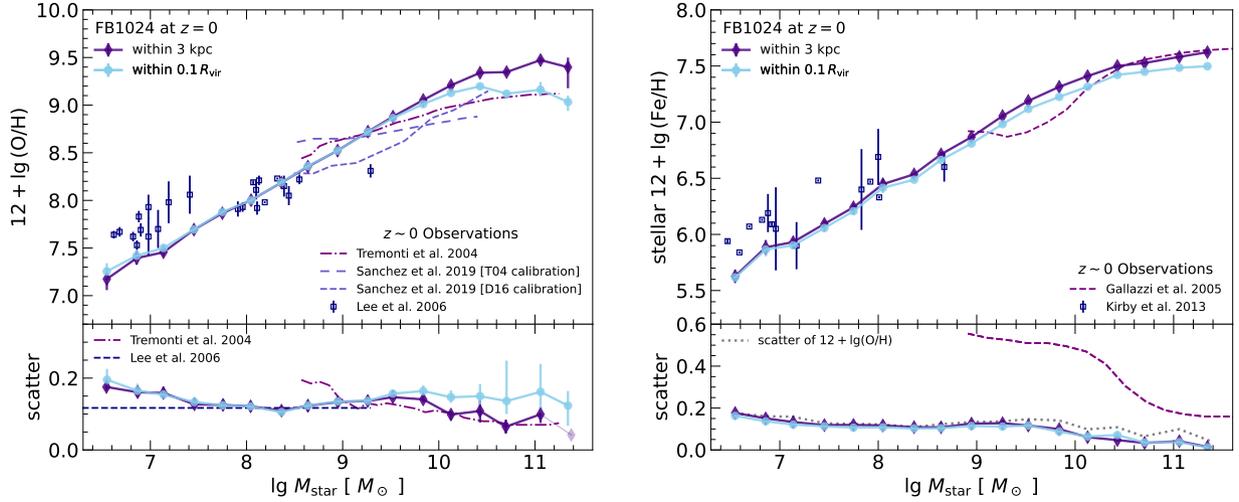


Figure 8. Relationship between the gas-phase oxygen abundance (left) or stellar iron abundance (right) and galaxy stellar mass at $z = 0$ in FIREbox and in observations. In the upper left panel, solid lines show the logarithm of the average oxygen abundance plus 12 for FIREbox galaxies in bins of stellar mass for a 3 kpc fixed physical radius (purple diamonds) or within $0.1 R_{\text{vir}}$ (light blue circles). Error bars (16–84 percentiles) are obtained via bootstrapping. Observational data (Tremonti et al. 2004; Lee et al. 2006; Sánchez et al. 2019) are included in the figure as dot-dashed lines, square symbols, and dashed lines. The scatter (one half of the 16–84% percentile range) of the logarithmic oxygen abundance at a fixed stellar mass is shown in the lower left panel. FIREbox predicts that the stellar mass – gas phase metallicity relation has low scatter ($\sim 0.1 - 0.2$) both in massive and low mass galaxies. The panels on the right hand side are analogous to the panels on the left but for the stellar iron abundance instead of the gas-phase oxygen abundance. Observational data is from Gallazzi et al. (2005) (dashed lines) and Kirby et al. (2013) (square symbols). Broken-linear dependences capture well the scaling of the gas-phase oxygen abundance and stellar iron abundance with stellar mass in FIREbox, see Table 2. The scatter of the stellar mass – stellar metallicity relation in FIREbox increases towards lower stellar masses but it is generally lower than the scatter of the stellar mass – gas phase metallicity relation (the dotted line in the bottom right panel reproduces the scatter of the latter relation for a 3 kpc aperture radius as shown in the bottom left panel).

that cosmological simulations with the FIRE-2 physics model are a significant step towards overcoming this challenge.

The MZR in FIREbox shows clear evidence of a flattening at the massive end. This flattening has been observed for many metallicity calibrators (e.g., Tremonti et al. 2004; Sánchez et al. 2019). Given its presence in FIREbox, we infer that the flattening of the MZR as reported by observations is likely not merely a consequence of aperture bias (Kirby et al. 2013). Instead, provided the equilibrium view of galaxy formation is correct, the flattening can be explained by the mass loading factors approaching, and falling below, unity in massive galaxies (Finlator & Davé 2008; Muratov et al. 2015). The relation between mass loading factor η and equilibrium metallicity is $Z_{\text{eq}} \propto y/(1 - R + \eta)$, see Finlator & Davé (2008) and Lilly et al. (2013), where y is the metal yield and $R \sim 0.5$ the mass return fraction (Krumholz & Dekel 2012). The equilibrium metallicity is approximately independent of the mass loading factor for $\eta \ll 1$.

The MZR can be well fit with a broken linear relation given by equation (2) with $y = 12 + \lg(\langle \text{O}/\text{H} \rangle)$ and $x = \lg M_{\text{star}}$. The fit parameters are provided in Table 2. For the 3 kpc aperture radius, the MZR is sub-linear with a slope of ~ 0.6 at low stellar masses and almost flat with a slope of ~ 0.2 at high stellar masses. The transition between the two regimes occurs at a break stellar mass of $\sim 10^{10.3} M_{\odot}$.

Focusing on the scatter of the MZR, FIREbox predicts a value of $\sim 0.1 - 0.15$ for much of the probed stellar mass range, in agreement with observations (Tremonti et al. 2004; Lee et al. 2006). Furthermore, the scatter is predicted to decrease slightly at the massive end if the 3 kpc aperture is used in line with results by Tremonti et al. (2004). However, as shown in the lower left panel of Fig. 8, the scatter is almost independent of stellar mass if an $0.1 R_{\text{vir}}$ aperture radius is adopted.

FIREbox predicts a relation between stellar iron abundance and stellar mass that is in approximate agreement with observational data (Gallazzi et al. 2005; Kirby et al. 2013), except perhaps at the lowest masses ($M_{\text{star}} < 10^8 M_{\odot}$). This overall behavior is consistent with the results of FIRE-2 zoom-in simulations (Gandhi et al. 2022). The relation between iron abundance and stellar mass follows the same general trend as the MZR and can also be approximated well by a broken linear function (equation 2 with $y = 12 + \lg(\langle \text{Fe}/\text{H} \rangle)$), see Table 2 for the best fit parameters. At low stellar masses, the slope is sub-linear and slightly smaller (0.53 for the 3 kpc aperture radius) than the slope of the MZR. The latter is expected given that the stellar metallicity relation is effectively a convolution of the MZR and the stellar growth history. The stellar metallicity relation significantly flattens (slope 0.13) in massive galaxies, similar to the MZR.

Interestingly, FIREbox predicts a much smaller scatter in stellar metallicities at given stellar mass than reported in the observational study by Gallazzi et al. (2005). The authors of the latter study point out that their high scatter may reflect, at least partly, the high observational uncertainties in measuring stellar metallicities. In fact, the stellar mass – stellar metallicity relation predicted by our simulation is even tighter than the MZR with a scatter of less than 0.05 in $M_{\text{star}} > 10^{10.5} M_{\odot}$ galaxies. We speculate that this lower scatter is a consequence of the stellar metallicity being a (SFR weighted) time-average of the gas phase metallicity.

3.6 Galaxy stellar mass functions

The stellar mass function (SMF) of galaxies provides an important point of comparison to observational data for galaxy formation simulations. Here, we use observational data spanning $z = 0 - 8$ (Baldry et al. 2012; Moustakas et al. 2013; Tomczak et al. 2014; Song et al.

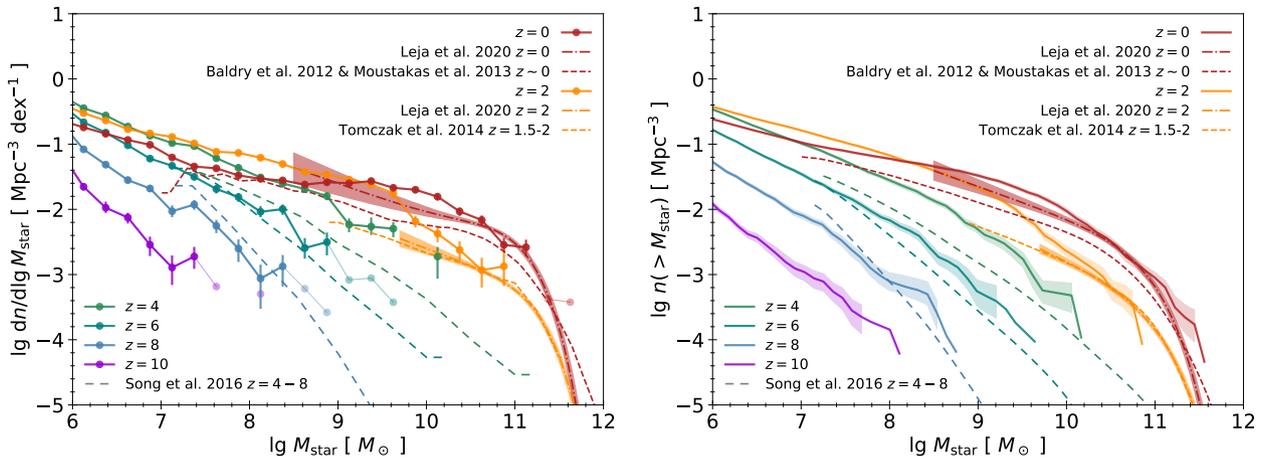


Figure 9. Stellar mass function (SMF) predicted by FIREbox for $z = 0 - 10$ and a comparison with observational estimates. In the left panel (right panel), circles (solid lines) show the differential (cumulative) SMF of all galaxies with $M_{\text{star}} > 10^6 M_{\odot}$ in the simulation volume. The abundance of galaxies is re-weighted to account for cosmic variance in the halo mass function, see Appendix A. Uncertainties (16-84%) of the differential and cumulative SMFs are calculated via bootstrapping and shown by error bars (left panel) or shaded regions (right panel). The panels also show observational estimates of the SMF at various redshifts (Baldry et al. 2012; Moustakas et al. 2013; Tomczak et al. 2014; Song et al. 2016; Leja et al. 2020). FIREbox predicts a SMF at $z = 0$ similar to recent estimates by Leja et al. (2020) based on non-parametric modeling except for a moderate excess at both low and high stellar masses. The $z = 0$ SMF is generally higher than those based on more traditional stellar mass estimates (e.g., Baldry et al. 2012; Moustakas et al. 2013). FIREbox struggles in reproducing the differential SMF in galaxies with $M_{\text{star}} \sim 10^{8.5} - 10^{10} M_{\odot}$ at $z \leq 4$ as a result of limited numerical convergence (see text). Interestingly, FIREbox predicts a high-mass turn-over in the SMF at low z , even though AGN feedback is not included.

2016) as provided by Behroozi et al. (2019). In addition, we compare with SMF estimates from the recent work by Leja et al. (2020). All data is converted (if necessary) to a Chabrier (2003) IMF.

