

Effect of molecular hydrogen self-shielding modeling on galaxy formation in cosmological simulation

1 THỊNH HỮU NGUYỄN,^{1,2} KIRK S. S. BARROW,¹ SUSIE BYROM,¹ AND VARUN SATISH¹

2 ¹*Department of Astronomy, University of Illinois at Urbana-Champaign, Urbana, IL 61801, USA*

3 ²*Center for AstroPhysical Surveys, National Center for Supercomputing Applications*

4 *Urbana, IL 61801, USA*

ABSTRACT

6 Accurately modeling molecular hydrogen H_2 is an important task in cosmological simulations because it affects star formation and galaxy evolution. One fundamental property of molecular hydrogen
7 is the ability to self-shield, a phenomenon in which the Lyman-Werner UV absorption line bands become optically thick at high H_2 column density and H_2 in a cloud's outer layer can shield H_2 inside.
8 Historically, numerical approximations have been utilized to avoid intensive ray-tracing calculations without significantly changing results. This paper evaluates the use of the Sobolev-like approximation
9 in self-shielding modeling and tests whether it agrees with the results from a more rigorous ray tracing method in the cosmological simulation context. We run two sets of high-resolution zoom-in
10 cosmological simulations, each set with two self-shielding models, to investigate the models' effects
11 on galaxy evolution in the early stage and the late stage of the Reionization era. We find that the
12 approximation model underestimates the level of H_2 self-shielding in a low gas density environment,
13 causing halos to lose a lot of H_2 when compared with the ray tracing model. The susceptibility of
14 H_2 against high-energy radiation in simulations with the approximation model prevents smaller halos
15 from forming stars, while bigger halos seem to be uninfluenced by the choice of self-shielding model
16 in terms of stellar mass. Within a halo, we show that the discrepancy between the approximation
17 and the ray-tracing model is more prominent in the halo's outer region due to its low gas density.
18 On a large scale, the approximation model has fewer metal-contaminated regions in the intergalactic
19 medium, increases IGM heating, and speeds up the reionization process. These results show that the
20 use of Sobolev-like approximation to model H_2 self-shielding alters various properties of galaxies and
21 the large-scale universe, emphasizing a need for caution when employing this technique in running
22 cosmological simulations.

27 **Keywords:** Astronomical simulations(1857) — Radiative transfer simulations(1967) — Galaxy forma-
28 tion(595) — Reionization(1383)

1. INTRODUCTION

30 Molecular hydrogen is a building block for star formation. For a gas cloud to collapse into a star, the cloud's
31 self-gravity must be sufficiently large to overcome its
32 pressure gradient. In the absence of other environmental effects, to achieve the collapse, the gas cloud usually
33 needs to have sufficient mass or a high enough cooling
34 rate so that the cooling time is smaller than the free-fall
35 time. Since the cooling time generally decreases when
36 the gas density increases during the collapse, this leads
37 to catastrophic cooling and the gas pressure being lost
38 against gravity, resulting in a collapse. Depending on
39 the temperature and density, there are multiple radiative
40 cooling mechanisms for a cloud to release its internal
41 energy. For primordial gas clouds with atomic hydro-
42 gen HI being the dominant component, Bremsstrahlung
43 emission, atomic hydrogen's recombination, collisional
44 ionization, and collisional excitation processes can help
45 cool the gas down to at best the virial temperature of
46 $10^4 K$, below which the cooling rate is too low (Thoul &
47 Weinberg 1995). However, if molecular hydrogen H_2 is
48 available or is created from atomic hydrogen, it can fur-
49 ther stimulate cooling by opening up new cooling chan-
50 nels through its rotational and vibrational energy levels.
51 This allows the gas to cool to ≈ 100 Kelvin degrees (Galli
52 & Palla 1998), making it possible for the cloud to col-
53 lapse into stars. This connection between star formation
54 and H_2 can be reflected through the Kennicutt-Schmidt
55 law (Schmidt 1959; Kennicutt 1998) and various obser-

⁵⁸ vational evidence in nearby disk galaxies (Wong & Blitz
⁵⁹ 2002; Kennicutt et al. 2007; Leroy et al. 2013).

⁶⁰ Ultraviolet (UV) radiation emitted by nearby active
⁶¹ stars can photodissociate molecular hydrogen via the
⁶² Solomon process (Solomon 1965 - private communica-
⁶³ tion reported in Field et al. 1966, Stecher & Williams
⁶⁴ 1967). When absorbing a Lyman-Werner (LW) pho-
⁶⁵ ton (11.2-13.6 eV), a molecular hydrogen molecule is
⁶⁶ excited from the ground state to an excited electronic
⁶⁷ state. Instead of radiatively decaying back to the bound
⁶⁸ state, about 15 percent of the molecules have their elec-
⁶⁹ trons decay into the vibrational continuum, which sub-
⁷⁰ sequently dissociates the molecule into atomic hydrogen.
⁷¹ Dissociation rates through this mechanism can be in-
⁷² hibited through H_2 self-shielding, a phenomenon where
⁷³ the column density is large enough that the H_2 in the
⁷⁴ cloud's outer layer absorbs the LW radiation and hence
⁷⁵ shields the inner region. Previous studies point out the
⁷⁶ importance of including self-shielding in preserving the
⁷⁷ amount of molecular hydrogen required for star forma-
⁷⁸ tion. When simulating a disc galaxy, (Christensen et al.
⁷⁹ 2012) notices an increase in the amount of cold gas and
⁸⁰ a clumpier interstellar medium when incorporating self-
⁸¹ shielding in their simulation. Safranek-Shrader et al.
⁸² (2017) finds that self-shielding is crucial in the devel-
⁸³ opment of H_2 in the disc's mid-plane, which accounts
⁸⁴ for 10-15 percent of the total gas mass. Therefore, the
⁸⁵ hydrogen self-shielding mechanism becomes pivotal in
⁸⁶ preserving the amount of molecular hydrogen and regu-
⁸⁷ lating star formation.

⁸⁸ Through modeling a semi-infinite, static slab of gas
⁸⁹ irradiated on one surface, Draine & Bertoldi (1996) pro-
⁹⁰ poses an analytical expression to model H_2 self-shielding
⁹¹ factor that includes the effect of line overlap. As shown
⁹² in Equation (37) of their work, the self-shielding factor
⁹³ is a function of the H_2 column density. In the past, com-
⁹⁴ puting the column density for multiple 3D directions was
⁹⁵ prohibitively computationally expensive (Shang et al.
⁹⁶ 2010; Wolcott-Green et al. 2011). Therefore, multi-
⁹⁷ ple methods have been suggested to approximate the
⁹⁸ self-shielding effect while trying to alleviate its demand-
⁹⁹ ing computational cost. A method is to define a lo-
¹⁰⁰ cal characteristic length scale across which the H_2 num-
¹⁰¹ ber density is constant. This characteristic length can
¹⁰² be either the Jeans length (Shang et al. 2010; Johnson
¹⁰³ et al. 2011), the Sobolev length (Sobolev 1957; Yoshida
¹⁰⁴ et al. 2006), or the Sobolev-like length that is computed
¹⁰⁵ from the density-gradient (Gnedin et al. 2009; Gnedin
¹⁰⁶ & Kravtsov 2011). Rather than a single characteris-
¹⁰⁷ tic length, Hartwig et al. (2015a) approximates the 3D
¹⁰⁸ column densities by creating spherical maps of the col-
¹⁰⁹ umn density around each Voronoi cell with 48 equal-area

¹¹⁰ pixels and also taking into account the Doppler effect
¹¹¹ from the relative velocities of the infalling gas particles.
¹¹² Another non-local method is the six-ray approximation
¹¹³ (Yoshida et al. 2003, 2007; Glover & Mac Low 2007a,b),
¹¹⁴ where the H_2 column density is integrated along six
¹¹⁵ directions along three Cartesian axes centered at each
¹¹⁶ particle's position. Many cosmological simulations use
¹¹⁷ one of these approximations to reduce the computational
¹¹⁸ costs, for example, the Christensen et al. 2012's simula-
¹¹⁹ tion, the COLDSTIM simulation (Maio et al. 2022), and
¹²⁰ the Renaissance Simulations (O'Shea et al. 2015).

¹²¹ However, there are limitations to the applicability of
¹²² approximate treatments in various test problems when
¹²³ compared to the accurate full ray-tracing calculation. In
¹²⁴ the context of photodissociation of H_2 in protogalaxies
¹²⁵ and direct-collapse black hole formation, Wolcott-Green
¹²⁶ et al. (2011) show that the Sobolev length, the density
¹²⁷ gradient, and the six-ray approximation methods over-
¹²⁸ estimate the H_2 shielding degree by an order of mag-
¹²⁹ nitude in low-density regions of $n < 10^4 \text{ cm}^{-3}$. Also
¹³⁰ in the context of direct-collapse black hole, when com-
¹³¹ paring with their non-local approximation detailed in
¹³² Hartwig et al. (2015a), Hartwig et al. (2015b) find that
¹³³ the Jeans approach returns a critical flux value J_{crit} -
¹³⁴ the lowest flux required for a halo with virial temper-
¹³⁵ ature above 10^4 K to collapse to a supermassive black
¹³⁶ hole seed - two times larger than the non-local approx-
¹³⁷ imation, leading to a disparity in the predicted number
¹³⁸ density of black hole seeds. Greif (2014) investigate the
¹³⁹ collapse of primordial star-forming clouds with an accu-
¹⁴⁰ rate H_2 line emission model and notice that the Sobolev
¹⁴¹ method brings about a thermal instability for the col-
¹⁴² lapsing cloud and an order-of-magnitude overestimation
¹⁴³ of the escape fraction for high optical depth. When eval-
¹⁴⁴ uating the triggered Population III star formation at the
¹⁴⁵ limb of the HII region, Chiaki & Wise (2023) find that
¹⁴⁶ while the density-gradient method matches well with the
¹⁴⁷ ray-tracing method, the Jeans length approximation re-
¹⁴⁸sults in an overestimation of the number of the Pop-
¹⁴⁹ulation III stars at the front of the shock wave. The
¹⁵⁰ authors suggest that this is because the thickness of the
¹⁵¹ H_2 ring of the shock front is typically smaller than the
¹⁵² Jeans length, and thus the local approximation is inap-
¹⁵³ propriate. In their large-scale galactic discs simulations,
¹⁵⁴ Safranek-Shrader et al. (2017) notices that the Sobolev
¹⁵⁵ method underpredicts the H_2 abundance in the disc by
¹⁵⁶ a factor of 5, while the six-ray and the Jeans length
¹⁵⁷ methods perform better, which is contrary to the find-
¹⁵⁸ ings that Jeans length method is ineffective in previ-
¹⁵⁹ ous studies. Thus, the validity of these approximation
¹⁶⁰ methods is highly problem-dependent and they cannot

be used as a general substitution for the full ray-tracing calculation.

