Triggered Population III star formation: the effect of $\text{H}_2$ self-shielding

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ABSTRACT

The multiplicity of metal-free (Population III) stars may influence their feedback efficiency within their host dark matter halos, affecting subsequent metal enrichment and the transition to galaxy formation. Radiative feedback from massive stars can trigger nearby star formation in dense self-shielded clouds. In model radiation self-shielding, the $\text{H}_2$ column density must be accurately computed. In this study, we compare two local approximations based on the density gradient and Jeans length with a direct integration of column density along rays. After the primary massive star forms, we find that no secondary stars form for both the direct integration and density gradient approaches. The approximate method reduces the computation time by a factor of 2. The Jeans length approximation overestimates the $\text{H}_2$ column density by a factor of 10, leading to five numerically enhanced self-shielded, star-forming clumps. We conclude that the density gradient approximation is sufficiently accurate for larger volume galaxy simulations, although one must still caution that the approximation cannot fully reproduce the result of direct integration.

Key words: early universe: hydrodynamics — H II regions — ISM: molecules — methods: numerical — stars: formation — stars: Population III —

1 INTRODUCTION

The first generation of metal-free (Population III or Pop III) stars are crucial astronomical objects. Main-sequence Pop III stars emit copious amounts of ultraviolet (UV) photons, which can have either positive or negative effects on star formation. Ionizing photons with energies $\geq 13.6$ eV can induce star formation in the interstellar medium (ISM) by enhancing the fraction of electrons, which catalyze formation reactions of hydrogen molecules (Ricotti, Gnedin, & Shull 2001; Johnson & Bromm 2006; Yoshida et al. 2007). Dissociating photons in the Lyman-Werner (LW) band (11.2–13.6 eV) can suppress star formation by destroying $\text{H}_2$ (Stacy et al. 2012; Hirano et al. 2015). Massive Pop III stars die with supernova (SN) events, which can also affect star formation (Klein, McKee, & Colella 1994; Nakamura et al. 2006; Chiaki et al. 2013; Magg et al. 2022). Sufficiently weak explosions can compress the surrounding gas and trigger star formation in a dense shell. Strong explosions can completely destroy ambient gas clumps and suppress star formation. Additionally, Pop III SNe supply the first elements heavier than lithium (metals) and their condensates (dust grains).

Additional cooling from metals and grains can lead the formation of first low-mass stars, by inducing the fragmentation of clouds (Omukai 2000; Schneider et al. 2003). The efficiency of radiation and SN feedback depends not only on the initial mass function (IMF) of Pop III stars but also on the number of Pop III stars per host dark matter minihalo (MH). Even with the state-of-the-art numerical simulations, it is challenging to predict the IMF and multiplicity within MHs.

Researchers have made valiant efforts to constrain the IMF of Pop III stars for the past two decades (Bromm et al. 1999; Abel et al. 2002; Yoshida et al. 2003). In metal-free collapsing clouds, hydrogen molecular cooling primarily induces fragmentation. $\text{H}_2$ cooling is inefficient at densities $\gtrsim 10^4$ cm$^{-3}$, where local thermal equilibrium is established. The mass scale of fragments can be estimated to be the Jeans mass

$$M_J = 2 \times 10^3 M_\odot \left( \frac{\mu}{1.23} \right)^{-3/2} \left( \frac{n_{\text{H}}}{10^4 \text{ cm}^{-3}} \right)^{-1/2} \left( \frac{T}{200 \text{ K}} \right)^{3/2},$$

(1)

(Matsuda, Satō, & Takeda 1969). Multi-dimensional simulations showed that the Pop III stellar mass lies in a range of $\sim 10$–1000 $M_\odot$ (Hirano et al. 2014; Susa et al. 2014).

The multiplicity of Pop III stars is also crucial for the
numerical simulations have shown that, through the fragmentation of turbulent clouds or accretion discs, binaries and star clusters form at scales of \( \sim 10^{-19} \) AU (Turk et al. 2009; Greif et al. 2012; Susa 2019; Wollenberg et al. 2020). Sugimura et al. (2020) found that hierarchical binary/triplet systems form from an accretion disc \( \sim 10^8 \) yr after the formation of the primary protostar. The primary binary system consists of massive stars (60–70 M\(_\odot\)) with a separation of \( \sim 10^8 \) AU. One star hosts a small triplet system with moderately massive companions (\( \sim 10 \) M\(_\odot\)) at distances of \( 10^3–10^4 \) AU.