The realized halo mass function (HMF) in FIREbox differs from the true HMF because of the finite box size and limited numerical resolution. Similarly, the realized SMF in FIREbox differs from the SMF that would be obtained if the exact same physical model were applied to an infinitely large cosmological volume. To account for the latter, we opt to apply a re-weighting approach, see Appendix A. This re-weighting procedure differs from similar methods to constrain SMFs from observational data (e.g., Efstathiou et al. 1988; Weigel et al. 2016) in that it aims to correct for variations in halo abundance instead of limits in stellar mass or luminosity.

Fig. 9 shows both the differential and the cumulative SMF in FIREbox for $z = 0 - 10$. At $z \geq 6$, the shape and normalization of the SMF in FIREbox agrees reasonably well with observations. The low mass slope of the simulated SMF decreases with decreasing redshift in qualitative agreement with Song et al. (2016). At $z \leq 4$, the SMF in FIREbox is higher than observed, especially for galaxies of $M_{\text{star}} \sim 10^9 - 10^{10} M_{\odot}$. A similar, but weaker, behavior has been reported in previous SAMs and hydrodynamical simulations (e.g., Vogelsberger et al. 2014; Somerville et al. 2015). At low redshift, FIREbox overpredicts the abundance (or stellar masses) compared with traditional SMF estimates (Baldry et al. 2012; Moustakas et al. 2013) but is in much better agreement with recent studies in which stellar masses are inferred from a non-parametric modeling of the star formation histories of galaxies Leja et al. (2020), especially for MW analogs with $M_{\text{star}} \sim 10^{10.5} M_{\odot}$. We note that FIREbox simulations are not tuned to reproduce any of the SMFs, in contrast with most other cosmological simulation suites (e.g., Vogelsberger et al. 2014; Schaye et al. 2015; Pillepich et al. 2018a), i.e., our results are predictions directly based on the FIRE-2 physics model.

We re-iterate two main areas of disagreement in Fig. 9. First, at low to intermediate stellar masses ($M_{\text{star}} \sim 10^{8.5} - 10^{10} M_{\odot}$), FIREbox overestimates the observed SMF at $z \leq 4$. A comparison with high resolution ($m_b < 10^4 M_{\odot}$) FIRE zoom-in simulations

shows that galaxies in moderately low mass ($M_{\text{halo}} \sim 10^{11} M_{\odot}$) halos have lower stellar masses at increased numerical resolution, see Appendix B. Unfortunately, this implies that the stellar masses of such galaxies are not converged at the resolution of FIREbox.

Secondly, at high stellar masses, FIREbox appears to over-predict galaxy abundances. Here the stellar masses are converged, see Appendix B. Given that FIREbox does not include AGN feedback, a mismatch at the massive end is not unexpected. However, the shape of the simulated SMF at the massive end ($M_{\text{star}} > 10^{10.5}$) may still be marginally consistent with the observations by Leja et al. (2020) if we account for the low numbers of massive galaxies in FIREbox and the associated large statistical errors. In any case, FIREbox appears to show a turn-over in the SMF at the massive end, above which the SMF becomes significantly steeper, which is qualitatively similar to observations. We highlight this point since the break in the SMF is often attributed to AGN feedback which is not included here. Hence, while galaxy quenching by AGN feedback may be needed to reproduce the exact position and shape of the SMF at the high-mass end, it may not be the primary reason that the SMF shows a break. We discuss the physical origin of this turn-over in more detail in the next section.

Finally, FIREbox suggests that the SMF decreases by up to ~ 0.3 dex with decreasing redshift at the lowest stellar masses ($M_{\text{star}} < 10^9 M_{\odot}$) between $z = 2$ and $z = 0$, which is qualitatively similar to the behavior of the low mass end of the HMF over this redshift range. Whether this trend is consistent with observations is currently not known given that $M_{\text{star}} \sim 10^9 M_{\odot}$ is close to the mass completeness limit of galaxy surveys exploring the SMF at $z = 1 - 2$ (Tomczak et al. 2014; Leja et al. 2020). Also, semi-empirical models do not necessarily predict this trend (Behroozi et al. 2019). Future, deeper observations may be required to test this prediction of our model.

3.7 Stellar mass – halo mass relation

The galaxy stellar mass – halo mass relation (SHMR) is closely related to the SMF. The latter can be obtained from the former (and

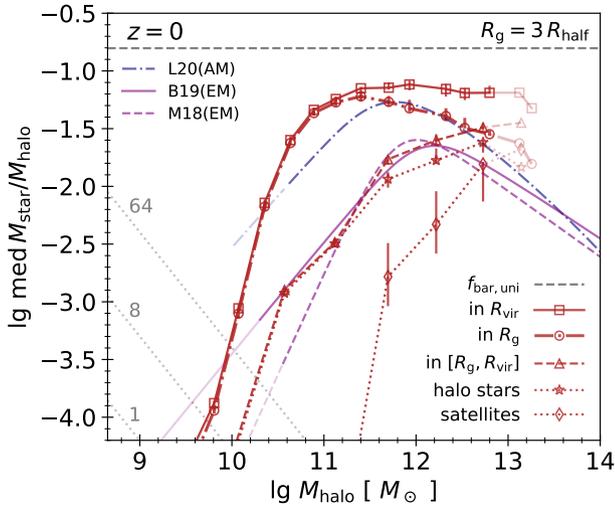


Figure 10. Median stellar mass fractions of central galaxies and their parent halos in FIREbox at $z = 0$. Different symbols refer to different mass components in the simulation. The galaxy stellar mass – halo mass relation (SHMR) is shown by circles. The galaxy stellar mass is defined as the stellar mass within 3 times the stellar half-mass radius, see section 2.6. Squares show the total stellar mass – halo mass relation. The galaxy and total stellar masses differ because of the stellar mass component outside the central galaxy but within the halo (triangles). The latter is further split into the stellar mass within identified sub-halos (diamonds) and stellar mass outside identified sub-halos (stars). Gray dotted lines correspond to 1, 8, and 64 star particles of mass $m_b = 6.3 \times 10^4 M_\odot$ in halos of a given mass (from bottom to top). Estimates of the galaxy stellar mass – halo mass relation (SHMR) via abundance matching (AM, Leja et al. 2020, dot-dashed line) and empirical modeling (EM, Moster et al. 2018; Behroozi et al. 2019, dashed and solid lines) are also shown. Extrapolations beyond the stellar mass range of the observational data are shown by a light colored line. The galaxy stellar fraction decreases with increasing halo mass for $M_{\text{halo}} > 10^{11.5} M_\odot$, while the total stellar fraction scales only weakly with M_{halo} over the $10^{11.5-13} M_\odot$ mass range. The increase in the stellar mass outside massive galaxies is driven by an increasing halo star contribution and, for $M_{\text{halo}} > 10^{12} M_\odot$, by a higher lock-up of stars in satellite galaxies.

vice versa) with the help of the HMF. We use this ansatz (abundance matching, AM) to calculate the SHMR from the SMFs provided by Leja et al. (2020). For simplicity of the calculation we ignore the scatter (~ 0.2 dex, Reddick et al. 2013; Zu & Mandelbaum 2015) of the SHMR. Given that FIREbox matches approximately the $z = 0$ SMF of Leja et al. (2020), we also expect a reasonable agreement with the derived SHMR. An alternative method of estimating the SHMR from observational data is empirical modeling (Moster et al. 2018; Behroozi et al. 2019). Here, we expect some level of disagreement, however, as these models are based on the SMFs derived from traditional SED-fitting, see discussion of Fig. 9.

The SHMR of central galaxies in FIREbox at $z = 0$ is given in Fig. 10. The ratio between galaxy stellar mass and halo mass rises quickly with increasing mass for $M_{\text{halo}} < 10^{11} M_\odot$, it reaches a peak near $M_{\text{halo}} \sim 10^{11.4} M_\odot$ with a maximum value ~ 0.42 dex below the universal baryon fraction, and then decreases slowly toward larger masses. We obtain a qualitatively similar result if we define the galaxy radius as $R_g = 0.1 R_{\text{vir}}$ instead of $3 R_{\text{half}}$ (not shown). However, in this case, the decline of the galaxy stellar fraction with increasing halo mass is shallower and the peak is shifted to $M_{\text{halo}} \sim 10^{11.7} M_\odot$.

Overall, the SHMR of FIREbox agrees with the AM prediction based on the Leja et al. (2020) SMF for $\sim 10^{11.5} - 10^{13} M_\odot$ halos and for our fiducial choice $R_g = 3 R_{\text{half}}$. However, we point out the shift

in the peak position (by about 0.4 dex) and the higher stellar mass in simulated halos with $M_{\text{halo}} \sim 10^{10.5} - 10^{11.4} M_\odot$. The latter result may also partly explain the overestimate of the extra-galactic stellar component around simulated MW analogs discussed in section 3.4 as their stellar halos are largely built from tidally disrupted galaxies in $\sim 10^{11} M_\odot$ halos (e.g., Purcell et al. 2007). As expected, empirical estimates (Moster et al. 2018; Behroozi et al. 2019) differ significantly from the simulation estimates with the former showing overall lower stellar masses in $M_{\text{halo}} > 10^{10} M_\odot$ halos.

We now further investigate the decrease of the galaxy stellar fraction in massive galaxies seen in FIREbox. A similar behavior has been found empirically and it is often attributed to AGN feedback (Croton et al. 2006). Given the lack of the latter in FIREbox, there are several remaining possibilities which could explain this result. First, more massive halos could lose a larger fraction of their gas, e.g., by stellar feedback driven outflows, before they are converted to stars. We can discount this possibility since $10^{12} M_\odot$ halos contain about 75% of the universal baryon fraction, see section 3.4. Furthermore, a more detailed study of the baryon content of FIREbox halos (Feldmann et al. in prep) shows that the baryon fraction of massive halos does not strongly decrease with increasing halo mass. Secondly, more massive halos could convert a smaller amount of the available baryons into stars potentially due to, e.g., the formation of a stable virial shock which keeps much of baryons in a hot, dilute state (Birnbom & Dekel 2003; Kereš et al. 2005; Faucher-Giguère et al. 2011; Stern et al. 2020). Finally, a similar amount of baryons may be converted into stars but the distribution of the stars could be more extended in more massive halos, e.g., a larger fraction of the stellar mass could reside in satellite galaxies or in a stellar halo.

To investigate these latter possibilities, we also show in Fig. 10, the total stellar mass in halos, the stellar mass in satellite galaxies, and the stellar mass in halo stars (defined as stars within a halo but outside any galaxy). While the ratio between galaxy stellar mass and halo mass decreases with increasing halo mass for $M_{\text{halo}} > 10^{11.5} M_\odot$, the stellar mass within the halo (total stellar mass) is an approximately constant fraction of the halo mass over the $M_{\text{halo}} = 10^{11.5} - 10^{12.5} M_\odot$ regime, with potentially a weak decline at the highest halo masses. Hence, we can largely exclude the second possibility mentioned above and conclude that a change in the spatial distribution of the stellar component, rather than a change in the baryonic conversion efficiency, drives the high-mass turn-over in the SMFs seen in Fig. 9 and the reduction of the galaxy stellar fraction in massive halos seen in Fig. 10.