In this paper, we expand the investigation by comparing the Sobolev-like density-gradient approximation model (Gnedin et al. 2009) with the detailed ray-tracing methods in the context of star formation during the Reionization period. This will help further examine and inform the community about the applicability of these approximations in modeling H_2 in different contexts. In Section 2, we will describe our simulation, the implemented H_2 self-shielding models, and our methodology for analysis. Section 3 analyzes the effect of these models on star formation and galaxy evolution. This section will be subdivided into smaller sections that discuss the effect of self-shielding model on individual galaxies and on the large scale universe. Finally, in Section 4, we discuss the implications of the findings and summarize the paper.

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2. METHOD

2.1. Cosmological simulations

We run and analyze outputs from a radiation-hydrodynamic adaptive mesh refinement simulation ENZO (Bryan et al. 2014). Two cosmological simulations are generated to explore the self-shielding effect in the early stage of the Reionization period, which are referred to as *EarlyRe-ray* and *EarlyRe-apx*. *EarlyRe-ray* uses detailed ray-tracing calculation for self-shielding and *EarlyRe-apx* uses a local approximation of the column density when computing the H_2 self-shielding factor. The self-shielding model is set by the `RadiativeTransferOpticallyThinH2` radiation parameter of ENZO, where a value of 1 enables an optically thin H_2 dissociating Lyman-Werner radiation field and a value of 0 uses ray-tracing for the calculation. The two simulations are initialized with an identical list of parameters and initial conditions except for the `RadiativeTransferOpticallyThinH2` parameter. We evolve the two simulations from $z = 100$ to $z \approx 10.89$, each output is 1 Myr apart.

Both simulations assume a flat Λ CDM cosmology and are run with the cosmological parameters obtained from Planck Collaboration et al. (2016): $\Omega_M = 0.3065$, $\Omega_\Lambda = 0.6935$, $\Omega_b = 0.0483$, $h = 0.679$, $\sigma_8 = 0.8154$, and $n = 0.9681$. The total moving volume is 13 (Mpc/h) 3 and the root grid dimension is 256^3 . The total number of dark matter particles is $\approx 10^{7.82}$ particles. Inside the total volume, we create a smaller zoom-in region using three additional levels of nested refinement to create an effective grid size resolution of $2632.5 \times 2512.9 \times 2871.9$ kpc 3 at the last snapshot at

redshift of 10.89. In the zoom-in region, the most refined dark matter particle mass is $2.7 \times 10^4 M_\odot$. As the density passes a certain threshold, the grids inside this zoom-in region can further be refined adaptively up to 2^{13} times the root grid dimensions. This allows a maximum spatial resolution down to 3.07 pc at the last time step, which allows the tracking of large molecular clouds through initial collapse. We use radiative star cluster particle (Wise & Cen 2009) and Population III star particle (Abel et al. 2007) for our star formation prescription.

2.2. Halo tracking and merger tree algorithms

To identify the halos in the simulations, we employ SHINBAD (Barrow et al 2025, in preparation), an all-in-one algorithm that both finds halos and builds merger trees based on robust energy definition and particle tracking of dark matter particles. (A few more sentences about SHINBAD by Kirks). We exclude all the halos that are outside the refined region of the simulation box - the region containing only the highest and the second-most highest resolution dark matter particles - to ensure that the halos are physical.

2.3. Numerical H_2 self-shielding models

A H_2 self-shielding process happens when a molecular cloud has a sufficiently high column density that its outer layer absorbs all the Lyman-Werner UV photons, effectively shielding the molecules within it against photodissociation. Via modeling a semi-infinite, static slab of gas that is irradiated on one surface, Draine & Bertoldi (1996) express a self-shielding-accounted photodissociation rate as

$$k_{\text{diss}}(N_{H_2}, T) = f_{sh}(N_{H_2}, T) \cdot k_{\text{diss}}(N_{H_2} = 0, T), \quad (1)$$

where $f_{sh}(N_{H_2}, T)$ is a self-shielding factor or shielding function, and $k_{\text{diss}}(N_{H_2} = 0, T)$ is the dissociation rate in a optically-thin regime. At a low temperature (hundreds of K), the self-shielding factor can be approximately computed from only the H_2 column density,

$$f_{sh} = \min \left[1, \left(\frac{N_{H_2}}{10^{14} \text{cm}^{-2}} \right)^{-3/4} \right]. \quad (2)$$

This is controlled by setting the ENZO radiation parameter `RadiativeTransferH2ShieldType` = 0, which is also its default value. We use this expression to calculate the self-shielding factor in the EarlyRe-apx simulation. It is important to note that the convention of f_{sh} value is slightly counter-intuitive: the f_{sh} value of 0 means full self-shielding is available, and the f_{sh} value of 1 means there is no self-shielding. We also acknowledge that Draine & Bertoldi (1996) lists a more accurate

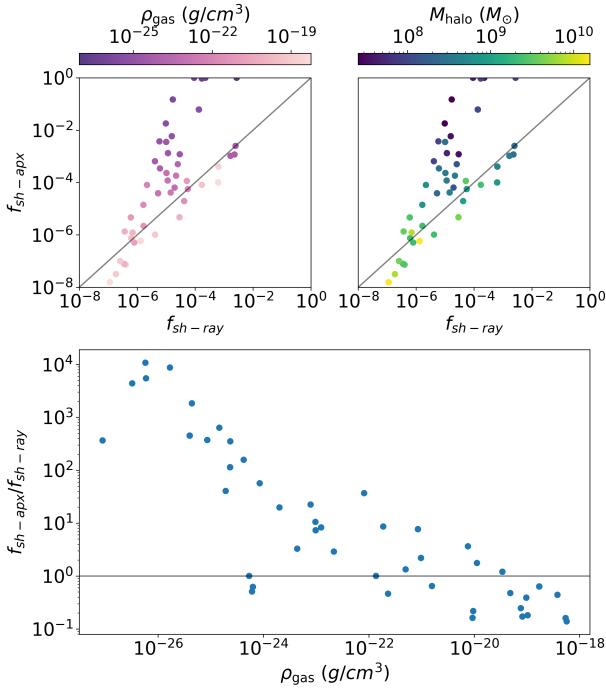


Figure 1. Comparison between the self-shielding factor between the *EarlyRe-ray* and the *EarlyRe-apx* simulation, evaluated at $z = 10.9$. Two gas cells with the highest gas density and highest gas density gradients are chosen in 31 halos in different mass range to evaluate the self-shielding factors. (Top) The relationship between the self-shielding factors calculated by the Sobolev-like approximation model and the ray-tracing model, colored by the cell’s gas density (top left) and the host halo’s mass (top right). (Bottom) The ratio between the approximated and the ray-traced self-shielding factors is plotted as a function of gas density. The Sobolev-like approximation tends to overestimate the amount of H_2 self-shielding in the high gas density regime and underestimate it in the low gas density regime.

formula to calculate f_{sh} that takes temperature as a parameter to include the effect of line overlap. Gnedin & Draine (2014) shows that the model accounting for line overlap enhances H_2 self-shielding primarily in low metallicity environment of below 10% solar and only has minor effect on galaxy’s star formation. Wolcott-Green et al. (2011) also emphasizes that the non-line-overlap equation (Equation 2) is derived with the assumption of cold gas that is colder than a few hundreds K. However, line overlap is often ignored with literature (Gnedin & Kravtsov 2011; Christensen et al. 2012), and using the line-overlap formula does require additional computational resources that we save to run the ray-tracing scheme. Thus, we limit the scope of this paper to the approximated expression of self-shielding at low temperatures, and the analysis on the line-overlap model will be addressed in future work.

To avoid the high computational expense of finding the H_2 column density in multiple 3D directions, previous studies employ different techniques to approximate it (see Section 1). In this paper, we compare the results from two methods: a direct integration from ray tracing and a Sobolev-like length approximation (Gnedin et al. 2009; Wolcott-Green et al. 2011). Even though demanding more computational time, the ray tracing treatment ensures a more accurate radiative transfer calculation. ENZO uses the adaptive ray tracing technique (Wise & Abel 2011) that is based on the HEALPix (Hierarchical Equal Area isoLatitude Pixelation, Gorski et al. 2005) scheme. The column density is integrated along a HEALPix rays,

$$N_{H_2} = \int n(H_2) ds. \quad (3)$$

The Sobolev-like treatment is a local approximation in which the number density n_{H_2} is assumed to be constant within a characteristic length scale L_{char} . In the Sobolev-like approximation, the characteristic length scale is defined as a distance over which the cell’s gas density ρ diminishes. The gas beyond this distance is sparse enough that its influence on shielding is negligible, and thus molecular hydrogen is dissociated in an optically thin fashion. The column density is then computed by

$$N_{H_2} \approx n_{H_2} L_{\text{char}} = n_{H_2} \frac{\rho}{|\nabla \rho|} \quad (4)$$

The approximation is enabled by setting the ENZO parameters `RadiativeTransferOpticallyThinH2 = 1` and `RadiationShield = 2`.