In this paper, we focus on another channel of multiple Pop III star formation, so-called “triggered star formation” (Elmegreen & Lada 1977; Whitworth et al. 1994; Hosokawa & Inutsuka 2005, 2006). After the primary star forms in a MH, it emits ionizing photons if the star is sufficiently massive (\( \gtrsim 10 \) M\(_\odot\)). The overpressurized H II region and associated D-type ionization front drives a shock wave, creating a dense shell. It potentially can host star formation if the abundance of H\(_2\) is sufficiently large (\( y(H_2) \gtrsim 10^{-3}\)) and becomes self-gravitating. The H\(_2\) fraction in the D-type front can be reduced by LW photons emitted by the primary star. With a sufficiently large column density \( N_{H_2} \gtrsim 10^{24} \) cm\(^{-2}\) of hydrogen molecules, the self-shielding effect becomes important (Shull 1978; Federman, Glassgold, & Kwan 1979), where the dissociation rate \( k_{\text{diss}} \) is reduced by a shielding factor \( f_{\text{SH}} \) that is a non-linear function of \( N_{H_2} \) (Draine & Bertoldi 1996). Therefore, an accurate estimate of \( N_{H_2} \) is essential to model star formation, if any, in the D-type front.

It is ideal to calculate the column density by integrating the H\(_2\) number density \( n(H_2) \) from the source. Gas is generally optically thin in the LW band, and photons can propagate farther distance than ionizing photons. Radiation transport is especially difficult and computationally expensive in multi-dimensional simulations. To save the computational time, approximation methods are often used, where the column density is calculated using a typical length scale (shielding length) defined at each fluid element. Previous works have often used the length scale associated with the density or velocity gradient. The former characterizes the length scale of the density structure. The latter, so-called the Sobolev length, characterizes the length scale where a molecule cannot absorb redshifted photons (Sobolev 1960). Another common choice is the local Jeans length, which typically characterizes the size of a collapsing cloud. Although it should be irrelevant to an expanding H II shell, this approximation is used in cosmological simulations, where not only radiative feedback but also star formation take place.

Several groups have studied the validity of the local approximation in various test problems. Greif (2014) studied the escape probability of H\(_2\) line emission to evaluate the cooling efficiency of Pop III star-forming clouds. They found that the Sobolev method underestimates the column density because the scale length of velocity gradient is significantly smaller than the bulk infall velocity due to turbulent motions. Wolcott-Green et al. (2011) and Hartwig et al. (2015) investigated the effect of H\(_2\) self-shielding of background LW emission in the context of direct-collapse black hole formation. Wolcott-Green et al. (2011) found that the Sobolev approach can reproduce the shielding factor of the direct integration method while Hartwig et al. (2015) found that the Jeans approach overestimates the LW intensity. Safranek-Shrader et al. (2017) studied the self-shielding effects of H\(_2\) and CO dissociation in a galactic disc. They compared direct ray-tracing and a variety of local approximations: the Jeans, Sobolev-length and density-gradient approach. They showed that the local approximation, especially the Jeans approach, in contrast with the findings of Hartwig et al. (2015), can reproduce the result of the full ray-tracing calculation well. In this work, we study the effect of the local approximation on the efficiency of triggered star formation, by comparing the full ray-tracing calculation with the density gradient and Jeans length approaches.

Another important numerical parameter is the threshold density \( n_{\text{th,1h}} \) above which star formation is assumed to occur. Stars will form if the gas density grows up to \( \gtrsim 10^{15} \) cm\(^{-3}\) in a timescale shorter than the dynamical time (Greif et al. 2012). To resolve the gas dynamics in such dense regions, numerical timesteps are limited by the short Courant timescales (\( \lesssim \upmu t \)). In Mpc-scale cosmological simulations of first-generations of stars and galaxies, several authors use \( n_{\text{th,1h}} = 10^{10}–10^{17} \) cm\(^{-3}\) (Smith et al. 2015; Schauer et al. 2021). Since the D-type front simultaneously contracts and expands with the thermal pressure from the inner H II region at comparable timescales, the density may only tentatively exceed the threshold value if \( n_{\text{th,1h}} \) is too small. In this work, we will test the convergence for \( n_{\text{th,1h}} = 10^6 \) and \( 10^8 \) cm\(^{-3}\).