Taking a closer look, we see that stars that do not belong to identified sub-halos (“halo stars”) make up the majority of the stellar mass outside of centrals in $M_{\text{halo}} \lesssim 10^{12} M_\odot$ halos. In more massive halos, stars locked up in satellite galaxies also contribute at a significant level. For Milky-Way like systems ($M_{\text{halo}} \sim 10^{12} M_\odot$), FIREbox predicts that the ratio between the stellar mass outside the central galaxy and the galaxy stellar mass is $\sim 0.45 \pm 0.05$ (if $R_g = 3 R_{\text{half}}$) and $\sim 0.13 \pm 0.03$ (if $R_g = 0.1 R_{\text{vir}}$), i.e., a sizable, but definition-dependent fraction of the total stellar mass resides outside central galaxies. A similar conclusion was reached by Pillepich et al. (2014) who analyzed the stellar mass outside galaxies for a set of cosmological volume (Vogelsberger et al. 2014) and zoom-in (Guedes et al. 2011; Marinacci et al. 2014) simulations using $R_g = 2 R_{\text{half}}$. They reported ratios ranging from ~ 0.1 to 0.6, depending on the simulation suite, for Milky-Way like halos, similar to our findings. We conclude that the decrease of the galaxy stellar fraction with increasing halo mass in FIREbox is driven primarily by an increasing contribution of a smooth halo star component and, at the highest masses, by a higher amount of stars in satellite galaxies.

4 COSMIC EVOLUTION OF GAS, STARS, AND STAR FORMATION

A major achievement of observational efforts with the Hubble and Spitzer Space Telescopes, as well as ground-based instruments, has been to map out the cosmic star formation history and stellar mass build-up from the Cosmic Dawn to the present time (Lilly et al. 1996; Madau et al. 1996; Hopkins & Beacom 2006; Madau & Dickinson 2014; Bouwens et al. 2015). In addition, observations of the neutral and molecular hydrogen content have made it possible to study how star formation in galaxies is fueled, see, e.g., Walter et al. (2020). Clearly, these observations provide an important point of comparison for galaxy models. In this section, we compare the evolution of the cosmic density of SFR, stellar mass, and atomic and molecular gas in FIREbox to observational data to further validate, and explore the limitations of, the FIRE-2 physics model.

4.1 Cosmic star formation history and stellar mass

Fig. 11 analyzes the cosmic star formation history (CSFH) and the cosmic stellar growth history (CSGH) in FIREbox. Specifically, it plots the volume-averaged SFR density and the stellar mass density as a function of redshift both for all identified galaxies in the simulation volume and for sub-sets of galaxies based on their stellar mass. Star formation rates are averaged over the past 20 Myr. The abundances of simulated galaxies are re-weighted based on their halo masses as described in Appendix A. We use a Locally Weighted Scatterplot Smoothing approach (Cleveland 1979) to reduce the noise in our predictions for the CSFH and CSGH.

When analyzing the CSFH and CSGH for galaxies of different stellar masses, we find that cosmic star formation and stellar mass are dominated by low mass galaxies at high z ($M_{\text{star}} < 10^8 M_{\odot}$ at $z > 7$). With decreasing z , more massive galaxies take over as main contributors. Since Cosmic Noon, galaxies with $10^{10} M_{\odot} < M_{\text{star}} < 10^{11} M_{\odot}$ dominate both the CSFH and the CSGH.

We can compare the prediction of our simulation with the compilation of observational data by Madau & Dickinson (2014). We take the data as is except that we adjust stellar masses and SFRs for the assumption of a Chabrier (2003) IMF using the conversion factors provided by authors. The observational data only includes sufficiently luminous galaxies ($L > 0.03L_{*}$) which corresponds to a stellar mass threshold of approximately $M_{\text{star,lim}} = 10^{9.3} M_{\odot}$ over $z = 0 - 3$ (Madau & Dickinson 2014).

We integrate the fit to the CSFH reported by Madau & Dickinson (2014) to obtain the corresponding average CSGH as follows:

$$\rho_{\text{star}}(t) = [1 - R_{\text{eff}}(t)] \int_0^t \rho_{\text{SFR}}(t') dt', \quad (3)$$

where $R_{\text{eff}} = 0.27$ is the effective mass return fraction⁷, which depends not only on the IMF but also on $\lg M_{\text{star,lim}}$.

⁷ This value was adopted by Madau & Dickinson (2014) based on the asymptotic mass return fraction of a Salpeter (1955) IMF. While the asymptotic mass return fraction for a Chabrier (2003) (or Kroupa 2001) IMF is $R \sim 0.4$, it should be noted that R_{eff} and R are different quantities. In FIREbox, $R_{\text{eff}}(z) \sim 0.35 - 0.11z$ holds for $z = 0 - 6$ if $\lg M_{\text{star,lim}} = 10^{9.3} M_{\odot}$ is adopted. Given that R_{eff} evolves with z in a mass threshold dependent manner, we adopt a constant value $R_{\text{eff}} = 0.27$ for simplicity. For a non-zero mass threshold, R_{eff} can become smaller than zero (i.e., $1 - R_{\text{eff}} > 1$) at high z . The reason being that galaxies with masses below the threshold never contribute to ρ_{SFR} , but the stellar mass they form is included in ρ_{star} once the masses of their descendants exceed the threshold.

Comparing the simulation predictions (thick black line) and observations (thin gray line) in Fig. 11, we find excellent agreement over $z \sim 1.5 - 4.5$. At higher redshifts, the CSFH and CSGH of $M_{\text{star,lim}} > 10^{9.3} M_{\odot}$ galaxies falls short of the observational data. Here, however, the assumed equivalence between $L = 0.03L_{*}$ and $M_{\text{star,lim}} > 10^{9.3} M_{\odot}$ likely does not hold given the younger stellar ages and lower metallicities of high z galaxies. Generally, the inferred CSFH (or CSGH) decreases much faster with increasing z when galaxies with low stellar masses (here $\lg M_{\text{star}} < 10^{9.3} M_{\odot}$) are excluded given their increased contribution to the total CSFH and CSGH at higher z . We defer a detailed analysis of the high redshift properties of FIREbox galaxies to future work. At $z \leq 0.7$, the CSFH in FIREbox differs noticeably from observational data. At $z = 0$ the predicted SFR density exceeds observations by ~ 0.5 dex, while the stellar density is too high by $\sim 0.1 - 0.2$ dex.

To understand the origin of this discrepancy at low z we separate the FIREbox sample into various stellar mass bins and calculate their contribution to the cosmic SFR density. We compare the simulation data with observational estimates of the cosmic SFR density (Brinchmann et al. 2004; Juneau et al. 2005; Salim et al. 2007). In the following, we specifically compare with the work by Salim et al. (2007) but we found similar results when using the data by Brinchmann et al. (2004). The SFR density in low mass galaxies is in approximate agreement with observations. Specifically, FIREbox predicts a contribution of $10^8 M_{\odot} \leq M_{\text{star}} < 10^9 M_{\odot}$ galaxies that is about 0.25 dex lower than observed and a contribution from galaxies of intermediate mass ($10^9 M_{\odot} \leq M_{\text{star}} < 10^{10} M_{\odot}$) is about 0.3 dex higher than observed. In contrast, massive galaxies ($10^{10} M_{\odot} \leq M_{\text{star}} < 10^{11} M_{\odot}$ and $10^{11} M_{\odot} \leq M_{\text{star}}$) in FIREbox contribute at much higher levels to the cosmic SFR than found observationally (~ 0.5 dex and ~ 1 dex). Massive galaxies thus appear primarily responsible for the high cosmic SFR at low z , presumably because of the lack of AGN feedback in FIREbox.

To test whether the low quenched fraction in FIREbox can explain the high cosmic SFR, we reduce the cosmic SFR in each stellar mass bin by the expected fraction f_Q of quenched galaxies given by Behroozi et al. (2019). Specifically, we use $f_Q = 20\%$, 45% and 90% for the stellar mass bins of $10^9 M_{\odot} \leq M_{\text{star}} < 10^{10} M_{\odot}$, $10^{10} M_{\odot} \leq M_{\text{star}} < 10^{11} M_{\odot}$, and $10^{11} M_{\odot} \leq M_{\text{star}}$. As shown in Fig. 11, a reduction by f_Q brings the simulation predictions in much better agreement with observations.

Even though FIREbox underestimates the fraction of massive, quenched galaxies at low z , the properties of star forming galaxies themselves appear well reproduced (see section 3). Hence, we can infer that the physical mechanism(s) responsible for quenching of star formation should not affect the galaxy scaling relations (e.g., the molecular gas sequence or the mass–metallicity relations) of the population of star forming galaxies too severely. Furthermore, going back in time, we see that the stellar feedback model in FIREbox explains well the evolution of the average SFR and stellar mass density at $z \gtrsim 1 - 5$. In other words, FIREbox does not leave much room for AGN feedback to affect the CSFH and CSGH at early cosmic times. Instead, the role of AGN feedback at $z > 1$ may be to turn quiescent galaxies with low, but non-zero sSFRs into the truly passively evolving galaxies observed at those redshifts (Kriek et al. 2006; Straatman et al. 2016).