Figure 1 compares the self-shielding factor f_{sh} between the ray-tracing model and the Sobolev-like approximation model. At the time step corresponding to $z = 10.9$, we select 31 halos that contain stars or overlap with another halo that contains stars. For each halo, we select two gas cells to evaluate the self-shielding factor: (1) the gas cell with the highest gas density, and (2) the gas cell with the highest gas density gradient. Each scatter point in Figure 1 represents a selected gas cell. In the approximation model, the self-shielding factor of a gas cell is calculated using Equations 2 and 3. For the ray-tracing model, since the simulation output does not store the photodissociation rate calculation, we need to re-compute the self-shielding factor using Equation 2 with an attenuated LW flux-weighted average column density. The LW flux from each star to a selected gas cell is calculated as follows. Firstly, the intrinsic spectrum of a star particle is generated using the Flexible Stellar Population Synthesis (fsps) with the age and metallicity of the star particle as inputs. We assume an initial

mass function from Davé (2008) evaluated at $z = 0$, and we use the MIST isochrone library and MILES spectral library to generate the spectra. (may cite Susie's paper here or ask her for more information). Then, we calculate the attenuation by including both scattering and absorption due to H/He and metals (Ask Kirk to include how the absorption and scatterings are computed). With the scattering and absorption coefficients, we can compute the total optical depth and then the attenuation of the stellar spectrum from the source to the target gas cell. Lastly, we calculate the attenuated flux of each source to the gas cell, compute the LW flux-weighted average H_2 column density, and get the self-shielding factor from the ray-tracing model. It is important to note that we only include stars within the halo's virial radius to estimate the flux-weighted average H_2 density because stars outside the radius are too far from the selected gas cell to contribute considerably to the total flux at the selected gas cell.

Figure 1 demonstrates a clear disparity in the f_{sh} value between EarlyRe-apx and EarlyRe-ray. In particular, the approximation model tends to overestimate the amount of shielding for cells with a gas density larger than $10^{-20} g/cm^3$ by up to 1 dex. On the other hand, diffuse gas is subjected to underestimated H_2 self-shielding when the Sobolev-like approximation model is used. For highly diffuse gas, this underestimation can be up to 3–4 dex. This connection between gas density and f_{sh} implies a mass-dependent effect of the self-shielding approximation model on halos. The top right subfigure of Figure 1 shows that larger halos ($M_{\text{halo}} > 10^{9.5} M_\odot$) have their molecular cloud region over-shielded in the approximation model due to higher gas densities. On the other hand, the molecular clouds in small halos ($M_{\text{halo}} < 10^{8.5} M_\odot$) are under-shielded against LW radiation when using the Sobolev-like approximation. In some cases, the approximation returns no shielding effect even though those gas cells are still weakly shielded ($f_{sh} \approx 10^{-3}$ when ray-tracing is utilized). Only molecular gas clouds in halos whose mass is about $10^9 M_\odot$ are well modeled in the approximation model. The significance of this effect on star formation will be explored in Section 3.1.

2.4. Cross-matching halos

To examine how each individual halo is affected by the implementation scheme of H_2 self-shielding, we perform cross-matching between halos in the simulations with ray-tracing and their counterparts in the simulations with the Sobolev-like approximation. The match-

ing requirements are

$$\begin{aligned} 375 \quad & \frac{2}{3} < \frac{M_{\text{vir}_{\text{ray}}}}{M_{\text{vir}_{\text{apx}}}} < \frac{3}{2} \\ 376 \quad & \frac{d_{\text{COM}}}{R_{\text{vir}_{\text{ray}}}} < 0.5, \quad \frac{d_{\text{COM}}}{R_{\text{vir}_{\text{apx}}}} < 0.5 \\ 377 \end{aligned} \quad (5)$$

If there are multiple halos matching to one halo, we select the pair with lowest $\frac{d_{\text{COM}}}{R_{\text{vir}}}$ value. The virial mass and radius in Equation 5 come from SHINBAD and are calculated using only dark matter. We cross-match all the halos at the last timestep of the simulations and then trace back their merger tree (details in Subsection 2.2).

2.5. Star assignment

We uniquely assign each star particle in the simulation to one dark matter halo in a two-step fashion. For the first step, a star particle is assigned to a halo where it is first created. If a star particle is created inside the intersection of multiple halos, we will calculate the orbital energy of that star particle with respect to each halo's center to determine which halo the particle belongs to. The assigned halo is the one with lower relative total orbital energy. We assume that a star particle never leaves its assigned halo unless that halo merges with another one, in which case the star particle will become a member of the descendant halo of the merger. This assumption allows a quick assignment of stars to halos without the need to calculate the orbital energy of each star to multiple halos, which is computationally expensive. The assignment's first step starts from the first snapshot to the last snapshot of the simulation.

Even though stars do not generally leave a halo's potential well for isolated halos, the behavior becomes more complex during halo-halo interaction as stripping can occur and stars can be lost from one halo to another (Kannan et al. 2015). Therefore, the second step of our process is to address this shortcoming of the first step's assumption and to refine the star assignment result. In this step, we validate the output from the first step and check whether a star remains in its assigned halo's virial radius throughout its lifetime. If a star escapes the virial radius of its originally assigned halo, we assign that star to a new halo under two conditions: (1) the star's position must be within the new halo's virial radius and (2) the star's total orbital energy with respect to the new halo must be negative. Similar to the first step, if a star is located inside multiple potential new halos, we assign that star to the halo with the lowest negative orbital energy. If either Condition (1) or (2) fails at a certain timestep, this suggests that the star is stripped out of the potential well of all halos and thus we remove that star from the halo assignment process of that time step.

423 Once each star particle is uniquely associated with one
 424 halo, we calculate a halo's stellar mass and SFR exclu-
 425 sively based on its member star particles. This gravita-
 426 tional unbinding of star particles guarantees that each
 427 halo's stellar mass profile are not overlap and indepen-
 428 dent of each other.

429 2.6. Defining ISM, CGM, and IGM

430 The boundary of the interstellar medium (ISM), the
 431 circumgalactic medium (CGM), and the intergalactic
 432 medium (IGM) region in our analysis is defined as fol-
 433 lows. The ISM region (or the boundary of a galaxy)
 434 starts from the galaxy's center of mass to $R_{\text{bary},2000}$,
 435 which is the radius enclosing a baryonic (gas and stars)
 436 mass density 2000 times the universe's critical mass den-
 437 sity at a certain redshift. Even though there are multiple
 438 other definition of the boundary of galaxy in literature,
 439 such as using a fixed fraction of the virial radius, a fixed
 440 physical radius, or a radius that is scaled with mass or
 441 surface brightness (see Stevens et al. 2014 for a sum-
 442 mary of these techniques), our over-density approach
 443 helps define the galaxy more robustly and more phys-
 444 ically because it is redshift and density dependent. It
 445 also helps better define the galaxy during a close galaxy
 446 interaction when a half-mass radius or half-light radius
 447 approach may fail as another galaxy is in the target
 448 galaxy's virial radius. Depending on the redshift and the
 449 galaxy's compactness, $R_{\text{bary},2000}$ typically ranges from
 450 0.15 to 0.25 times the halo's virial radius, which falls
 451 in the same range as other galaxy's aperture definitions
 452 in cosmological simulations (Stevens et al. 2014). The
 453 CGM starts from $R_{\text{bary},2000}$ to $R_{\text{halo,vir}}$, and the IGM is
 454 the region outside of the virial radius of all halos.

455 Also, it is important to note that the baryonic center
 456 of mass does not always coincide with the halo's center
 457 of mass. Thus, in some cases, we shift the virial region
 458 to be centered on the gas and stellar mass instead of the
 459 dark matter mass; however, this shift is not large and
 460 does not affect our interpretation.

461 3. RESULTS

462 3.1. Effect on the molecular hydrogen content and star 463 formation

464 Because the column density approximation model di-
 465 rectly concerns the calculation of the molecular hydro-
 466 gen density, we first investigate the amount of H_2 in
 467 the ray tracing and approximation treatment. Figure 2
 468 shows the H_2 fraction (f_{H_2}), which is the ratio between
 469 the H_2 mass with the total gas mass, as a function of
 470 the total halo mass in three snapshots, one at the time
 471 where star particles first appear in the simulations ($z \approx$
 472 17.49), one at the time step in the middle of the simula-

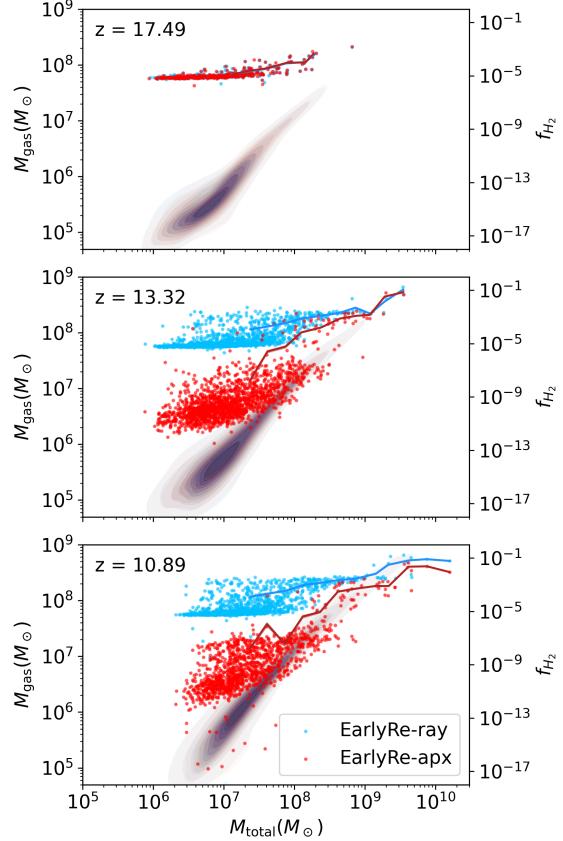


Figure 2. The relationship between the H_2 fraction and the total mass in the timestep where stars first appear, in the intermediate, and in the last timestep of the *EarlyRe* dataset. The contour plots show the M_{gas} distribution and the scatter points show the H_2 fraction of all halos in the simulation box.