We structure this paper as follows. In Section 2, we detail our cosmological hydrodynamics simulations and the relevant chemical processes. Then, we describe the results for the different schemes to estimate the H\(_2\) column density and star formation density threshold in Section 3. In Section 4, we compare the computational cost for direct integration and local approximation. We also discuss the ramifications of the different schemes on star formation and feedback in the early Universe. Finally, we summarize the paper in Section 5.

Throughout the simulations, we adopt the cosmological parameters \( \Omega_0 = 0.3089, \Omega_{\Lambda,0} = 0.2693, \Omega_M = 0.6911, \) and \( H_0 = 67.74 \) km s\(^{-1}\) Mpc\(^{-1}\) (Planck Collaboration et al. 2016). We run the simulations in comoving coordinates, but we describe physical quantities in proper coordinates throughout this paper, unless otherwise specified. We use the mass fraction of hydrogen nuclei \( X_H = 0.76 \). All the figures in this paper are created with the yt toolkit (Turk et al. 2011).\(^1\)

1 https://yt-project.org/.

2 METHOD

2.1 Cosmological simulation

We run a suite of cosmological simulations with the adaptive mesh refinement (AMR)/N-body simulation code Enzo (Bryan et al. 2014; Bromm-Smith et al. 2019). We solve the hydrodynamics equations with the piecewise parabolic method (PPM) in an Eulerian frame (Woodward & Colella 1984; Bryan et al. 1995), using a Harten-Lax-van Leer-Contact (HLLC) Riemann solver to accurately capture hydrodynamical shocks and compute advection of chemical
species across contact discontinuities. We follow the DM dynamics with an $N$-body particle-mesh solver (Efstathiou et al. 1985; Bryan & Norman 1997).

Computational cells are progressively refined by a factor of two in space when satisfying the following criteria:

(a) The baryon mass in a cell exceeds $3m_{\text{b},0} \times 2^{-0.2L}$ on a refinement level $L$, where $m_{\text{b},0}$ is the mean baryon mass on the root grid.
(b) The DM particle mass contained by a cell exceeds $3m_{\text{dm},0}$, where $m_{\text{dm},0}$ is the mean DM mass on the root grid.
(c) The local Jeans length $\lambda_J$ is resolved less than 64 cells.

The negative coefficient $-0.2$ in the exponent of criterion (a) invokes the super-Lagrangian refinement for the gas component while criterion (b) ensures Lagrangian refinement for the DM. When the baryon density starts to increase in the run-away collapse phase, cells are refined mostly on criterion (c). This criterion warrants that the local Jeans length is resolved sufficiently to prevent spurious fragmentation (Truelove et al. 1997; Turk et al. 2012).

We generate the initial conditions in a periodic box with a side length of $1\, \text{h}^{-1}\, \text{Mpc}$ (comoving) with MUSIC (Hahn & Abel 2011). We initially run a DM-only simulation with a base resolution $512^3$ and identify the most massive halo with a mass $5.97 \times 10^8 \, \text{M}_\odot$ at redshift $z = 7$ with a halo-finding code ROCKSTAR (Behroozi, Wechsler, & Wu 2013). After initially refining the halo Lagrangian region with two additional AMR levels, i.e., with higher spatial resolution by a factor of four, we restart the simulation adding the baryon component. With this zoom-in strategy, the effective resolution is $2048^3$, and the minimum DM particle mass is $12.4 \, \text{M}_\odot$.

### 2.2 Pop III star formation

The main coolant of a primordial cloud is molecular hydrogen. To calculate the fraction and cooling rate of H$_2$, we model the non-equilibrium chemistry with the chemistry/cooling library GRACKE (Smith et al. 2017; Chiaki & Wise 2019). We solve a chemical network of 15 primordial species, $e^-$, H$^+$, H, H$^-$, H$_2^+$, H$_2$, D$^+$, D, D$^-$, HD$^+$, HD He, He$^+$, He$^{2+}$ and HeH$^+$. This chemical network includes the collisional ionization/recombination of H/He and formation/dissociation of H$_2$/HD molecules. We compute the rates of radiative cooling including inverse Compton cooling, bremsstrahlung, H/He transition line cooling, H$_2$ vibrational transition line cooling and HD vibrational transition line cooling. We also consider chemical heating from H$_2$ formation, where the binding energy ($4.48 \, \text{eV per molecule}$) is converted to the thermal energy (see Omukai 2000).