4.2 Cosmic gas density

The evolution of the cosmic gas density is connected to the evolution of the cosmic star formation rate and stellar mass density. On the one

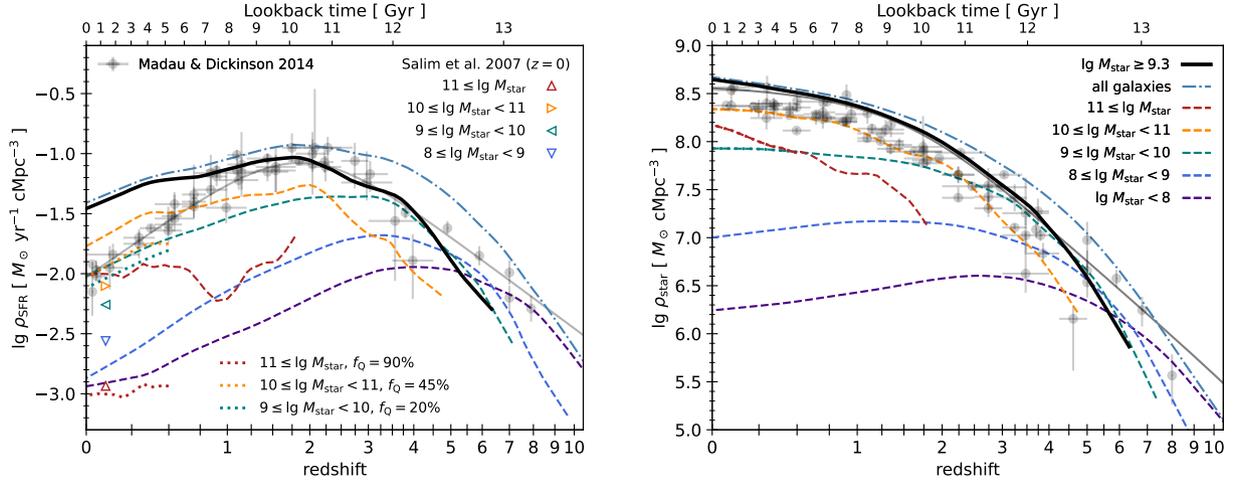


Figure 11. Cosmic star formation history (CSFH, left panel) and cosmic stellar growth history (CSGH, right panel) in FIREbox. Blue dot-dashed lines show the CSFH and CSGH of all identified galaxies in the simulation volume, while black solid lines correspond to the case when low mass galaxies with $\lg M_{\text{star}}/M_{\odot} < 9.3$ are excluded. Star formation rates (SFRs) of simulated galaxies are averaged over the past 20 Myr. The abundance of galaxies is re-weighted to account for cosmic variance in the halo mass function, see Appendix A. Dashed lines show the contributions of galaxies in various stellar mass ranges (see legend). Triangles are observational estimates of the cosmic SFR density at $z \sim 0.1$ for the same stellar mass ranges (Salim et al. 2007). Gray symbols and lines refer to an observational compilation by Madau & Dickinson (2014). The gray line in the right panel is the integral of the CSFR reduced by an effective stellar mass loss of 27%. The observational data is converted to a Chabrier IMF using the conversion factors of Madau & Dickinson (2014). The observational estimates of the CSFH and CSGH include galaxies above a luminosity threshold of $0.03L_{*}$, which corresponds approximately to a mass threshold of $\lg M_{\text{star}}/M_{\odot} \sim 9.3$ at $z = 0 - 3$. The CSFH in FIREbox is in good agreement with observations at $z \sim 1.5 - 4.5$. At $z < 1$, massive, low z galaxies often do not efficiently quench their star formation, resulting in an over-estimation of the CSFH possibly as a result of the lack of AGN feedback in FIREbox. Excluding a fraction f_Q of quenched galaxies (Behroozi et al. 2019) by hand (dotted lines) results in much better agreement with the observational estimate (triangles). Intermediate mass galaxies ($9 \leq \lg M_{\text{star}}/M_{\odot} < 10$, teal-colored dashed line) dominate the CSFH and CSGH at $z = 3 - 5$, and galaxies with $10 \leq \lg M_{\text{star}}/M_{\odot} < 11$ (orange dashed line) at $z \leq 2$. In contrast, most of the star formation and stellar mass build-up during the Epoch of Re-ionization takes place in galaxies with low stellar masses ($\lg M_{\text{star}}/M_{\odot} < 8$, purple line) and low SFRs ($< 0.03 M_{\odot} \text{ yr}^{-1}$).

hand, a larger fraction of the overall baryonic mass gets locked up in stars with increasing cosmic time, thus reducing the total gas density in the Universe. On the other hand, stellar feedback, a natural by-product of star formation, strongly affects the properties the cosmic gas, in particular the abundance of atomic and molecular hydrogen.

Several previous FIRE studies analyzed the H_1 content within the zoom-in regions around individual galaxies, but did not fully sample the intergalactic medium (e.g., Faucher-Giguère et al. 2015, 2016; Hafen et al. 2017; Stern et al. 2021a). With FIREbox, we can more rigorously quantify the integrated neutral hydrogen mass and column density distribution across cosmic history.

The left panel of Fig. 12 compares the evolution of the cosmic H_1 mass density in FIREbox with observational data compiled by Peroux & Howk (2020). Given the challenge in detecting the 21 cm hyper-fine transition emission line of atomic hydrogen beyond $z \sim 0.4$, the evolution of the H_1 mass fraction at higher z is primarily constrained by absorption spectroscopy of high column density systems, specifically Damped Lyman- α systems (DLAs). To ease the comparison, Fig. 12 thus reports the mass density of atomic hydrogen in FIREbox both restricted to DLAs (i.e., only counting H_1 with column densities above $2 \times 10^{20} \text{ cm}^{-2}$) as well as the overall amount. To this end, we estimate the column density of atomic hydrogen for each gas particle as $N_{\text{H}_1} = \Sigma_{\text{gas}} f_{\text{H}_1} X / m_{\text{H}}$, with Σ_{gas} calculated as described in section 2.2.

As the figure shows, the cosmic H_1 density in DLAs predicted by FIREbox is in good agreement with observational data once we re-weight the halo abundance to account for the finite box size. In particular, we find that the atomic hydrogen density of DLAs associated with halos changes by a factor ~ 2 between $z \sim 3 - 4$ and

today’s Universe. About 2-4% of the cosmic baryon density Ω_b is in atomic hydrogen at $z < 4$. A comparison with Fig. 11 reveals that the mass in stars exceeds the mass in atomic hydrogen at $z \lesssim 1.5 - 2$ in agreement with observational estimates (Driver et al. 2018).

Comparing the total amount of atomic hydrogen in FIREbox (solid black line) with the H_1 contribution by DLAs (dashed green line) we see that out to at least $z \sim 5$ the majority of the cosmic H_1 mass (50%-65%) is associated with DLAs (Wolfe et al. 1986; Lanzetta et al. 1991). Furthermore, almost all the atomic hydrogen at $z < 5$ resides in halos (blue dotted line), see also Villaescusa-Navarro et al. (2018). FIREbox predicts that the fraction of atomic hydrogen not within DLAs ($\sim 35 - 50\%$) exceeds the 10-20% contribution of atomic hydrogen from sub-DLAs ($10^{19} \text{ cm}^{-2} < N_{\text{H}_1} < 2 \times 10^{20} \text{ cm}^{-2}$) at those redshifts (Peroux et al. 2005; Zafar et al. 2013; Berg et al. 2019), suggesting that a larger fraction of hydrogen can be found at lower column densities than currently expected. Alternatively, the UV background adopted in FIREbox or the crude modeling of local shielding of UV/ionizing photons in FIRE (Hopkins et al. 2018) could perhaps explain this difference.

The fraction of atomic hydrogen in DLAs decreases noticeably towards higher redshifts in qualitative agreement with observations (Storrie-Lombardi & Wolfe 2000). For instance, FIREbox predicts that only $\sim 25\%$ of the cosmic H_1 mass is hosted by DLAs at $z = 8$. While the H_1 density in DLAs declines with increasing redshift at $z > 4$, an even stronger decline is seen for those DLAs that are associated with DM halos (blue solid line) during the Epoch of Re-ionization (EoR, here $z \sim 6 - 11$). For instance, we predict that the H_1 density in DLAs associated with halos is lower by over an order of magnitude at $z = 9$ compared with $z \sim 3$. Fully accounting for

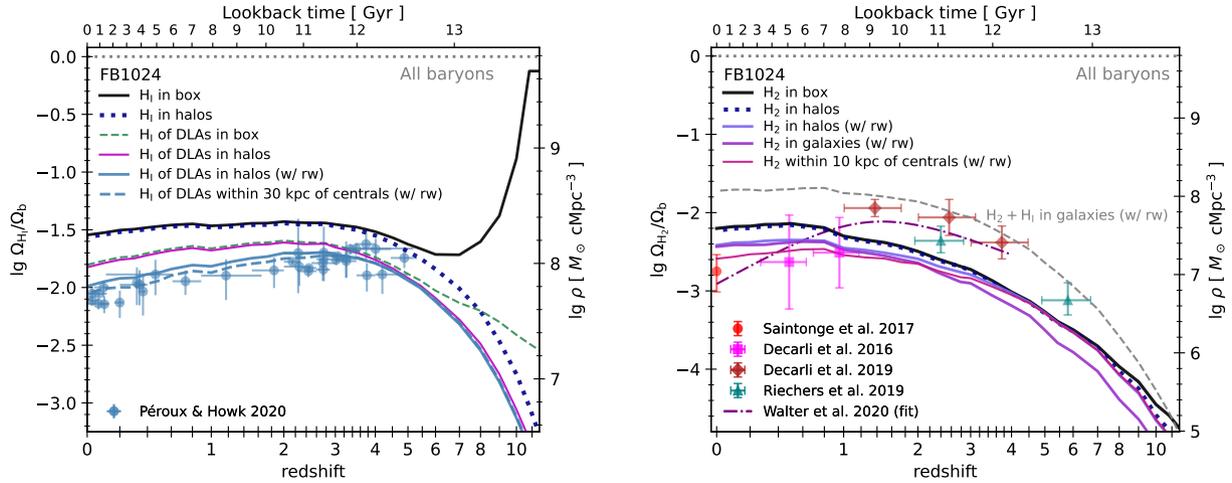


Figure 12. Cosmic evolution of the mass fractions of atomic and molecular hydrogen in FIREbox. (Left panel) The mass fraction of atomic hydrogen (H_I) in the simulation volume is shown by a black solid line. This mass fraction decreases from the beginning of re-ionization ($z \sim 11$) until $z \sim 7$. Between $z \sim 4$ and $z = 0$ the fraction in H_I in FIREbox remains approximately constant. At those times, the vast majority of atomic gas resides in DM halos (blue dotted line). A green dashed line shows the fraction of H_I with column densities above $2 \times 10^{20} \text{ cm}^{-2}$ (damped Lyman- α absorbers, DLAs). At high redshift ($z > 6$), DLAs can also be found outside the virial radii of dark matter halos identified in FIREbox. The cosmic H_I density in DLAs peaks around $z \sim 2 - 3$. Blue and pink solid lines show the mass fraction of atomic hydrogen in DM halos attributable to DLAs with and without re-weighting ('rw') by halo abundance, see Appendix A. The blue dashed line shows the H_I mass in DLAs within a 30 proper kpc radius around central galaxies. Also included in the panel are a compilation of observational data (Noterdaeme et al. 2009, 2012a; Delhaize et al. 2013; Rhee et al. 2013; Zafar et al. 2013; Crigton et al. 2015; Hoppmann et al. 2015; Rhee et al. 2016; Sánchez-Ramírez et al. 2016; Rao et al. 2017; Jones et al. 2018; Rhee et al. 2018; Bera et al. 2019; Hu et al. 2019) by Peroux & Howk (2020). Observational estimates for $z > 0.4$ were obtained via absorption spectroscopy and are thus typically limited to atomic hydrogen in DLAs. Simulations and observations agree well at those redshifts. (Right panel) The mass fraction of molecular hydrogen (H_2) in the simulation volume is shown by a black solid line. Other lines show the H_2 mass fraction in halos, in galaxies (here understood as the molecular hydrogen within a sphere of radius $0.1 R_{\text{vir}}$ located at the (sub-)halo center), and within 10 kpc of central galaxies, with and without re-weighting, see legend. The figure further includes observational estimates (Decarli et al. 2016; Saintonge et al. 2017; Decarli et al. 2019; Riechers et al. 2019) based on carbon-monoxide (CO) line emission with a CO-to- H_2 conversion factor $\alpha_{\text{CO}} = 3.6 M_{\odot} (\text{K km s}^{-1} \text{ pc}^2)^{-1}$. The cosmic H_2 mass fraction in FIREbox increases from early times until $z \sim 1$ in agreement with observations but does not decline steeply at later times as observations may imply. Mass fractions are reported in units of the cosmic baryonic density ($\rho_{\text{bar,uni}} \sim 6.2 \times 10^9 M_{\odot} \text{ cMpc}^{-3}$ for our adopted cosmology; left y axis) or in solar masses per comoving Mpc^3 (right y axis).

atomic hydrogen, especially during the EoR, thus requires modeling the contribution outside halos as well as from systems with column densities below those of DLAs.