473 tion run ($z \approx 13.32$), and one being the last time step of
 474 the run ($z \approx 10.9$). Each halo in the snapshot is repre-
 475 sented by a scatter point, the line represents the running
 476 average of each total mass bin, and the shaded region
 477 around the line is the standard deviation of the scatter
 478 points within each mass bin. The contour plots repre-
 479 sent the distribution of the halos in the $M_{\text{gas}} - M_{\text{total}}$
 480 space. According to Figure 2, both EarlyRe-ray and
 481 Early-apx simulations have similar gas mass distribution
 482 across all timesteps, showing f_{H_2} represents the amount
 483 of H_2 in the halos. However, f_{H_2} shows a notable dif-
 484 ference between the two radiative transfer treatments,
 485 especially at the later time step and in the lower-halo-
 486 mass regime. For halo mass smaller than $10^8 M_{\odot}$, the
 487 f_{H_2} in the ray-tracing treatment is larger than that of
 488 the Sobolev-like approximation treatment by 3 to 6 dex.
 489 This difference grows larger as the simulation evolves,
 490 reaching up to 12 dex at the last time step for small ha-
 491 los. The EarlyRe-ray simulation also develops a lower

492 limit for f_{H_2} of around 10^{-5} , whereas the f_{H_2} is al-
 493 lowed to reach much further value in the *EarlyRe-apx*
 494 simulation. This shows that the ray-tracing treatment
 495 models the self-shielding effect much better and thus
 496 helps preserve more molecular hydrogen in the halos.
 497 As pointed out in Figure 1, the approximation treat-
 498 ment considerably underestimates H_2 self-shielding in a
 499 low gas density regime and molecular hydrogen to get
 500 photodissociated more easily, inferring that smaller ha-
 501 los are the most susceptible to the choice of the model.
 502 At a higher mass range, the difference in f_{H_2} between
 503 the two models gradually diminishes. This is reasonable
 504 because larger halos have deeper gravitational potential
 505 well and have more dense cool gas regions where H_2 ex-
 506 ists. In these regions, the approximation model matches
 507 well with the ray-tracing model (as shown in Figure 1),
 508 leading to an agreement of f_{H_2} between the two runs.
 509

We proceed to investigate whether the self-shielding
 510 treatment affects the stellar mass of galaxies in the sim-
 511 ulation. Figure 3 shows the relationship between stellar
 512 mass and halo mass between the *Early-Ray* and *Early-*
 513 *apx* in the time step where stars first appear (top left
 514 panel), in the last time step of the dataset (bottom right
 515 panel), and in the intermediate time steps. Figure 4
 516 displays the number of halos that host stars as a func-
 517 tion of time for different halo mass bins. The stellar
 518 component of the halos is unbound by using the star
 519 assignment procedure described in Section 2.5. Even
 520 though the number of halos with stars is even between
 521 *EarlyRe-apx* and *EarlyRe-ray* in the beginning, there
 522 are more halos with stars in *EarlyRe-ray* at the end of
 523 the simulation, particularly halos with $M_{halo} < 10^9 M_\odot$.
 524 For ease of reference and lack of a better term, we will
 525 use the term "galaxy" to refer to a halo with stars, as
 526 opposed with halos with only gas and dark matter parti-
 527 cles. From 375 million years after the Big Bang to near
 528 the end of the simulation ($z \approx 11.88 - 11$), there are two
 529 to four galaxies more in the simulation with the ray-
 530 tracing treatment. Furthermore, at a similar halo mass,
 531 smaller halos in *EarlyRe-ray* tend to have more stars
 532 than their counterparts in *EarlyRe-ray* by several dex in
 533 solar mass. This indicates that the use of Sobolev-like
 534 approximation for H_2 self-shielding treatment inhibits
 535 star formation activity in small halos and dwarf galax-
 536 ies. On the other hand, halos whose dark matter mass
 537 is larger than $10^9 M_\odot$ show good agreement in stellar
 538 mass, suggesting that the stellar components of large
 539 halos are unaffected by our choice of H_2 self-shielding
 540 model. This observation aligns with Figure 2, where we
 541 see that H_2 is more accurately shielded in higher halo
 542 mass in *EarlyRe-apx*.

543 Even though we show that stars form easier in smaller
 544 halos when using a ray-tracing model, readers may
 545 notice in Figure 4 that star particles first appear in
 546 *EarlyRe-apx* simulation rather than *EarlyRe-ray*. The
 547 formation of the first galaxy in *EarlyRe-apx* occurs 16
 548 million years before that in *EarlyRe-ray*, and the two
 549 first galaxies both form in the same cross-matched halo
 550 whose dark matter mass is smaller than $10^9 M_\odot$ (for eas-
 551 ier reference, we will call this halo *Halo FS*). This is
 552 quite intuitive and contrasting to our arguments. How-
 553 ever, further investigation suggests that the timing dis-
 554 parancy in the formation of first stars is likely due to the
 555 simulation's numerical stochastic nature rather than a
 556 physical reason. We examine the gas properties of *Halo*
 557 *FS* in both models and notice that in *EarlyRe-apx*, for
 558 cold gas region with temperature lower than 100K, there
 559 is one gas cell with a gas density of $\approx 10^{-22} \text{ g/cm}^3$, 4 dex
 560 higher than the density of surrounding cells. This gas
 561 cell is also at a higher refinement level than what we
 562 observe in the cold gas region of *EarlyRe-ray*. In our
 563 simulations, a cell is refined by two criteria: by baryon
 564 mass or by particle mass. Because the baryon mass is
 565 relatively similar between the two models, the refine-
 566 ment of that gas cell is likely due to a high concentra-
 567 tion of dark matter particles. Thus, we speculate that
 568 at an earlier time step, the cell has more dark matter
 569 particles in *EarlyRe-apx* than in *EarlyRe-ray*, leading to
 570 it being subdivided. After the subdivision, the child cell
 571 increases in gas density and thus becomes more shielded.
 572 Higher self-shielding protects more H_2 and leads to more
 573 cooling, allowing gas to collapse and reach higher den-
 574 sity in that particular gas cell, which in returns provides
 575 more shielding to H_2 according to the approximation
 576 model. This runaway effect makes this gas cell very
 577 dense and filled with H_2 , eventually leading to star for-
 578 mation. However, this effect happens only in a single
 579 gas cell and should not be considered as a global effect
 580 of the approximation model. Apart from that single cell,
 581 the average H_2 mass in the halo is still higher and the
 582 average temperature in the halo is still lower in the ray-
 583 tracing simulation, which is consistent with the general
 584 observation.

585 3.2. Case study on star formation

586 In this section, we analyze the properties of two halos,
 587 one being the largest halo in the simulation and one
 588 having a halo mass of $\approx 1.7 \times 10^9 M_\odot$, which is in the
 589 mass range where the approximation in H_2 self-shielding
 590 fails to accurately model star formation, as suggested in
 591 Figure 3. We match the halos between *EarlyRe-ray* and
 592 *EarlyRe-apx* using the procedure in Section 2.4. These

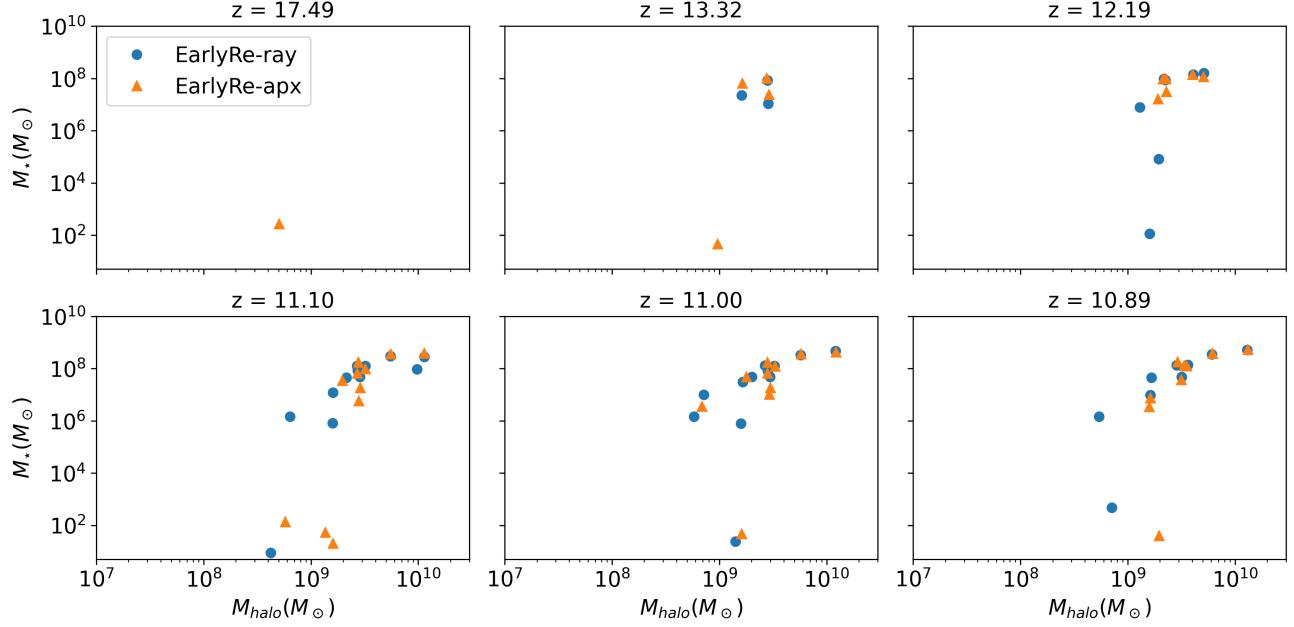


Figure 3. The relationships between stellar mass and total mass of all the halos in the timestep where stars first appear, in the intermediate timesteps, and in the last timestep of the *EarlyRe* dataset.

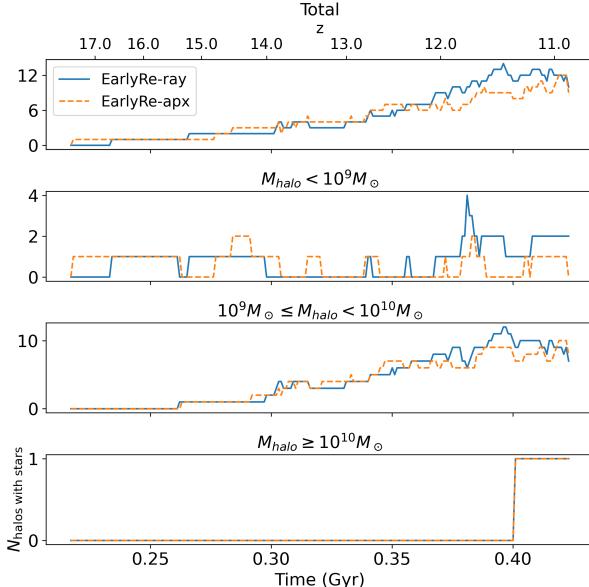


Figure 4. The comparison of the number of halos with stars as a function of time for each halo mass bin between the *EarlyRe-ray* and the *EarlyRe-apx* simulations.

two pairs of halos serve as examples to how the H_2 self-shielding modeling affects the galaxy properties.