When certain criteria with a molecular cloud are met, we assume that a Pop III star forms. In reality, a star forms after gas is accreted onto a protostellar hydrostatic core with a density of $n_{\text{H}} \sim 10^{19} \, \text{cm}^{-3}$ (Larson 1969; Greif et al. 2012). In this work, to save the computational cost, we insert a Pop III star particle in cells that satisfy the following criteria:

(i) the gas density exceeds a threshold density $n_{\text{H,th}}$,
(ii) the gas flow is convergent, $\nabla \cdot \mathbf{v} < 0$,
(iii) the cooling time is less than the dynamical time,
(iv) the H$_2$ fraction exceeds a threshold value, $y_{\text{th}}(\text{H}_2) = 10^{-3}$.

We assign the mass $M_{\text{PopIII}}$ of the star particle, randomly sampling from a Larson-type IMF

$$
\frac{dN}{d \log M_{\text{PopIII}}} \propto M_{\text{PopIII}}^{-1.3} \exp \left[-\left(\frac{M_{\text{thar}}}{M_{\text{PopIII}}}\right)^{1.6}\right],
$$

where $M_{\text{thar}}$ is a characteristic mass of Pop III stars. We set the minimum, maximum and characteristic mass to 1, 300 and 20 $\text{M}_\odot$, respectively. Secondary star formation may be affected by the structure of H II region created by the primary star, and the structure will change for different stellar masses. We test two cases with fixed primary stellar masses of $M_{\text{PopIII,1}} = 10.4$ and $40.0 \, \text{M}_\odot$, called M10 and M40, respectively.

Table 1. Initial parameters of each run

| Parameter                      | n6     | n8     | Note                      |
|--------------------------------|--------|--------|---------------------------|
| **ENZO**                       |        |        |                           |
| PopIIIOverDensityThreshold     | -1e6   | -1e8   | Minimum density for star formation. |

(b) Approximation methods for LW transfer.

| Parameter                      | TestA | TestB | TestC | Note                      |
|--------------------------------|-------|-------|-------|---------------------------|
| RadiativeTransferOpticallyThinH2 | 0     | 1     | 1     | Flag to use local approximation. |
| RadiativeTransferUseH2Shielding  | 1     | —     | —     | Flag to calculate the self-shielding function. |

**GRACKE**

| Parameter                      | TestA | TestB | TestC | Note                      |
|--------------------------------|-------|-------|-------|---------------------------|
| H2_self_shielding              | —     | 1     | 3     | Types of local approximation method. |

Note — (a) If a negative value is assigned, ENZO uses its absolute value in units of cm$^{-3}$.
(b) 1: Density gradient. 3: Jeans length.

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2 https://grackle.readthedocs.io/


### 2.3 Radiation feedback from a Pop III star

During the main sequence of a Pop III star, we solve the radiative transfer equation with the adaptive ray tracing module MORAY (Wise & Abel 2011). We calculate the number flux $P$ of ionizing/dissociating photons passing through each computational cell. From each radiation source, we integrate $P$ along rays in directions based on HEALPix (Hierarchical Equal Area Isolatitude Pixelization; Górski et al. 2005). The number of rays is $12 \times 4^6$ with a level $l$. The initial level (RadiativeTransferInitialHEALPixLevel) is set to 1, and rays are adaptively split as they travel away from the source. We set the minimum number of rays passing through a cell (RadiativeTransferRaysPerCell) to 5.1.

We divide the spectral energy distribution of the source into four energy bins of $(E_{\text{LW}}, E_{\text{H}}, E_{\text{He}}, E_{\text{He}^+}) = (12.8, 28.0, 30.0, 58.0) \text{ eV}$, corresponding to the dissociating, H, He and He$^+$ ionizing photons, respectively. In each energy bin, we do not consider frequency dependence of the cross-section and photon flux. Instead, we use the averaged values over each energy band to save numerical costs. The validity of this assumption is discussed in Section 4.4.1. Also, the energies are fixed regardless of the stellar mass for simplicity. We use the fits from Schaerer (2002) to calculate the emission rates of dissociating and H, He, and He$^+$ ionizing photons, $Q(\text{LW}), Q(\text{H}), Q(\text{He})$ and $Q(\text{He}^+)$, respectively, as a function of stellar mass.