The right panel of Fig. 12 shows the evolution of the cosmic H_2 mass density in FIREbox. We compare our model predictions with compilations of observational data (Peroux & Howk 2020; Walter et al. 2020). Given the tight empirical correlation between molecular hydrogen and star formation rate (Bigiel et al. 2008; Genzel et al. 2010; Saintonge et al. 2017; Feldmann 2020), at least in the local Universe, one might expect that the evolution of the H_2 mass density mirrors the evolution of the CSFH (Decarli et al. 2019; Tacconi et al. 2020), i.e., with a peak near Cosmic Noon and a noticeably decline towards low redshift. However, this is not what we see in Fig. 12. Instead, we find that the cosmic H_2 density in FIREbox increases with cosmic time until $z \sim 1$, after which it remains approximately constant down to $z = 0$. The latter results from two complementary effects. First, the CSFH in FIREbox (Fig. 11) decreases too gently at low z as a consequence of under-predicting quenching of star formation, see section 4.1. Secondly, the typical molecular depletion time of FIREbox galaxies increases with increasing cosmic time, qualitatively similar to observations (Tacconi et al. 2020). Hence, comparably more molecular gas is required at a later time to sustain the cosmic star formation activity. We postpone a detailed discussion of the depletion time of FIREbox galaxies to future work.

The evolution predicted by FIREbox differs from the findings of recent observational studies (Decarli et al. 2019; Walter et al. 2020),

even though it may be broadly in line with other observational measurements (Decarli et al. 2016; Saintonge et al. 2017; Riechers et al. 2019). While this difference may indicate a potential short-coming of the FIRE physics model, we note that molecular gas plays a somewhat limited role in FIREbox given the high density threshold of star formation (Hopkins et al. 2018). Furthermore, the neutral hydrogen density predicted by FIREbox exceeds the observed molecular density at all z suggesting there is sufficient neutral gas in FIREbox galaxies. Therefore, another possibility is that our approximate approach of estimating molecular fractions, see section 2.2, breaks down at higher z . However, Krumholz & Gnedin (2011) demonstrated that this approach predicts molecular fractions with an absolute error of better than 0.1 for more than 80% of the ISM mass of galaxies with a range of stellar masses and ISM conditions when compared to a non-equilibrium radiative transfer solution.

Observational biases are yet another concern. The abundance of molecular hydrogen is typically inferred indirectly from the line luminosity of carbon-monoxide (CO) molecules or from the continuum emission of dust grains. The latter method suffers from uncertainties in the dust-to-gas ratios and dust temperatures (Scoville et al. 2014; Liang et al. 2018, 2019) and includes a contribution from atomic gas (e.g., Scoville et al. 2014), while the former approach requires knowledge of the conversion factor between CO luminosity and H_2 mass. While this conversion factor is well constrained for molecular gas in the Milky-Way (Solomon et al. 1987; Bolatto et al. 2013), it has been shown to vary significantly with galaxy properties such as

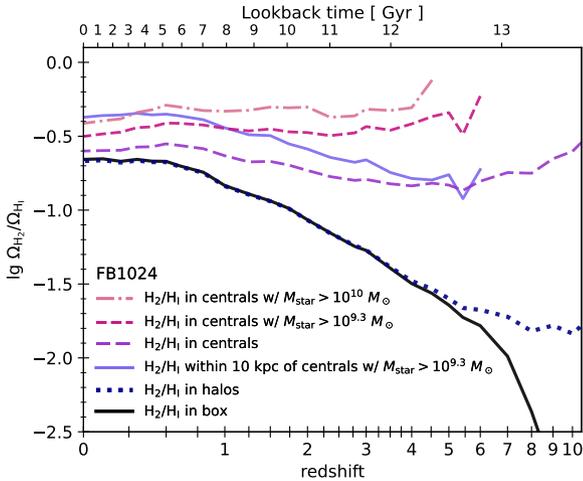


Figure 13. Evolution of the mass ratio between molecular and atomic hydrogen in FIREbox. The H_2 -to- H_1 ratio in the simulation volume (in DM halos) is shown by a black solid line (a blue dotted line), while a purple solid line refers to the ratio between M_{H_2} and M_{H_1} within 10 physical kpc around central galaxies with stellar masses exceeding $10^{9.3} M_{\odot}$. The H_2 -to- H_1 ratio within $0.1 R_{\text{vir}}$ of central galaxies (central galaxies with $M_{\text{star}} > 10^{9.3} M_{\odot}$, central galaxies with $M_{\text{star}} > 10^{10} M_{\odot}$) is shown by a long-dashed purple line (short-dashed red line, dot-dashed pink line). Although the cosmic abundance of molecular hydrogen relative to atomic hydrogen decreases towards higher redshift, the H_2 -to- H_1 ratio in central galaxies of a given stellar mass is relatively constant across most of cosmic history when measured within $0.1 R_{\text{vir}}$. In contrast, the H_2 -to- H_1 ratio measured in a fixed physical radius evolves more strongly with redshift. Atomic hydrogen dominates over molecular hydrogen in the interstellar medium of all but the most massive galaxies both in the present-day Universe and at early cosmic times.

metallicity and interstellar radiation field (Leroy et al. 2011; Feldmann et al. 2012; Bolatto et al. 2013). The conversion factor is thus a significant systematic for molecular gas estimates based on CO data, especially at higher z (Walter et al. 2020). Bringing the H_2 predicted by FIREbox at $z > 1$ in agreement with Decarli et al. (2019) and Walter et al. (2020) would require a conversion factor that is about 0.4 dex lower than the standard value for the Milky Way. We note that such a reduction in the conversion factor would also help mitigating the tension between the theoretically predicted and observed molecular gas fractions in galaxies at the Cosmic Noon (Narayanan et al. 2012), see also Lagos et al. (2015) and Popping et al. (2019).

The conversion factor for high z galaxies has been empirically constrained by comparing CO emission and dynamical masses (Daddi et al. 2010). This approach tacitly assumes, however, that gas in high redshift galaxies is predominantly molecular (e.g., Saintonge et al. 2013). To test this assumption, we plot in Fig. 13 the ratio between molecular and atomic hydrogen in FIREbox. The figure offers several insights.

First, it shows that with the possible exception of the most massive galaxies at high z , the cold gas in galaxies is never H_2 dominated. In fact, less than a third of neutral gas is in molecular form with the mass ratio between molecular and atomic hydrogen near or below 0.5. If taken at face value, this result suggests that the CO to H_2 conversion factor as inferred from dynamical masses could be significantly overestimated. Secondly, Fig. 13 shows that, when averaged over cosmic scales, the H_2 to H_1 mass ratio decreases strongly with increasing redshift. This result holds both for the gas phases in the box as well as the gas residing in DM halos. The latter plateaus at a mass ratio of $\sim 1.5\%$ at $z \gtrsim 8$, while the former continues to drop with increasing

z during the EoR. Finally, the H_2 to H_1 mass ratio within galaxies is almost independent of z . The normalization and redshift evolution of the latter depends on the mass of the selected galaxies (more massive galaxies tend to have a larger H_2 to H_1 mass ratio) as well as the radius enclosing the gas components. Calculating the mass ratio within $0.1 \times R_{\text{vir}}$ results in a flatter evolution than using a radius of fixed physical size.

4.3 Large scale distribution of atomic and molecular hydrogen

The column density distribution function (CDDF) measures the number of intervening systems per unit column density N and absorption length X (Bahcall & Peebles 1969). The CDDF provides an excellent point of comparison for theoretical models given that it probes cosmic gas under a range of physical conditions and in a variety of cosmic environments (Altay et al. 2011; McQuinn et al. 2011; Rahmati et al. 2015; Crain et al. 2017; Balashev & Noterdaeme 2018; Szakacs et al. 2022).

At $z < 0.4$, the CDDF of atomic hydrogen is observationally accessible via its 21-cm line emission (Zwaan et al. 2005; Péroux & Howk 2020), while $\text{Ly}\alpha$ absorption spectroscopy of background quasars can probe the CDDF at higher redshift (e.g., Prochaska & Wolfe 2009; Noterdaeme et al. 2009, 2012b). Intervening systems include both $\text{Ly}\alpha$ forest absorbers with $N_{\text{H}_1} < 10^{17.2} \text{ cm}^{-2}$ (e.g., Rauch 1998), Lyman limit systems ($10^{17.2} \leq N_{\text{H}_1}/\text{cm}^{-2} < 10^{20.3}$, e.g., Péroux et al. 2003), and Damped $\text{Ly}\alpha$ systems ($N_{\text{H}_1} \geq 10^{20.3} \text{ cm}^{-2}$, e.g., Wolfe et al. 2005). Observationally, the H_1 CDDF is approximately described by a single power-law over $N_{\text{H}_1} \sim 10^{13} - 10^{21} \text{ cm}^{-2}$ (Tytler 1987) with a break at higher column densities ($\sim 10^{20.5} - 10^{21} \text{ cm}^{-2}$; Péroux et al. 2003). The shape of the H_1 CDDF is almost invariant with redshift and its normalization shows only a moderate change (factor 2 between $z = 4$ and $z = 2.2$) with redshift (Zwaan et al. 2005; Prochaska et al. 2005; Prochaska & Wolfe 2009).

To calculate the CDDF, we project the atomic or molecular hydrogen density in the simulation box along a specified axis onto a 2-dimensional grid with resolution of 150 comoving pc which is comparable to the ~ 100 pc resolution of the PHANGS-ALMA survey at $z = 0$ (Leroy et al. 2021b). In more detail, we use a combination of smooth and tipgrid for the deposition of the H_1 and H_2 masses onto the grid⁸. First, smooth computes a smoothing length for every particle as half of the distance to the n th neighbor particle. We found that $n = 80$ provides a good balance between over-smoothing and too high particle noise for this application. Next, the simulation region is divided into n_s equally spaced slabs of depth $\Delta L = 15/n_s \text{ cMpc } h^{-1}$ for the chosen spatial direction. The advantage of using slices is that it reduces the chance of line-of-sight overlap between separate absorbing systems. However, we find practically little difference in the estimated CDDF over much of the column density and redshift range of interest when varying n_s between 1 and 10. In the following, we use $n_s = 10$ but report the CDDF only if it differs by less than 5% from the CDDF calculated with $n_s = 1$. Next, tipgrid projects particles in the same slab onto a two-dimensional grid by depositing the atomic or molecular hydrogen mass of each gas particle via the SPH scatter approach with a cubic spline kernel and the smoothing lengths calculated beforehand. The CDDF is then obtained from the column density distributions of the pixels of all slabs normalized to ΔX , where the absorption distance ΔX is related to the comoving slab depth ΔL via $\Delta X = \Delta L \frac{H_0}{c} (1+z)^2$.