Figures 5 and 6 show the projection of various properties at the last time step and the time evolution of those properties for the two halos in our case study. As hinted earlier by Figure 2, gas mass stays consistent between *EarlyRe-apx* and *EarlyRe-ray* throughout the halo's evolution and thus is unaffected by the choice of

H_2 self-shielding modeling. The gas density projection plot also looks relatively similar between our two runs. However, even though there is an agreement on total gas content, the amount of H_2 is considerably different in two simulations. For the largest halo, the mass of H_2 starts to diverge around $z \approx 14$, and *EarlyRe-ray* has about 10 times more H_2 in that halo than *EarlyRe-apx*. For the smaller halo, the discrepancy in the H_2 content is much more severe. Early in the simulation, the ray-tracing model consistently returns about 0.5 dex more mass than the approximation model. At $z \approx 11.5$, while *EarlyRe-ray* witnesses a quick rise in molecular gas, *EarlyRe-apx* maintains the same level of H_2 , intensifying the difference to be up to 2 dex in M_{H_2} between the two simulations at the last snapshot. This difference in H_2 matches our observation in Figure 2. In addition to H_2 mass, the distribution of molecular hydrogen is also different. In both halos that we use as examples, molecular hydrogen exists in clumps of high density ($\approx 10^{-21} \text{ g/cm}^3$) with respect to the surrounding. These clumps are located inside the galaxy (indicated by the white circle in the figures) and are concentrated in the galactic center. Outside of these clumps, H_2 gas density is quite low, reaching down to 10^{-36} g/cm^3 , proving that H_2 is completely photo-dissociated. In contrast, the halos in the *EarlyRe-ray* set displays a much more uniform distribution of molecular hydrogen. While H_2 density is still highest at the halo's center, H_2 density in the surrounding region is only 2-3 dex lower, showing that H_2 is able to exist and form in the outer part

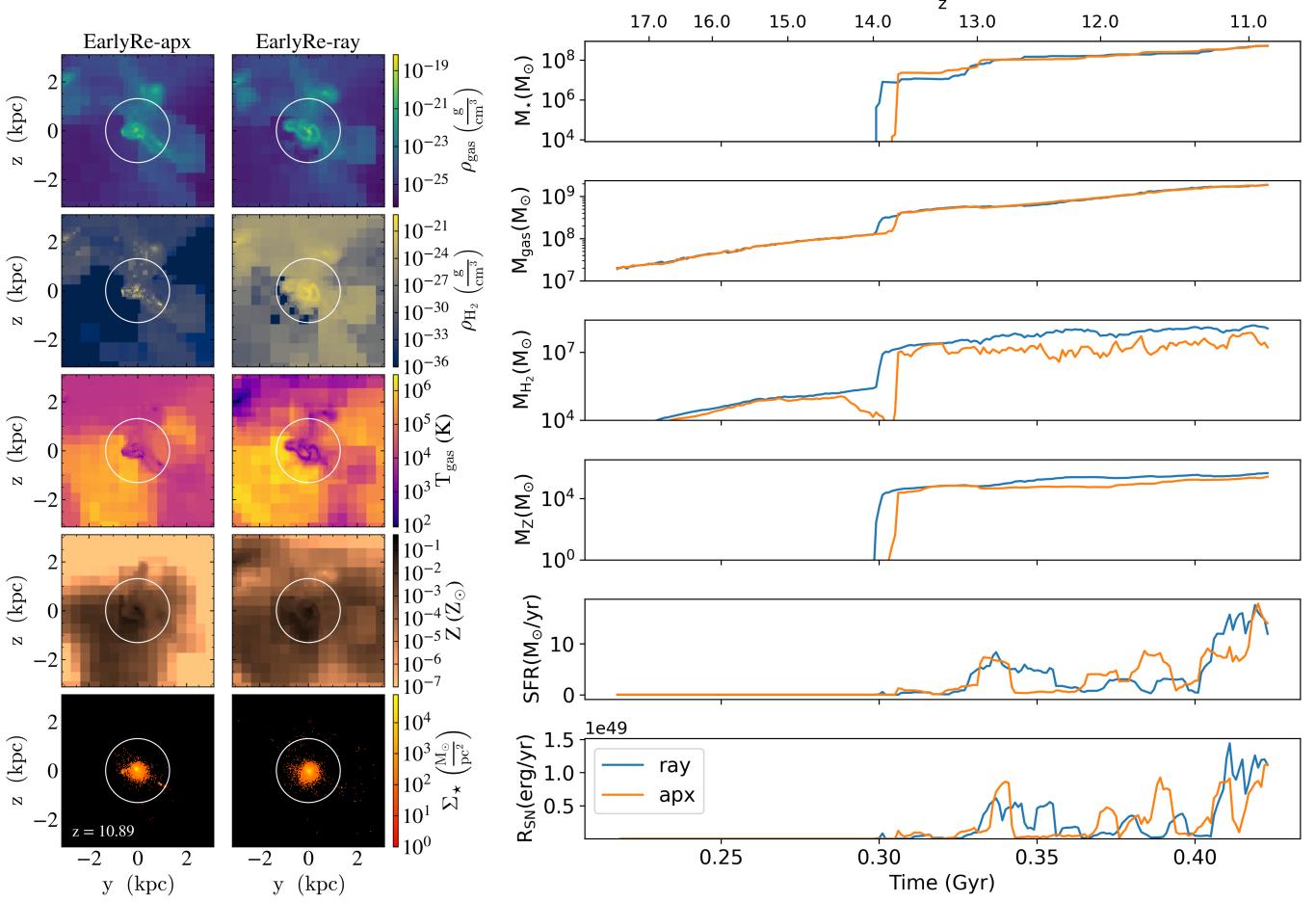


Figure 5. (Left) The gas density, H_2 density, temperature, metallicity, and stellar surface density projection plot of Halo 0 ($M_{\text{halo}} \approx 1.3 \times 10^{10} M_\odot$ at $z = 10.89$) within one virial radius. The white circle represents the boundary of the galaxy, which is defined as the radius enclosing the baryonic density 2000 times larger than the critical density of the universe. (Right) The time evolution of different properties in Halo 0 between the *EarlyRe-ray* and *EarlyRe-apx* simulations.

of the galaxy and even in the CGM. Indeed, the existence of H_2 outside the galactic center is what causes the discrepancy in the H_2 fraction between *EarlyRe-apx* and *EarlyRe-ray*. More details on the topic of ISM and CGM will be discussed in Section 3.3.

With regards to stellar mass, the different in self-shielding modeling results in greater differences in smaller halos than in bigger halos, as pointed out in Figure 3. For the case of the biggest halo in the simulation, Figure 5 shows that the stellar mass of the halo converge after $z \approx 13$, even though *EarlyRe-ray* forms its first stellar particles a few million years earlier. On the other hand, for the smaller halo in Figure 6, the halo modeled with ray-tracing forms stars approximately 20 million years prior to the *EarlyRe-apx*'s counterpart. Furthermore, throughout most of this halo's evolution, the stellar mass in *EarlyRe-ray* stays about several dex higher

in the *EarlyRe-apx* version and relatively converge at the last snapshot. Thus, this shows that the choice of H_2 self-shielding model affects the timing of star formation in halos while the stellar mass between two models will eventually converge. While the ray-tracing model might initially boost star formation due to higher amount of H_2 , this effect will be counteracted by increased stellar feedback later, leading to a balanced average on stellar mass.

In addition to the difference in stellar mass, the star formation history shows that the halo in the ray-tracing model experience more prolonged period of star formation while the halo in the approximation model experience shorter but stronger star formation episode (**more detailed explanation maybe?**). This behavior also happens in other large halos in the simulation box (for the brevity purpose, they are not shown in the paper).

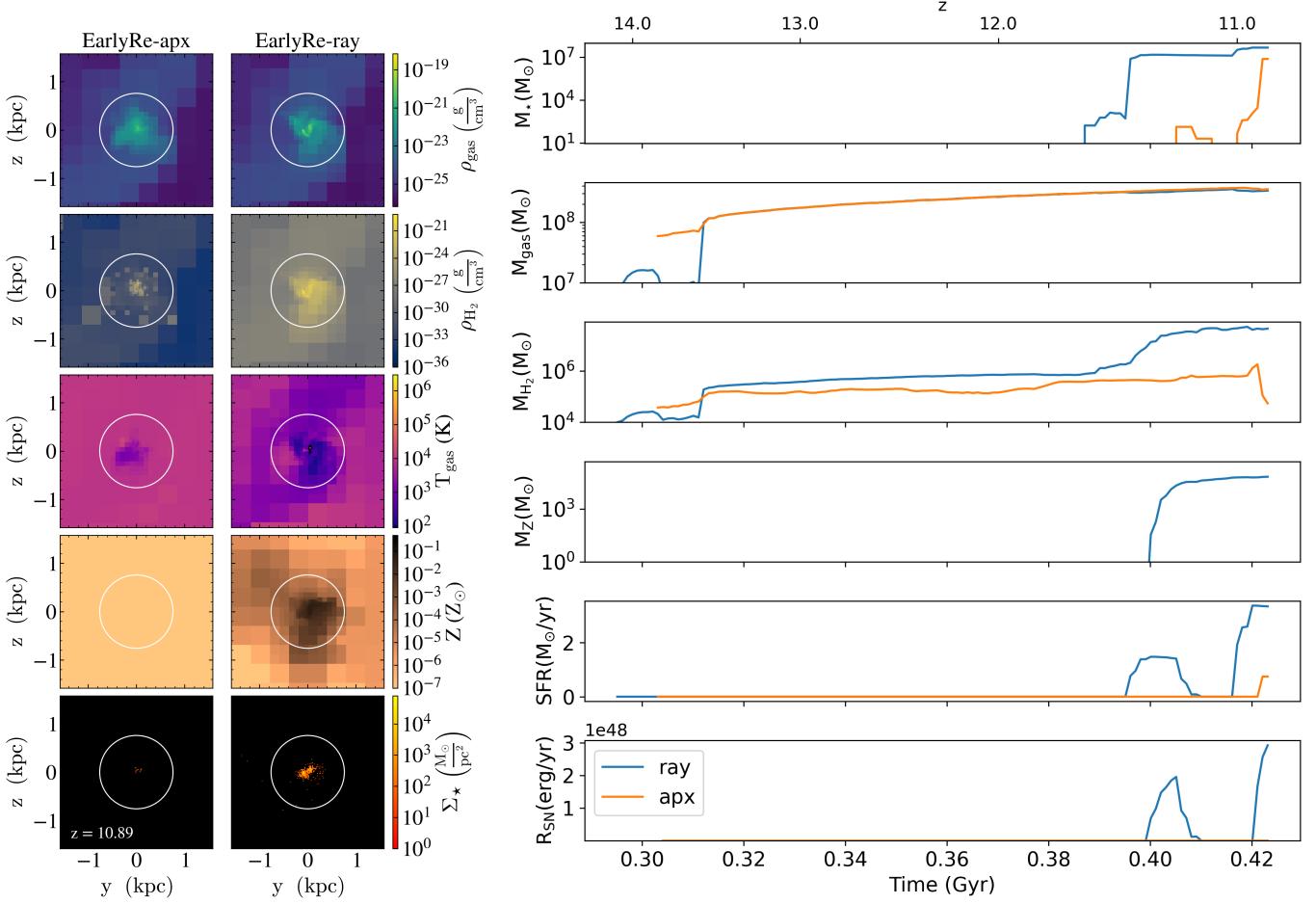


Figure 6. Same as Figure 5, but for another halo whose $M_{\text{halo}} \approx 1.7 \times 10^9 M_{\odot}$ at $z = 10.89$.