For ionizing photons, we solve the radiative transfer equation for all runs. We calculate the optical depth along a ray segment passing through a cell with a size $dr$ as

$$d\tau = \sigma_i n_i dr,$$

where $\sigma_i$ and $n_i$ is the absorption cross-section (taken from Verner et al. 1996) and number density of a species $i = \{\text{H}, \text{He}, \text{He}^+\}$, respectively. The photon flux is reduced by

$$dP_{\text{ion},i} = P_{\text{ion},i}(1 - e^{-d\tau})$$

across the ray segment. Then we calculate the photoionization rate as

$$k_{\text{ion},i} = \frac{dP_{\text{ion},i}}{n_i V_{\text{cell}} dr},$$

during a photon integration timestep $dr$, where $V_{\text{cell}}$ is a cell volume, from a single ray. The total photoionization rate is the sum of all the rays passing through the cell. To calculate the photodissociation rate, we test the following three methods.

#### TestA Direct integration of $H_2$ number density

In this test, we compute the H$_2$ dissociation rate $k_{\text{diss}}$ using the number of LW photons $P_{\text{LW}}$ entering a computational cell as

$$k_{\text{diss}} = \sum_{\text{rays}} \frac{P_{\text{LW}} n_{\text{H}_2} \Omega_i r^2 dr}{A_{\text{cell}} V_{\text{cell}} dr},$$

where $A_{\text{cell}}$ is the face area of the computational cell, $r$ is a
distance between the source and the cell, $\Omega_{\text{sc}}$ is the solid angle of a HEALPix cell. We use a reaction cross-section $\sigma_{\text{H}_2} = 3.71 \times 10^{-15} \text{ cm}^2$ of H$_2$ (Abel et al. 1997). In the cell, photons are attenuated as

$$dP_{\text{LW}} = P_{\text{LW}} \left[ f_{\text{sh}}(N_{\text{H}_2} + dN_{\text{H}_2}) - f_{\text{th}}(N_{\text{H}_2}) \right],$$

where $f_{\text{sh}}(N_{\text{H}_2})$ is a shielding function. We use the fitting function

$$f_{\text{sh}}(N_{\text{H}_2}) = \frac{0.965}{(1 + x/v_{\text{th},5})^2} + \frac{0.035}{(1 + x)^{0.5}} \times \exp\left[ -8.5 \times 10^4 (1 + x)^{0.5} \right]$$

(Wolcott-Green et al. 2011), by setting the parameter $\text{RadiativeTransferH2ShieldType} = 1$, where $x = N_{\text{H}_2}/5 \times 10^{14} \text{ cm}^{-2}$ and $v_{\text{th},5} = v_{\text{th}}/10^5 \text{ cm s}^{-1}$. The column density is directly integrated as

$$N_{\text{H}_2} = \int n(\text{H}_2) ds$$

along a HEALPix ray $s$.

**TestB Local approximation with the density gradient**

In local approximations, the dissociation rate is estimated as

$$k_{\text{diss}} = f_{\text{sh}}(N_{\text{H}_2}) \frac{Q(\text{LW}) \sigma_{\text{H}_2}}{4\pi r^2}$$

using the functional form $f_{\text{sh}}(N_{\text{H}_2})$ given in Eq. (8). We compute the column density as

$$N_{\text{H}_2} = n(\text{H}_2) l_{\text{sh}}$$

with a length scale $l_{\text{sh}}$ (shielding length) defined with physical quantities of each fluid element. In **TestB**, we estimate $l_{\text{sh}}$ as the density gradient

$$l_{\text{sh},D} = \frac{\rho}{|\nabla \rho|},$$

where $\rho$ is the density of a cell.

**TestC Local approximation with the Jeans length**

In this test, we use the same local approximation as **TestB** (Eq. 11), but the shielding length is calculated from the local Jeans length

$$l_{\text{sh},J} \equiv \lambda_J = \left( \frac{\pi c_s^2}{G \rho} \right)^{1/2},$$

where $c_s$ is the sound speed of a fluid.

### 2.4 Star formation density threshold

The threshold density $n_{\text{H}_2,\text{th}}$ can affect the efficiency of Pop III star formation. For **M10**, we compare two cases with $n_{\text{H}_2,\text{th}} = 10^6$ and $10^8 \text{ cm}^{-3}$, hereafter called **n6** and **n8**, respectively. The former value is often used in small-volume cosmological simulations of the first galaxies (Skinner & Wise 2020; Schauer et al. 2021) and lower values in larger-volume simulations (Wise et al. 2012; Xu et al. 2016; Jeon, Besla, & Bromm 2021). For **M40**, we test only the case with $n_{\text{H}_2,\text{th}} = 10^8 \text{ cm}^{-3}$. In this paper, we mainly show the result for **M10n6** as a fiducial case. We run simulations of **TestA**, **B** and **C** for each $n_{\text{H}_2,\text{th}}$, and Table 1 summarizes the initial parameters in the runs.