⁸ <https://github.com/N-BodyShop/smooth>

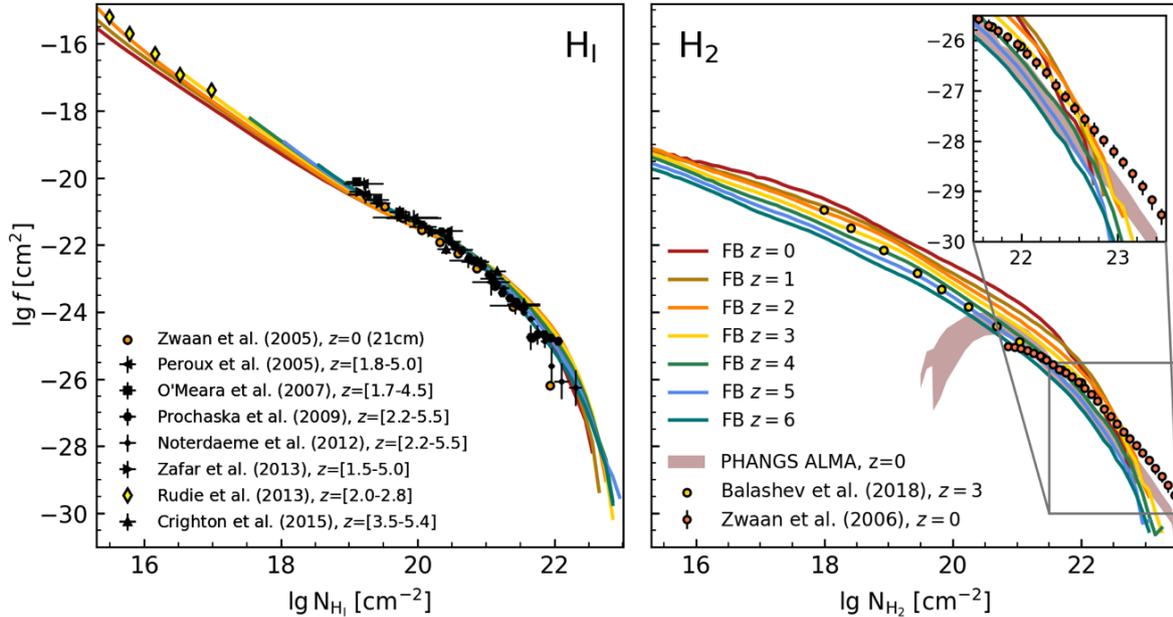


Figure 14. Column density distribution functions (CDDFs, f) of atomic and molecular hydrogen in FIREbox. The CDDF $f(N, z)$ quantifies the number of intervening systems per unit path length $X(z)$ and unit column density N . (Left) The CDDF of atomic hydrogen in FIREbox reproduces well the observed H_I CDDF from quasar absorption line spectroscopy and 21 cm emission line surveys (Zwaan et al. 2005; Peroux et al. 2005; O’Meara et al. 2007; Prochaska & Wolfe 2009; Noterdaeme et al. 2012b; Zafar et al. 2013; Rudie et al. 2013; Crighton et al. 2015) but with some apparent deviations at $N_{\text{H}_I} > 10^{21} \text{ cm}^{-2}$. We note that the observational estimate for $z = 0$ assumes optical thin emission which may not hold at high column densities (Zwaan et al. 2005). (Right) The CDDF of molecular hydrogen in FIREbox and observational estimates by PHANGS (Szakacs et al. 2022) and by Zwaan & Prochaska (2006) and Balashev & Noterdaeme (2018). In agreement with the literature, the H_I CDDF does not strongly evolve with cosmic time. In contrast, the H_2 CDDF at $N_{\text{H}_2} \leq 10^{22} \text{ cm}^{-2}$ increases by more than one order of magnitude between $z = 6$ and $z = 0$.

The left panel of Fig. 14 compares the CDDF of atomic hydrogen in FIREbox with a compilation of observational data over $z = 0 - 5.5$. Overall the agreement is good, especially at $N_{\text{H}_I} < 10^{21} \text{ cm}^{-2}$. FIREbox predicts that the H_I CDDF does not strongly evolve with cosmic time in agreement with observations. FIREbox overestimates the incidence of low redshift systems with the highest column densities ($N_{\text{H}_I} > 10^{21} \text{ cm}^{-2}$). However, the observational estimate for $z = 0$ assumes optical thin emission which may result in an underestimate at the highest column densities (Zwaan et al. 2005).

The right panel of Fig. 14 shows our prediction for the CDDF of molecular hydrogen (H_2) and compares it with observational data (Zwaan & Prochaska 2006; Balashev & Noterdaeme 2018; Leroy et al. 2021b; Szakacs et al. 2022). The H_2 CDDF is in broad agreement with the observations at $z = 3$ but shows some differences at low z , in particular a steeper decrease with increasing column density for large N_{H_2} and a higher normalization at low column densities. In contrast to the H_I CDDF, the normalization of the H_2 CDDF shows a noticeable dependence on redshift, increasing by over one order of magnitude from $z = 6$ to $z = 2$ at all column densities reflecting the overall increase in the cosmic molecular gas density (Peroux & Howk 2020), see also Fig. 12. Between $z = 2$ and $z = 0$, the H_2 CDDF slightly decreases at the highest column densities ($N_{\text{H}_2} \gtrsim 10^{22} \text{ cm}^{-2}$) and increases at lower column densities, leading to a change in its shape. While the H_2 CDDF is “bottom-light” compared with the H_I CDDF, it increases monotonically with decreasing column densities down to at least $N_{\text{H}_2} \sim 10^{16} \text{ cm}^{-2}$, i.e., there is no indication of a turn-over in the H_2 CDDF as seen in the observational study of Szakacs et al. (2022) presumably due to sensitivity and incompleteness limits.

5 SUMMARY AND CONCLUSIONS

We have introduced the FIREbox suite, a set of galaxy formation simulations in a cosmological volume ($L = 22.1 \text{ cMpc}$) run down to $z = 0$ with the GIZMO gravity-hydrodynamics solver in mesh-less hydrodynamics mode (Hopkins 2015) and with the FIRE-2 physics model (Hopkins et al. 2018). The FIREbox volume contains about 20-30 Milky-Way analogs as well as over a thousand lower mass galaxies enabling the study of representative samples of highly resolved galaxies. The main simulation analyzed in this paper (FIREbox), has a baryonic mass resolution of $m_b \sim 6.3 \times 10^4 M_\odot$ and a spatial resolution of $\sim 20 \text{ pc}$ in dense interstellar gas, comparable to state-of-the-art zoom-in simulations. The high numerical resolution combined with the fully cosmological setting results in an unprecedented dynamic range ($\gtrsim 10^6$) for a galaxy formation simulation. FIREbox is able to capture simultaneously the multiphase structure of the interstellar medium in galaxies and the impact of baryonic physics on cosmological scales. Importantly, FIREbox is not tuned to specific observational data, such as the stellar mass function, but rather it implements comparably well-understood physical processes in a self-consistent fashion without adjusting model parameters. As such it provides a true prediction of galaxy formation theory in a ΛCDM Universe. Modeled baryonic processes include gas cooling, star formation, stellar winds, supernova feedback, and radiative feedback (photo-ionization, photo-electric heating, and radiation pressure). Feedback from active galactic nuclei is currently not included.

In this work, we have focused on validating our methodology by comparing basic predictions of FIREbox with observational data across cosmic time. Specifically, we have analyzed various fundamental galaxy scaling relations as well as the cosmic evolution of

gas masses, stellar masses, and SFRs, highlighting successes and failures of the FIRE-2 model. Future studies based on FIREbox will discuss, e.g., the morphologies of the simulated galaxies, their star formation rates and depletion times, and the link between galaxy and halo formation. Our main findings are as follows:

- FIREbox predicts average SFRs of star forming galaxies in good agreement with observations both at $z = 0$ and $z = 2$ (Fig. 5). The slope of the star forming sequence is slightly sub-linear at $z = 0$ (~ 0.85) and near linear at $z = 2$ (~ 0.95).

- FIREbox underestimates the presence of massive, quiescent galaxies at low z (Fig. 6). While FIREbox naturally accounts for a variety of environmental and stellar feedback driven quenching channels, additional sources, such as AGN feedback, are thus necessary to fully suppress star formation in massive galaxies at low z .

- Simulated galaxies have atomic and molecular gas masses (for a given stellar mass) in good agreement with observational data at $z = 0$, see Fig. 7. According to FIREbox, these gas sequences extend down to (at least) $M_{\text{star}} \sim 10^7 M_{\odot}$ and they are well described by broken power-laws over 4 orders of magnitude in stellar mass.

- FIREbox broadly reproduces the observed mass–metallicity relation at $z = 0$ over many orders of magnitude both for gas phase metallicities as well as stellar metallicities, see Fig. 8. In addition, the simulation predicts a low scatter ($\lesssim 0.1$ dex) for both relations. Both mass–metallicity relations are well fit by broken power-laws.

- FIREbox predicts a stellar mass function (SMF) at $z = 0$ similar to recent estimates by Leja et al. (2020) based on non-parametric modeling except for a moderate excess at both low and high stellar masses (Fig. 9). Our predicted $z = 0$ SMF is generally higher than those based on more traditional stellar mass estimates (e.g., Baldry et al. 2012; Moustakas et al. 2013). At intermediate redshifts ($z \sim 2 - 4$), FIREbox over-predicts the SMF at low-to-intermediate galaxy masses ($M_{\text{star}} \sim 10^{8.5} - 10^{10} M_{\odot}$). A comparison with FIRE-2 zoom-in simulations reveals that reaching a mass resolution of $m_b < 10^4 M_{\odot}$ may be needed to sufficiently lower stellar masses in halos of $M_{\text{halo}} \sim 10^{11} M_{\odot}$. A re-run at 8 times better mass resolution (FIREbox^{HR}) than the current FIREbox simulation would be desirable and is left as a future goal. At high $z \geq 6$, the SMF in FIREbox agrees well with estimates by Song et al. (2016).