The prolonged star formation period leads to prolonged supernova rate, thus affecting the metal mixing and metal distribution of the galaxy. As supernovas go off in longer time period, more metals are produced at once and thus it takes a longer time for the metals to mixed with the surrounding gas. This leads to what we see in the metallicity projection plot, where metals are less mixed and more uniformly distributed in the *EarlyRe-ray* set. More metals also results in more efficient cooling of gas, which is reflected in the temperature projection plot. These behaviors are more prominent in smaller halos, showing again that smaller halos are more susceptible by H_2 self-shielding modeling than of bigger halos.

3.3. Effect on the galaxy and CGM

In this section, we more closely examine the effect of H_2 self-shielding modeling on the ISM, the CGM, and the IGM to help further explain the previous observations we have on star formation.

Following the two case studies we examined in Section 3.2, Figures 7 and 8 show the gas and H_2 phase plot of the largest halo in the simulation ($M_{\text{halo}} = 1.3 \times 10^{10} M_{\odot}$) and a smaller halo of mass $M_{\text{halo}} \approx 1.7 \times 10^9 M_{\odot}$. The plots are separated into the galaxy (top row) region and the CGM region (bottom row). One noticeable disparity between *EarlyRe-ray* and *EarlyRe-apx* is the inefficiency of the gas to cool down below $10^4 K$ due to the lack of molecular hydrogen in the region. With atomic hydrogen HI being the only dominant component, processes such as Bremsstrahlung emission, atomic hydrogen's ionization and excitation processes can only help cool the gas down to $10^4 K$, while the existence of H_2 can introduce more energy levels to lower gas temperature. Thus, we can see a high concentration of gas at $10^4 K$ at low to intermediate density ($\rho_{\text{gas}} \leq 10^{-22} \text{ g/cm}^3$) when using the approximation model. The gas in *EarlyRe-apx* can only cool down to lower temperature after reaching a density of $\approx 10^{-22} \text{ g/cm}^3$ - the limit which the approximation

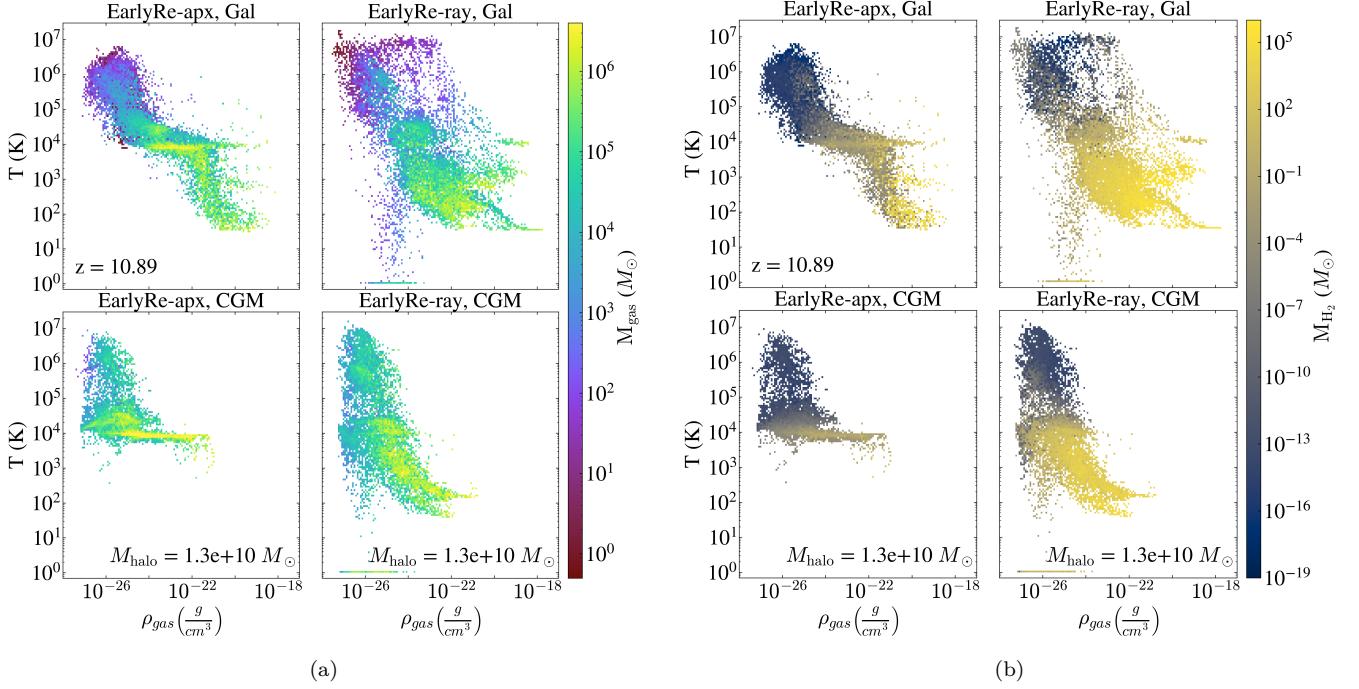


Figure 7. The gas phase plot colored by gas mass (Sub-figure (a)) and by molecular hydrogen mass (Sub-figure (b)) of the largest halo ($M_{\text{halo}} = 1.3 \times 10^{10} M_{\odot}$) in our simulation set, evaluated at the last time step $z = 10.89$. For each sub-figure, the left column shows the halo in *EarlyRe-apx*, and the right column shows its counterpart in *EarlyRe-ray*. The top row in each subfigure shows the phase plot using the gas cells within the galaxy region ($r \leq R_{\text{bary},2000}$), and the bottom row shows the phase plot using the gas cells in the CGM region ($R_{\text{bary},2000} < r \leq R_{\text{vir}}$).

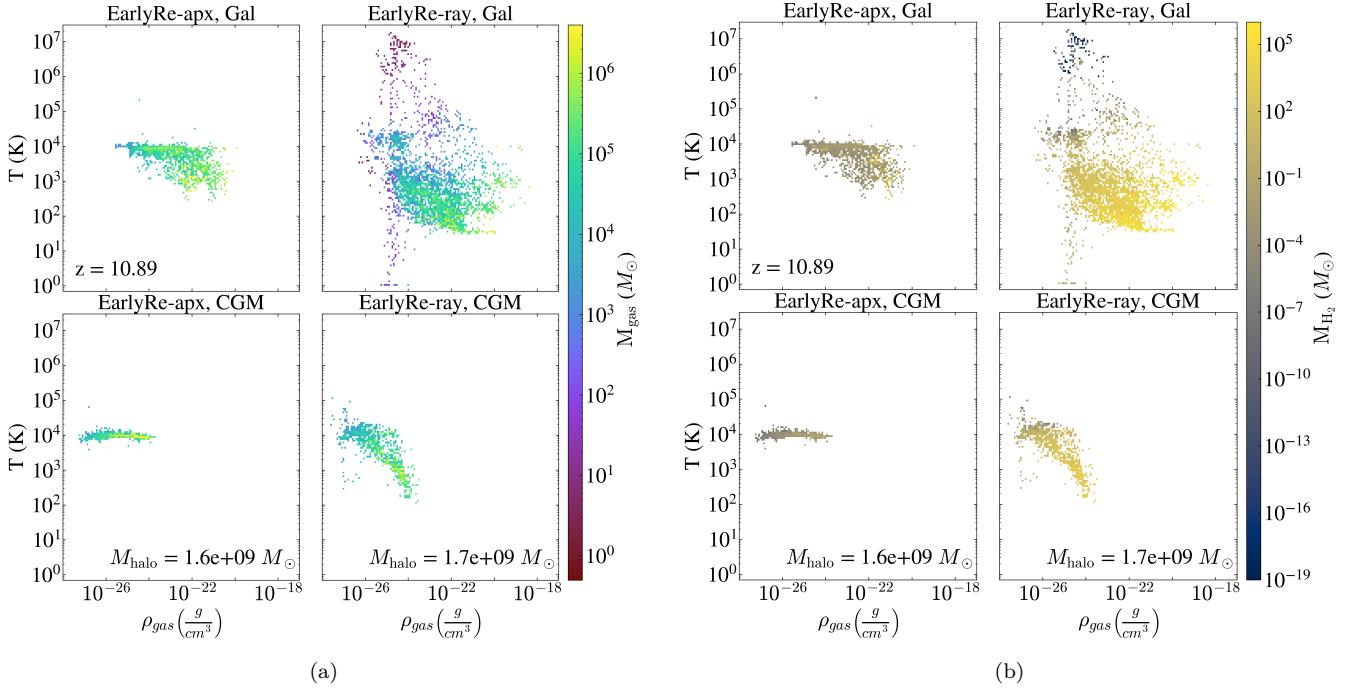


Figure 8. Similar to Figure 7, for a halo with $M_{\text{halo}} \approx 1.7 \times 10^9 M_{\odot}$ at $z = 10.89$.