We terminate our simulations 0.1 Myr after the formation of the primary star, that is shorter than the lifetime (~ 10 Myr) of a star with a mass ~ 10 M$_\odot$. We confirm that the number of Pop III stars is unchanged by running the simulation for **TestB** until the lifetime of the primary star. We output snapshots at every 5000 yr to analyze the star formation history. Hereafter, we measure the time $t_{\text{sf}}$ from the primary star formation.

### 3 RESULTS

#### 3.1 Number of forming Pop III stars

In this section, we present the results for **M10n6**. At a redshift of $z = 25.1$ in a MH with a virial mass of $3.39 \times 10^8 \text{ M}_\odot$ and virial radius of 86.8 pc, H$_2$ molecules form through the reactions

$$\text{H} + e^- \rightarrow \text{H}^- + \gamma \quad (\text{Reaction 7}),$$

$$\text{H}^- + \text{H} \rightarrow \text{H}_2 + e^- \quad (\text{Reaction 8}),$$

catalyzed by free electrons (H$^-$-process; Peebles 1980). The gas temperature decreases below ~ 1000 K through radiative cooling of H$_2$. A cloud collapses in a runaway manner. When the density reaches $10^9 \text{ cm}^{-3}$, we insert the primary Pop III star. With our random seed, the mass of the primary star is assigned to 10.4 M$_\odot$. Its lifetime is $t_{\text{sf}} = 16.9$ Myr, and the photon emission rates are $(Q(\text{LW}), Q(\text{H}), Q(\text{He}), Q(\text{He}^+)) = (5.42 \times 10^{57}, 1.78 \times 10^{57}, 2.84 \times 10^{43}, 7.96 \times 10^{57}) \text{ s}^{-1}$. An H II region forms around the star through the absorption of ionizing photons, and modifies the density structure in the ISM. Photons in the LW band dissociate H$_2$ molecules and affect the formation of any secondary star.

The subsequent star formation history varies for different local approximation methods. Table 2 summarizes the properties of Pop III stars forming during the first 0.1 Myr after the primary star forms. Only one Pop III star forms for **TestA** and **B**, while six stars form for **TestC**. In **TestC**, the secondary stars with (random) mass form $20-30 \text{ M}_\odot$ form at distances $D = 0.1-0.7 \text{ pc}$ from the primary star at the time $t_{\text{sf}} = 20-60$ kyr. Compared to **TestA**, the number of Pop III stars is consistent for **TestB** and overestimated for **TestC**.

In the following subsections, we describe the evolution of the H II region for **TestA** and **B** (Section 3.2) and interpret the secondary star formation in case **TestC** (Section 3.3). Then, we describe the result for **n8** in Section 3.4.

#### 3.2 Evolution of H II regions

Fig. 1 shows the slices of density, temperature and the number fraction $y(\text{H}_2)$ of H$_2$ to hydrogen nuclei at $t_{\text{sf}} = 17.1$ kyr, just before the secondary star formation for **TestC**. In this figure, we plot the results only for **TestC**. The distribution of density and temperature for **TestA** and **B** is almost the same as **TestC**, but $y(\text{H}_2)$ is smaller than for the two other tests by eight orders of magnitude in the dense shell outside the H II region.
Fig. 2 shows the density, temperature, \( e^- \) and \( \text{H}_2 \) fraction, column density and photodissociation rate along a ray from the source to the density maximum. The UV photons with energies \( E \geq 13.6 \text{eV} \) emitted by the primary star ionizes the adjacent gas. The temperature increases to \( \sim 5 \times 10^4 \text{K} \), comparable to the surface temperature of the star. Due to the strong thermal pressure (\( \sim 10^{-5} \text{dyn/cm}^2 \)), the density declines to \( \sim 400 \text{cm}^{-3} \) in the ionized region. Just outside the ionizing front (I-front), a dense shell (D-type front) forms. We define the D-type front as the region with densities above 0.1 times the maximum density (orange hatched region in Fig. 2). In the region between the I-front and D-type front, the gas is partly ionized with an electron fraction of \( y(e) \sim 10^{-3} \). The \( \text{H}_2 \) fraction increases through the \( \text{H}^- \) process (Reactions 7 and 8), and a so-called “\( \text{H}_2 \)-ring” appears (Fig. 1c). We define the \( \text{H}_2 \)-ring as the region with \( \text{H}_2 \) fractions above 0.1 times the maximum, \( y_{\text{max}}(\text{H}_2) \sim 10^{-7} \) (purple hatched region in Fig. 2). In Fig. 2, we plot the D-type front and \( \text{H}_2 \)-ring for Test\( \text{A}\), but their positions are almost the same for the other tests.