- The galaxy stellar-to-halo mass ratio in FIREbox increases with increasing halo mass at $M_{\text{halo}} < 10^{11} M_{\odot}$, peaks near $M_{\text{halo}} < 10^{11.5} M_{\odot}$, and then declines towards the massive end in qualitative agreement with empirical estimates. The FIRE-2 physics models thus predicts a peak in the galaxy baryonic conversion efficiency even without the inclusion of AGN feedback. However, as our study of the SMF highlights, the stellar masses at the massive end tend to be too high if no additional feedback sources are included, i.e., the decline in the stellar mass – halo mass ratio is too shallow. The galaxy baryonic conversion efficiency reaches a peak at intermediate halo masses because the fraction of stellar mass residing outside galaxies, i.e., in a stellar halo and in satellite galaxies, increases strongly with increasing halo mass at the massive end (Fig. 10). In contrast, the ratio between the stellar mass in the halo and the halo mass declines only weakly at the massive end after peaking near $M_{\text{halo}} = 10^{12} M_{\odot}$.

- The halos of Milky-Way analogs have a baryon fraction of $11.6^{+0.5}_{-0.4}\%$, which is only about 25% lower than the universal baryon fraction. This percentage is higher than the empirical estimate of 7% of detected baryons. The observationally ‘missing’ baryons are located in various components including ionized gas with temperatures below 2×10^5 K and an extra-galactic stellar component.

- The cosmic star formation history (CSFH) and the stellar mass

build-up in FIREbox broadly match observational estimates at $z > 1$. At low z , FIREbox over-estimates the cosmic SFR density by a factor of ~ 3 . This mismatch is driven to a large degree by the under-prediction of the quenched fraction in FIREbox which results in too high a star formation activity in halos hosting $M_{\text{star}} > 10^{10} M_{\odot}$ galaxies.

- The cosmic H_1 density is in broad agreement with observations and shows little evolution with redshift. The cosmic H_2 density increases monotonically with increasing cosmic time until $z \sim 1$ after which it remains approximately constant, see Fig. 12. The near constancy of the cosmic H_2 density at $z < 1$ is in tension with some observational data (Walter et al. 2020). This tension could be reduced if higher z galaxies have a lower H_2 mass per CO luminosity compared with Milky-Way like galaxies in the nearby Universe.

- Finally, we compare the column density distribution functions (CDDF) of atomic and molecular hydrogen in FIREbox with observations finding good agreement for H_1 , see Fig. 14. In contrast to the H_1 CDDF, the normalization of the H_2 CDDF shows a noticeable dependence on redshift, increasing by over one order of magnitude from $z = 6$ to $z = 2$ at all column densities reflecting the overall increase in the cosmic molecular gas density (Péroux & Howk 2020).

FIREbox makes it possible to explore the predictions of the FIRE-2 physics model statistically, by providing a representative sample of highly resolved galaxies across cosmic history. However, the current iteration of FIREbox should be understood as a first step in this direction with much work yet to be done. While the model is broadly successful in reproducing a number of observational constraints, we also noted various areas of tension or disagreement. In particular, FIREbox is unable to produce massive, quenched galaxies in the appropriate numbers and also predicts a cosmic star formation rate density that is too high at late times. It is possible that the inclusion of feedback from super-massive black holes will remedy these shortcomings (Su et al. 2021; Wellons et al. 2022). However, adding AGN feedback also increases the uncertainty of the model predictions as it introduces significant modeling degeneracies.

Additional work is also needed in both completing the accounting of the relevant processes and in modeling them at the required resolution level. For instance, magnetic fields and cosmic ray pressure can affect the cloud structure on small scales (Hennebelle & Inutsuka 2019) or result in low velocity galactic winds (Booth et al. 2013; Girichidis et al. 2016). Recent progress on modeling these physical processes is encouraging (Chan et al. 2019; Hopkins et al. 2020) and we hope to include them in the future. FIREbox, with its focus on comparably well understood physics, provides a robust base-line prediction for such future model extensions.

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DATA AVAILABILITY STATEMENT

The data supporting the plots within this article are available on reasonable request to the corresponding author. A public version of the GIZMO code is available at <http://www.tapir.caltech.edu/~phopkins/Site/GIZMO.html>. FIRE data releases are publicly available at <http://flathub.flatironinstitute.org/fire>.

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APPENDIX A: RE-WEIGHTING

We estimate the true (ensemble average) halo mass function (HMF) for our adopted cosmology with the help of HMFcalc⁹ (Murray et al. 2013). Specifically, we select the ‘Behroozi+2013 (Tinker Extension to High-z)’ fitting function (Behroozi et al. 2013) and a CAMB transfer function. We then calculate the HMF for the virial halo criterion (Bryan & Norman 1998) over a $\lg M_{\text{vir}}/M_{\odot} = 7 - 15$ range in steps of $\Delta \lg M_{\text{vir}} = 0.05$.

The realized cumulative HMF in the simulation volume V can be estimated as the number of halos above a certain mass $x = \lg M_{\text{h}}$ divided by the simulation volume, i.e.,

$$\hat{\Phi}(x) = \sum_{\{i: x_i \geq x\}} \frac{1}{V}. \quad (\text{A1})$$

The idea of the re-weighting approach is to replace the equal weights of $1/V$ in the sum above with halo dependent weights. Specifically, approximating the true cumulative HMF $\Phi(x) = \int_x^{\infty} \phi(x') dx'$

⁹ <https://hmf.icrar.org>

with the following sum over the halos in the simulation volume

$$\Phi(x) \approx \sum_{\{i: x_i \geq x\}} \phi(x_i) \Delta x_i, \quad (\text{A2})$$

suggests that we can replace $1/V$ with weights $w_i = \phi(x_i) \Delta x_i$. Here, the line elements Δx_i represent the typical spacing in logarithmic halo mass between halos with $\lg M_h$ near x_i and $\phi(x)$ is the true differential HMF. We calculate the line elements Δx_i as d_i/N_i by counting the number of halos (N_i) in a top hat kernel of diameter d_i and centered on x_i . The diameter is chosen such that the kernel includes a fixed number of halos $N_i = 100$ subject to strict lower and upper bounds of $d_i \geq 0.05$ and $d_i \leq 0.5$. Before the weights are calculated, the masses of halos in hydrodynamical simulations are converted to the masses expected for a corresponding dark-matter-only simulation by matching the cumulative abundances of halos in FIREbox runs with and without baryonic physics.

The weights w_i exceed $1/V$ for underrepresented halos in the simulation volume thus boosting their contribution and vice versa for overrepresented halos. Once we assign weights w_i to all halos, we can thus calculate re-weighted properties and mass functions in a straightforward manner. For instance, differential stellar mass functions can be obtained via a weighted histogram, while cumulative stellar mass functions sum all the weights of the host halos of galaxies above a certain stellar mass.

In case re-weighting is used, only halos containing more than 300 DM particles obtain updated weights. Halos excluded from re-weighting obtain the standard weight $w_i = 1/V$. Sub-halos are assigned the weights of their parent main halos.

We show a test of the re-weighting approach in Fig. A1. Without re-weighting, the cumulative and differential HMFs in FIREbox can exceed the expectations from HMFcalc by up to ~ 0.2 dex, especially at $z \leq 2$. After re-weighting, the HMFs typically match the reference HMFs close to statistical errors.

APPENDIX B: COMPARISON WITH FIRE-2 ZOOM-IN SIMULATIONS

The SMF in FIREbox shows a higher abundance of moderately low mass galaxies ($M_{\text{star}} \sim 10^9 - 10^{10} M_{\odot}$) than is seen in galaxy surveys. Here, we compare FIREbox to other FIRE-2 zoom-in simulations to explore whether this difference is caused by the numerical resolution or the different set-up of FIREbox as a cosmological volume simulation. Overall, we include 41 separate FIRE-2 zoom-in simulations which target halos over a broad range of halo masses $M_{\text{halo}} \sim 10^{11} - 10^{13} M_{\odot}$ and are run to $z = 1$ or $z = 0$, see Table B1.

We derive cumulative SMFs for galaxies in zoom-in simulations in an approximate fashion via abundance matching of the stellar masses of galaxies (M_{star}) and the masses of their host halos (M_{halo}). Ignoring scatter, the cumulative SMF $\Phi_{\text{star}}(\lg M_{\text{star}})$ equals the cumulative HMF $\Phi(\lg M_{\text{halo}})$ and we can thus plot M_{star} vs $\Phi_{\text{star}}(\lg M_{\text{star}})$ for each galaxy from a zoom-in simulations. Cumulative HMFs are obtained from HMFcalc as described in Appendix A.

The left panel of Fig. B1 shows the SMF of central galaxies in FIREbox. We exclude satellite galaxies since the primary galaxies in zoom-in simulations are usually selected to be centrals or isolated galaxies. In each case, the abundances of the main (or isolated) halos are re-weighted to match the expected HMF of all halos (see Appendix A) to allow a more direct comparison with the SMF of zoom-in runs.

At high z , the SMF in FIREbox is in good agreement with the SMF predicted via abundance matching from the zoom-in runs. At

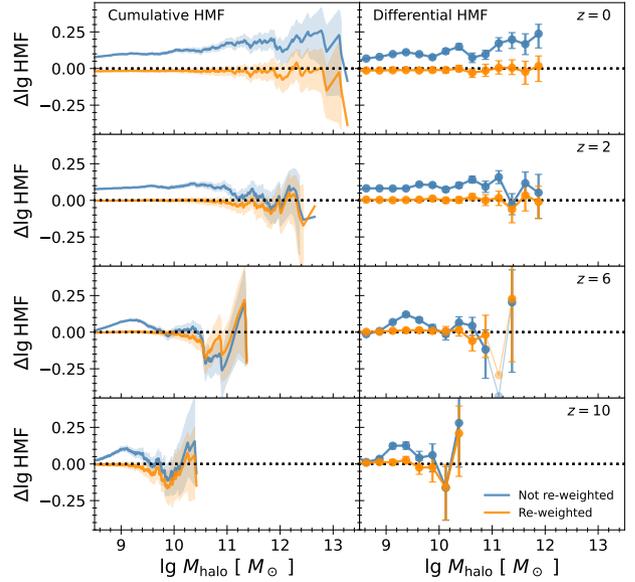


Figure A1. Halo mass function (HMF) in FIREbox relative to the reference HMF at $z = 0 - 10$ with and without re-weighting. Halo masses in the simulation are first converted to halo masses in a corresponding dark-matter-only simulation via abundance matching. Subsequently, the empirical cumulative (left panels) and differential (right panels) HMF from the simulation are compared with the reference HMF (HMFcalc; Murray et al. 2013). Without re-weighting (blue lines), the HMF of FIREbox can overestimate the reference HMF by up to ~ 0.2 dex. In contrast, the re-weighted cumulative and differential HMFs (orange lines and symbols) match their reference HMF nearly within statistical errors (shaded regions and error bars are the 16th to 84th percentiles calculated via bootstrapping).

low z , however, FIREbox predicts a higher abundances for $M_{\text{star}} \sim 10^9 - 10^{10} M_{\odot}$ galaxies compared both with the available FIRE-2 zooms (Fig. B1) and observations (Fig. 9). We now investigate the origin of difference in some detail.