model can better predict the H_2 self-shielding factor, according to Figure 1. When the gas is dense enough, the self-shielding of H_2 is approximated by *EarlyRe-apx* more accurately, leading to more H_2 to exist and gas to cool down. Indeed, according to the H_2 phase plot, H_2 exists most abundantly at the gas density of $\rho_{H_2} \geq 10^{-22} \text{ g/cm}^3$. The phase plot also re-affirm that the amount of H_2 existed in the *EarlyRe-apx*'s galaxy is much smaller than that of *EarlyRe-ray*, as pointed out in Figure 5. On the other hand, the large amount of molecular hydrogen in *EarlyRe-ray* existing even at low density helps cool down more of the gas. This allows gas to become denser. For example, the densest gas cell in the *EarlyRe-ray*'s galaxy in Figure 7 reaches the density above 10^{-18} g/cm^3 , about 10 to 100 times higher than the densest region in the *EarlyRe-apx*'s galaxy. It is important to note that for the radiative star cluster model and the Population III star model used in our simulation, their overdensity thresholds for a star particle to form are 10^7 and 10^6 , respectively. At the last time step ($z = 10.89$), these overdensity thresholds correspond to a gas density threshold of 4.5×10^{-20} and 4.5×10^{-21} . This suggests that both *EarlyRe-ray* and *EarlyRe-apx* galaxies are able to form stars; however, since *EarlyRe-ray* has more denser gas cells, it can form stars easier and quicker. **(so why the two stellar mass is the same?)** Furthermore, this effect is more prominent for lower halo. When using the approximation model, the gas within the *EarlyRe-apx*'s galaxy shown in Figure 8 cannot cool down below 10^3 K or gets denser than 10^{-20} g/cm^3 , while its counterpart can reach below 10^2 K and about 10^{-18} g/cm^3 thanks to much more H_2 being available.

In the CGM, gas has lower density and thus H_2 is more susceptible to destruction by LW radiation when using the approximation model. For both halos in our case studies, there is very little H_2 existing in the CGM in the *EarlyRe-apx* simulation. This keeps the gas in the CGM relatively hot at the minimum of 10^4 K . In contrast, for *EarlyRe-ray* simulation, H_2 still exists in sufficient quantity outside of the galaxies that the CGM gas can cool down to a few hundred kelvins. Therefore, the use of the self-shielding model significantly effect the temperature and density profiles of both the galaxy and the CGM.

The effect of the self-shielding model on different region of the halo is further illustrated in Figure 9, which shows the comparison between *EarlyRe-ray* and *EarlyRe-apx* with respect to the gas mass fraction and the H_2 fraction in four radial bins. We crossmatch and select halos whose gas is resolved enough for us to locate the baryonic center of mass and distinctly separate

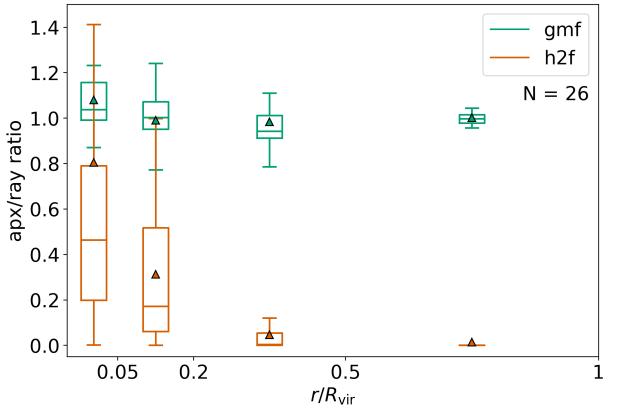


Figure 9. The comparison of the gas mass fraction (gmf) and H_2 fraction (h2f) in different radial bins (0 to $0.05 R_{\text{vir}}$, 0.05 to $0.2 R_{\text{vir}}$, 0.2 to $0.5 R_{\text{vir}}$, and 0.5 to $1 R_{\text{vir}}$) between the *EarlyRe-ray* and the *EarlyRe-apx* simulations at $z = 10.89$. The sample size for the statistics is 26 halos. The box represents the first and third quartile of the sample. The whiskers extend from the box to the further point within 1.5 times the inter-quartile range. The median is shown as a line in the box and the mean is shown as a triangle point.

the halo into multiple bins. We end up with 26 halos, including halos without any stars, to calculate the statistics. The figure shows that while the gas mass fraction remains consistent between the two models across all radial bins, the ratio of H_2 fraction between the approximation and the ray tracing model shows a declining trend towards larger ratio. The H_2 fraction in *EarlyRe-apx* agrees with *EarlyRe-ray* only in the inner most region of the galaxy ($r < 0.05 R_{\text{vir}}$) where gas is at high density and thus the self-shielding factor is accurately calculated by the approximation model. As we go to the outer radius, gas density decreases and thus H_2 in *EarlyRe-apx* is under-shielded, leading to a decrease in the ratio of H_2 fraction. Further into the CGM ($r > 0.2 R_{\text{vir}} \approx R_{\text{bary},2000}$), the approximation model fails to estimate the self-shielding factor, leading to a clear absence of molecular hydrogen in this region when compared with the ray-tracing model.

It is important to note that we have an outlier in Figure 9 where a halo with mass $M_{\text{halo}} = 3.6 \times 10^{10} M_{\odot}$ has a H_2 fraction within $0.05 R_{\text{vir}}$ about 8 times larger in *EarlyRe-apx* compared to *EarlyRe-ray*. To ensure the readability of the figure, we exclude this outlier from the figure; however, you can still see its effect on pulling the mean value away from the median value. The reason for this big difference is because for this particular halo, the gas in the inner region is much more compact and reaches a higher density in *EarlyRe-apx*. In particular, the densest gas cell in the *EarlyRe-apx*'s halo is about 10^{-19} g/cm^3 , 10 times higher than the *EarlyRe-*

ray's counterpart. At $\rho_{\text{gas}} \approx 10^{-19} \text{ g/cm}^3$, according to Figure 1, the Sobolev-like approximation typically overestimate the self-shielding amount, leading to more H_2 being able to form. More H_2 forming corresponds to more cooling, leading to the collapse of gas and increase in gas density. This results in a runaway effect that causes this halo to have noticeably high amount of H_2 in its inner region when using the approximation model. However, this halo is the only case where the H_2 fraction is considerably higher when using the approximation and it only happens near the galactic center. In most of the cases, this runaway effect only happens locally at a few dense gas cells (as also shown in the H_2 clumps in Figures 5 and 6) that it does not change the average H_2 fraction of the whole galactic region.

3.4. Effect on the large-scale universe and reionization

We extend our analysis to the whole simulation box to investigate the effect of H_2 self-shielding modeling on a large-scale universe. Figure 10 shows the projection plots at different snapshots within the simulation's refined region, which is about 1/10000 volume of the whole simulation box. While the large-scale structure of gas is similar between two simulations, the distribution of other properties differ greatly. The amount of molecular hydrogen in the IGM is much lower when using the Sobolev-like approximation method, especially after stars start to form in the simulation. Newly formed stars produce LW radiation that propagate the whole simulation's refined region and destroy H_2 in the low gas density region where the approximation model under-predicts the amount of shielding. The lowest H_2 density in the IGM of *EarlyRe-apx* is less than 10^{-36} g/cm^3 , while the H_2 density in the most diffuse region of *EarlyRe-ray* is nearly 10 dex higher. As the simulation progresses, H_2 is recreated surrounding the supernova's superbubbles and the galactic filaments. As we can see in the temperature projection plot, supernova explosions heat up and ionize the surrounding gas. The electron and proton created from the ionization provide ingredients for H_2 to form (Galli & Palla 1998, see Table 1). However, near the supernova explosion when the temperature becomes too hot, H_2 can then be destroyed via collisional mechanisms. These explains the accumulation of H_2 around galaxies and galactic filaments and the temporary absence of H_2 close to galaxies after stellar feedback in Figure 10. At high gas density region inside galaxies, H_2 can form via a three-body interaction between three atomic hydrogen (Palla et al. 1983) or via grain catalysis (Gould & Salpeter 1963).

As pointed out in Section 3.2, galaxies in *EarlyRe-ray* experience more prolonged star forming period than

their counterparts in *EarlyRe-apx* and thus more metals are pushed out simultaneously in each period. This leaves shorter time for pristine gas to mix in to reduce the gas metallicity. Furthermore, more metals being produced at once helps contaminate the IGM more easily. When metals get out to the IGM, because of the medium's very low gas density for mixing, metallicity does not decrease over time, creating more extended metal-rich regions spanning out to the IGM in the ray-tracing simulation. It is important to note that this difference in metallicity originates from the difference in star formation history rather than the amount of metals being produced because the galaxies in two simulations have relatively similar stellar mass and total supernova energy, as shown in Figure 5.

As suggested by Figure 10, the universe in *EarlyRe-apx* is much hotter at $z \approx 10.9$ than its counterpart in *EarlyRe-ray*. Because cosmic reionization is linked to the heating of the IGM (D'Aloisio et al. 2019), we expect that reionization is affected by the choice of self-shielding modeling. Figure 11 shows the distribution of neutral hydrogen fraction χ_{HI} within the refined region between our two simulations. The χ_{HI} value of 0 corresponds to complete ionization of atomic hydrogen. High-energy radiation from galaxies ionizes hydrogen, decreasing χ_{HI} in the surrounding IGM regions. χ_{HI} can go up again during recombination between protons and electrons to form neutral hydrogen, which is efficient at temperature lower than 10^4 K (Wise 2019). In all time steps shown, *EarlyRe-apx* displays more extended and prominent region of ionized hydrogen, expanding out to the further IGM region. On the other hand, hydrogen is less ionized in *EarlyRe-ray*, and ionized hydrogen is limited around the galaxy filament (shown in the top two rows of Figure 10). This observation is quantified in Figure 12 where we plot the volume-weighted average of χ_{HI} within the simulation's refined region as a function of time. At the start of both simulations, the universe is dominated with neutral hydrogen ($\chi_{\text{HI}} \approx 1$). However, about 0.32 Gyr after the Big Bang ($z \approx 13.5$), the volume-weighted average of the neutral hydrogen fraction starts to drop considerably in the approximation model when the ray-tracing model only shows a slight decline. By the end of the simulation, while more than 90% of hydrogen is still neutral in *EarlyRe-ray*, only about 65% of hydrogen remains as such in *EarlyRe-apx*. While both simulations are not run long enough to cover the whole reionization epoch, Figure 12 suggests that the reionization may be complete earlier in *EarlyRe-apx* than in *EarlyRe-ray*, even though the reionization's start time is similar. This illustrates that the use of Sobolev-like approximation to model H_2 self-shielding speeds up