At the time \( t_{\text{SF}} = 17.1 \text{ kyr} \), the radius of the D-type front reaches \( \sim 0.1\text{ pc} \) (Fig. 2). The gas flow is convergent, and the density increases up to \( \sim 10^6 \text{ cm}^{-3} \), comparable to \( n_{\text{H},\text{in}} \). Therefore, the D-type front naturally satisfies the criteria (i) and (ii) for star formation. If \( \text{H}_2 \) fraction is larger than \( y_{\text{th}}(\text{H}_2)\), the criteria (iii) and (iv) will be also satisfied. For Test\( \text{A}\) and \( \text{B} \), due to ineffective shielding, a sufficient fraction of dissociating photons can penetrate into the D-type front, and the formation of secondary stars is prevented. We discuss the result in a quantitative manner in subsequent sections.

(a) Test\( \text{A}\)

For Test\( \text{A}\), the density reaches the maximum value of \( n_{\text{H},\text{max}} = 6.88 \times 10^6 \text{ cm}^{-3} \) in the D-type front at a distance \( 0.170 \text{ pc} \) at the time \( t_{\text{SF}} = 17.1 \text{ kyr} \). Since \( n_{\text{H},\text{max}} \) is comparable to \( n_{\text{H},\text{in}} \), the criteria (i) and (ii) will be satisfied if the convergence continues. Just inside the D-type front, the \( \text{H}_2 \)-ring forms at a distance \( 0.0960 \text{ pc} \), where the fraction of \( \text{H}_2 \) reaches only up to \( y(\text{H}_2) = 2.95 \times 10^{-7} \). The column density increases rapidly in the \( \text{H}_2 \) ring, and it reaches a plateau of \( N_{\text{H}_2} \sim 7 \times 10^{14} \text{ cm}^{-2} \) (red curves in Fig. 2). At the density maximum, the column density is \( N_{\text{H}_2} = 6.98 \times 10^{14} \text{ cm}^{-2} \). With the temperature 856 K, the shielding fraction is \( f_{\text{sh}} = 0.704 \) (Eq. 8), that is, dissociation photons are only marginally shielded in the \( \text{H}_2 \)-ring. Since \( \text{H}_2 \) molecules cannot avoid dissociation, the \( \text{H}_2 \) fraction declines down to \( y(\text{H}_2) \sim 10^{-10} \). The star-formation criteria (iii) and (iv) are not satisfied, and thus secondary stars do not form.

(b) Test\( \text{B} \)

For Test\( \text{B}\), only one Pop III star forms during the simulation, which is the same result as Test\( \text{A}\). However, this does not necessarily mean that the Sobolev-like approximation can reproduce the result of direct integration. The D-type front is a potential star forming site, because its density (\( 6.74 \times 10^6 \text{ cm}^{-3} \)) is comparable to \( n_{\text{H},\text{in}} \) at \( t_{\text{SF}} = 17.1 \text{ kyr} \). The shielding length \( l_{\text{sh,D}} = 0.111 \text{ pc} \) at the density maximum characterizes the length scale of the D-type front (0.139 pc). The column density is estimated as the product of \( \text{H}_2 \) fraction at the density maximum and the thickness of the D-type front. As we have discussed in the previous section, the \( \text{H}_2 \)-ring mostly contributes to the column density at the density maximum for Test\( \text{A}\). This indicates that the local approximation fails to capture the contribution of the spatially separated region. The column density is indeed underestimated to be \( N_{\text{H}_2} = 2.95 \times 10^{13} \text{ cm}^{-2} \), compared to the value \( 6.98 \times 10^{14} \text{ cm}^{-2} \) for Test\( \text{A}\) by a factor of 20, because the \( \text{H}_2 \) fraction is smaller in the D-type front than in the \( \text{H}_2 \)-ring. Nevertheless, since the shielding factor \( f_{\text{sh}}(N_{\text{H}_2}) \) is insensitive to \( N_{\text{H}_2} \) at \( N_{\text{H}_2} \lesssim 5 \times 10^{14} \text{ cm}^{-2} \), \( f_{\text{sh}} = 0.982 \) is comparable to the value for Test\( \text{A}\). Consequently, secondary stars do not form as for Test\( \text{A}\).
3.3 Secondary star formation for TestC