First, we would like to test whether a selection bias toward more isolated galaxies in zoom-in simulations could be responsible. To this end, we plot in the right hand panel of Fig. B1 the SMF of isolated galaxies in FIREbox. A galaxy is isolated if it does not lie within 3 times the virial radius of another main halo. A comparison with the left hand panel of Fig. B1 and with Fig. 9 reveals that the SMF in FIREbox in the stellar mass regime of interest does not strongly depend on the isolation criterion (all vs central vs isolated galaxies). Hence, differences in galaxy isolation do not appear to be responsible for the excess in moderately low mass galaxies in FIREbox at low z .

Also, we can largely exclude a statistical effect related to the scatter in the SHMR relation. This scatter is empirically constrained to about 0.2 dex in massive halos (see e.g., Reddick et al. 2013; Zu & Mandelbaum 2015), while numerical simulations (e.g., Schaye et al. 2015; Pillepich et al. 2018a; Feldmann et al. 2019) as well as semi-analytic (e.g., Somerville et al. 2012) and empirical models (e.g., Hearin & Watson 2013) suggest that the scatter increases with decreasing halo mass to potentially ~ 0.3 dex at $M_{\text{halo}} \sim 10^{11} M_{\odot}$ (Wechsler & Tinker 2018). However, Fig. B1 highlights that all FIRE-2 zoom-in simulations (out of a dozen) with $M_{\text{star}} \sim 10^9 - 10^{10} M_{\odot}$ at $z = 0$ have lower abundances, i.e., lower stellar masses for a given halo mass.

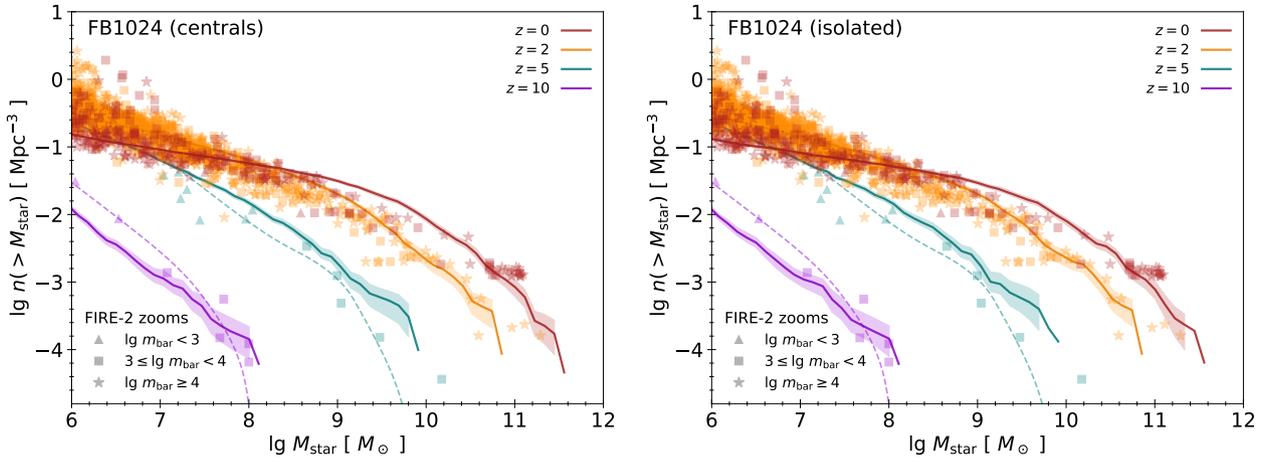


Figure B1. Comparison between FIRE-2 cosmological zoom-in simulations and FIREbox. Solid lines in the left (right) panel show the cumulative galaxy stellar mass function (SMF) of central (isolated) galaxies with $M_{\text{star}} > 10^6 M_{\odot}$ in FIREbox. A galaxy is isolated if it is the central galaxy of a main halo and it does not lie within 3 times the virial radius of another main halo. The abundance of galaxies is re-weighted, see Appendix A. The various symbols correspond to SMF estimates for central galaxies in FIRE-2 cosmological zoom-in simulations at $z = 10$ and $z = 5$ (Ma et al. 2018), $z = 2$ (Anglés-Alcázar et al. 2017b), and $z = 0$ (Hopkins et al. 2018), see Table B1. Dashed lines are fits provided in Ma et al. (2018). For individual zoom-in simulations, the abundance of galaxies is derived from the expected abundance of their halos. Circles, squares, and stars indicate zoom-in simulations with a baryonic mass resolution of $< 10^3 M_{\odot}$, $10^3\text{--}4 M_{\odot}$, and $> 10^4 M_{\odot}$. FIREbox agrees with the results of previous zoom-in simulations for massive galaxies but appears to predict a larger abundance of intermediate mass galaxies ($M_{\text{star}} \sim 10^9 - 10^{10} M_{\odot}$). This difference appears to be primarily related to the higher numerical resolution of zoom-in simulations of low mass galaxies. Restricting the analysis to isolated galaxies, as opposed to central galaxies, does not significantly lower the abundance of intermediate mass galaxies.

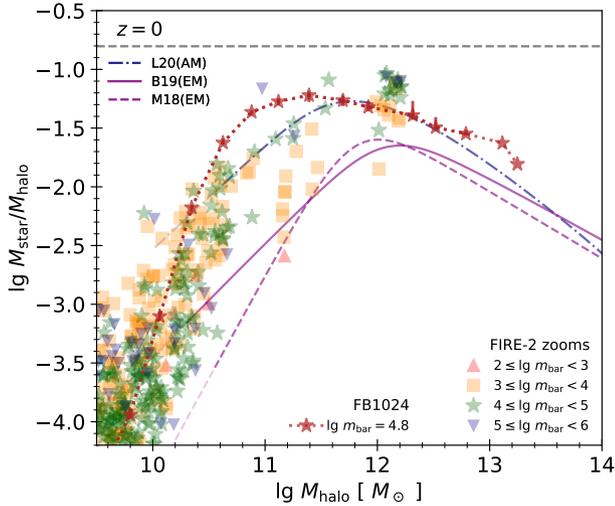


Figure B2. Ratio between the stellar mass of central galaxies and their parent halos in FIREbox and in FIRE-2 zoom-in simulations at $z = 0$. The dotted line and red stars show the median stellar-mass-to-halo-mass ratio in bins of halo mass for FIREbox galaxies, while all other symbols report the mass ratios of individual galaxies in FIRE-2 zoom-ins of different mass resolution (see legend). Stellar masses are measured within $R_g = 3 R_{\text{half}}$, see section 2.6. The figure includes estimates of the galaxy stellar mass – halo mass relation via abundance matching (AM, Leja et al. 2020, dot-dashed line) and empirical modeling (EM, Moster et al. 2018; Behroozi et al. 2019, dashed and solid lines), see also Fig. 10. In the FIRE-2 model, the $z = 0$ stellar mass of galaxies in halos of intermediate mass ($M_{\text{halo}} \sim 10^{11} M_{\odot}$) are noticeably resolution dependent. In contrast, at low ($< 10^{10.5} M_{\odot}$) and high ($\geq 10^{12} M_{\odot}$) halo masses, stellar masses show a much weaker (if any) resolution dependence.

In Fig. B2 we show the SHMR for central galaxies in both FIREbox and in the FIRE-2 zoom-ins. The figure highlights that stellar masses of galaxies in halos of intermediate mass ($M_{\text{halo}} \sim 10^{11} M_{\odot}$) are noticeably resolution dependent, varying by an order of magnitude

(with large scatter) when increasing the mass resolution by 3 orders of magnitude. In addition, it appears that central galaxies residing in such halos are more massive (by ~ 0.2 dex) in FIREbox compared with zoom-ins of a similar resolution. The latter result may indicate that the Lagrangian patches of the zoom-ins (or perhaps the box-size of FIREbox) are too small to adequately capture the cosmological environment at $z = 0$. Given the resolution dependence, we caution that our predictions for central galaxies residing in $M_{\text{halo}} \sim 10^{11} M_{\odot}$ halos (and thus the SMF of galaxies with $M_{\text{star}} \sim 10^9 - 10^{10} M_{\odot}$) are uncertain. In contrast, stellar masses in low mass ($< 10^{10.5} M_{\odot}$) and massive ($\sim 10^{12} M_{\odot}$) halos appear close to converged.

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Label	$m_b [10^3 M_\odot]$	z_{final}	cosmo	source
w/o Metal Diffusion				
m11a	2.1	0	<i>a</i>	A
m11b	2.1	0	<i>a</i>	A
m11c	2.1	0	<i>a</i>	A
m11q	0.9, 7.1	0	<i>a</i>	B
m11v	7.1	0	<i>a</i>	B
m12b	57	0	<i>a</i>	B
m12c	57	0	<i>a</i>	B
m12f	7.1, 57	0	<i>a</i>	C
m12i	7.1, 57	0	<i>a</i>	B
m12m	7.1, 57	0	<i>a</i>	B
m12q	57	0	<i>a</i>	B
A1	33	1	<i>c</i>	D
A2	33	1	<i>c</i>	D
A4	33	1	<i>c</i>	D
A8	33	1	<i>c</i>	D
w/ Metal Diffusion				
m11d	7.1	0	<i>b</i>	E
m11e	7.1	0	<i>b</i>	E
m11h	7.1	0	<i>b</i>	E
m11i	7.1	0	<i>b</i>	E
m11q	7.1	0	<i>a</i>	B
m12b	7.1, 57	0	<i>a</i>	F
m12c	7.1, 57	0	<i>a</i>	F
m12f	7.1, 57, 450	0	<i>a</i>	C
m12i	7.1, 57, 450	0	<i>a</i>	G
m12m	7.1, 57, 450	0	<i>a</i>	B
m12r	7.1, 57	0	<i>b</i>	H
m12w	7.1, 57	0	<i>b</i>	H

Table B1. FIRE-2 zoom-in simulations used as a point of reference for FIRE-box. The first three columns list the simulation identifier, baryonic mass resolution, and the final redshift reached by each simulation. The fourth column states the adopted cosmology of each run. All runs adopt a standard, flat Λ CDM cosmology with $h \sim 0.7$, $\Omega_m = 0.27-0.31$, and $\Omega_b \sim 0.0455-0.048$ broadly consistent with current observational constraints (Planck Collaboration et al. 2015). Specifically, cosmology *a* corresponds to $h = 0.702$, $\Omega_m = 0.272$, $\Omega_b = 0.0455$, cosmology *b* to $h = 0.68$, $\Omega_m = 0.31$, $\Omega_b = 0.048$, and cosmology *c* to $h = 0.697$, $\Omega_m = 0.2821$, $\Omega_b = 0.0461$. The final column lists the work that first describes the respective simulation with A: Chan et al. (2018), B: Hopkins et al. (2018), C: Garrison-Kimmel et al. (2017), D: Anglés-Alcázar et al. (2017b), E: El-Badry et al. (2018), F: Garrison-Kimmel et al. (2019), G: Wetzel et al. (2016), and H: Samuel et al. (2020). The first 15 lines (the last 12 lines) list runs without (with) metal diffusion due to sub-grid turbulence (Hopkins et al. 2018).