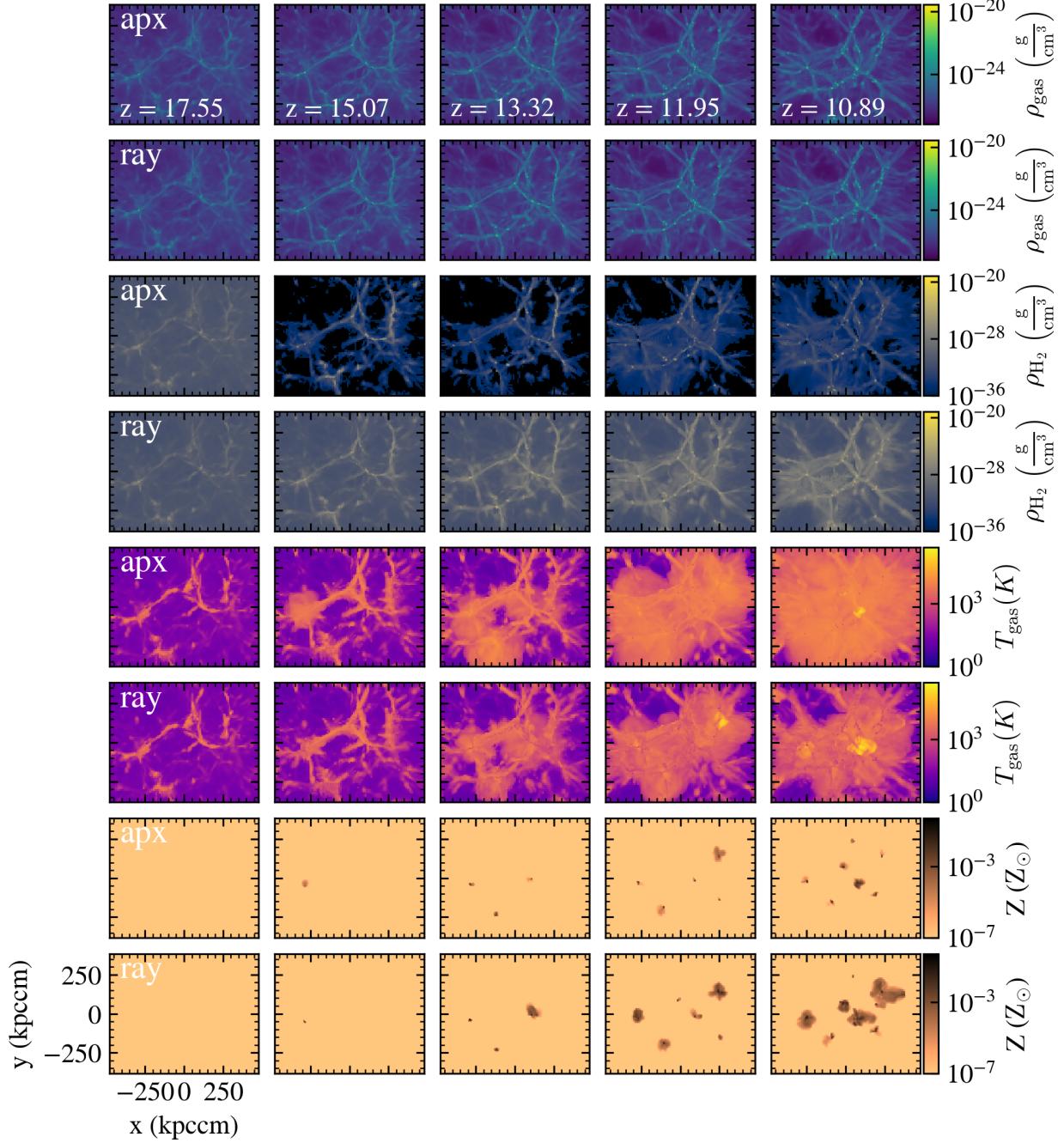


Figure 10. The gas density (1st and 2nd row), H_2 density (3rd and 4th row), gas temperature (5th and 6th row), and gas metallicity (7th and 8th row) within the simulation’s refined region between the *EarlyRe-apx* and *EarlyRe-ray* across five time steps.

the reionization process and thus affect our theoretical prediction and modeling of the reionization epoch.

4. DISCUSSION AND CONCLUSION

In this paper, using high-resolution zoom-in simulations, we run two radiative transfer models of molecular hydrogen self-shielding to examine their effect on galaxy evolution. The two models are the Sobolev-like approx-

imation that uses local gas property to estimate the H_2 photodissociation rate and the ray tracing model based on HEALPix scheme. In summary, our key findings are as follows:

- The Sobolev-like approximation for H_2 self-shielding underestimates the self-shielding factor at low gas density ($\rho_{\text{gas}} \leq 10^{-22} \text{ g/cm}^3$) while over-

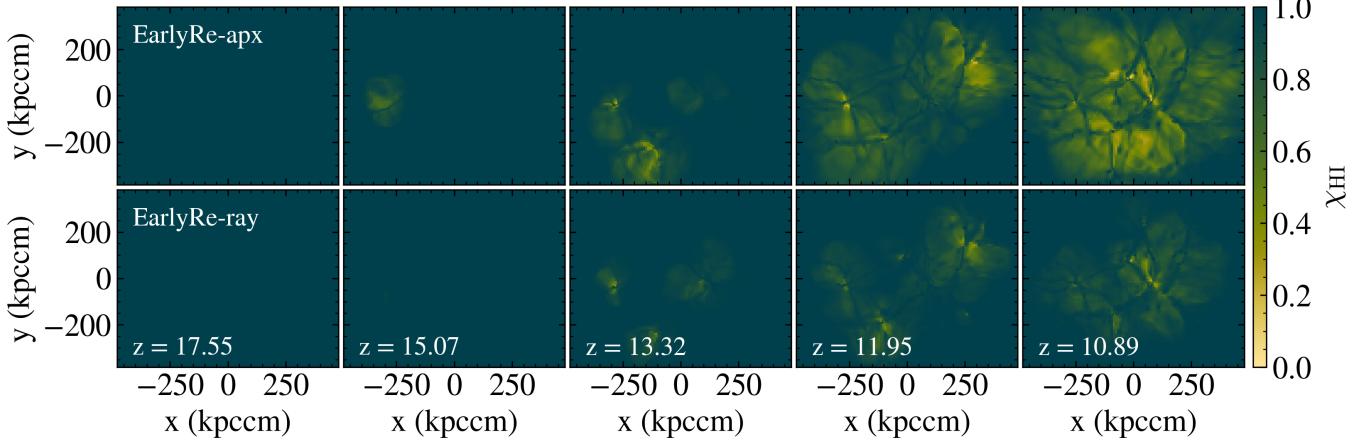


Figure 11. The neutral hydrogen fraction within the refined region between the *EarlyRe-ray* and *EarlyRe-apx* simulations across five time steps.

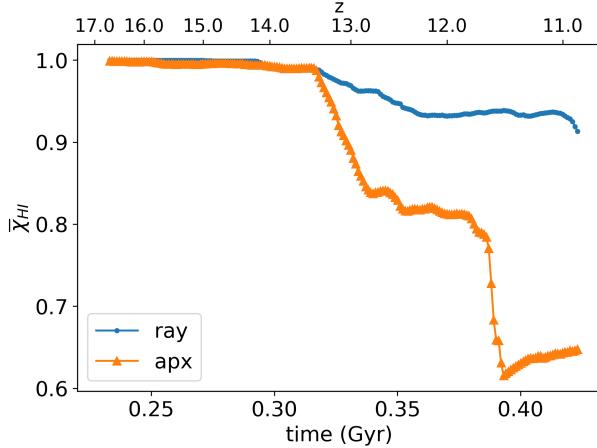


Figure 12. The comparison between the volume-weighted average of the neutral hydrogen fraction as a function of time between the *EarlyRe-ray* and the *EarlyRe-apx* simulations.

estimates the self-shielding factor at high gas density ($\rho_{\text{gas}} \geq 10^{-19} \text{ g/cm}^3$). This leads to halos in the simulation with the approximation model having their H_2 fraction several dex lower than their counterparts in the simulation with ray tracing model, especially for lower mass halo. (Figures 1 and 2)

- The Sobolev-like approximation affects star formation in cosmological simulation. Lower-mass halos ($M_{\text{halo}} < 10^9 M_\odot$) are harder to form stars due to the lack of molecular hydrogen fuel. Bigger halos are less affected and still converge in stellar mass between the two models. (Figures 3, 4)
- Even though there is convergence in the total stellar mass, the star formation history in the ray-tracing model shows more prolonged period of star

formation while the approximation model shows a more bursty behavior. The different star formation behavior results in metals being produced, distributed, and mixed differently in the two simulation. This leads to a discrepancy in the metallicity and temperature profile between the two simulations where the ray-tracing model shows a more metal-riched and cooler ISM. (Figures 5, 6, and 10)

- Because the CGM is less dense than the galaxy, the effect of the approximation is more prominent in the outer region of the halo. Also, halos in the simulation with ray-tracing have more cool diffuse gas than in the simulation with the approximation model. (Figures 7, 8, and 9)
- The Sobolev-like approximation also effect the timing of the reionization epoch in cosmological simulation, where it make the universe reionize much quicker than the prediction using the ray tracing model. (Figures 11 and 12)

These results show that using the Sobolev-like approximation has a considerable impact on the prediction made with cosmological simulation, particularly with regards to H_2 , star formation activity in dwarf galaxies, and reionization period. Studies on chemical distribution, phase profile, and temperature profile of ISM and CGM will also likely be affected by using the approximation. Therefore, predictions based on this model of H_2 self-shielding should be re-evaluated as needed. For future work, we want to expand this comparison to other self-shielding approximation models as discussed in Section 1. It is possible that one method performs better in one aspect and worse in another, which makes it im-

portant for the simulation users to be aware and apply them accordingly to their scientific questions.

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