For TestC, the shielding factor is overestimated, compared to TestA, that consequently overproduces Pop III stars. At $t_{\text{SF}} = 17.1$ kyr, just before the formation of the first secondary star, the dissociation rate $k_{\text{diss}} = 8.48 \times 10^{-12}$ s$^{-1}$ is much smaller than for TestA and B at the density maximum. A large fraction ($9.67 \times 10^{-4}$) of H$_2$ survives, and $y(H^-)$ exceeds the threshold value $10^{-3}$ at $t_{\text{SF}} = 20.6$ kyr. Feedback from the secondary stars further induces repetitive star formation. By $t_{\text{SF}} = 0.1$ Myr, six Pop III stars form.

This behavior occurs because the Jeans length approach overestimates the H$_2$ column density. For a fair comparison, we calculate $N_{\text{H}_2}$ with the three different methods from a snapshot for TestC at the time $t_{\text{SF}} = 17.1$ kyr (Fig. 3). The blue and green curves show the result for the direct integration and the density gradient approach, respectively. The Jeans length approach overestimates $N_{\text{H}_2} = 9.45 \times 10^{20}$ cm$^{-2}$ at the density maximum, compared to $4.87 \times 10^{19}$ and $9.19 \times 10^{19}$ cm$^{-2}$ for direct integration and density gradient approach by a factor of two and ten, respectively. Since the Jeans length originally characterizes the length scale of a quasi-static collapsing cloud, it is larger than the length scale of the D-type front contracting with the thermal pressure of the H II region. The shielding factor $f_{\text{sh}} = 8.36 \times 10^{-6}$ is smaller than the direct integration method, because $f_{\text{sh}}(N_{\text{H}_2})$ is a decreasing function of $N_{\text{H}_2}$ for $N_{\text{H}_2} \gtrsim 5 \times 10^{14}$ cm$^{-3}$ (Eq. 8). Dissociating photons cannot penetrate into the D-type front due to the high efficiency of self-shielding, and thus the H$_2$ fraction exceeds the critical value. After this point, secondary stars form in the D-type front.
$M_{\text{PopIII},1} = 10.4M_\odot$

$\n_{\text{H},\text{th}} = 10^6 \text{ cm}^{-3}$

$t_{\text{SF}} = 17.062 \text{ kyr}$

![Graph](image)

**Figure 3.** $\text{H}_2$ column density calculated with different schemes as a function of distance from the primary Pop III star on a ray from the source to the density maximum at the time 17.1 kyr after the primary star formation. From the snapshot of TestC, we calculate the column density by integrating $\text{H}_2$ density along the ray (red curve) and using density gradient $|\rho/\nabla \rho|$ (green curve). The blue curve is the same as the one in Fig. 2e. The purple and orange hatched regions represent the $\text{H}_2$-ring and D-type front, respectively, the same as Fig. 2.

### 3.4 Effect of the threshold density for star formation

In this section, we describe the results for a higher threshold density $n_{\text{H},\text{th}} = 10^6 \text{ cm}^{-3}$ (n8). The primary star forms at a redshift 25.0, 0.3 Myr later than n6. The stellar UV photons create an H II region, and a D-type front forms just outside a $\text{H}_2$-ring like the n6 case. As Table 2 summarizes, only one Pop III star forms in TestA and B, while three stars form in TestC when we terminate the simulations at the time $t_{\text{SF}} = 0.1$ Myr. For TestC, the number of Pop III stars becomes smaller than case n6 and approaches the value for TestA. However, the result still does not converge even for the high $n_{\text{H},\text{th}} = 10^6 \text{ cm}^{-3}$.

Fig. 4 shows density, temperature, $e^-$ and $\text{H}_2$ fraction, $\text{H}_2$ column density and dissociation rate along a ray from the primary star to the density maximum at $t_{\text{SF}} = 36.7 \text{ kyr}$, just before the secondary star formation for TestC. For TestA, the column density increases only up to $1.33 \times 10^{15} \text{ cm}^{-3}$ in the $\text{H}_2$-ring at a distance $6.29 \times 10^{-3} \text{ pc}$. The $\text{H}_2$-ring is optically thin ($f_{\text{abs}} = 0.987$), and almost all LW photons enter the D-type front at a distance $0.0308 \text{ pc}$ (red vertical line in Fig. 4). The $\text{H}_2$ fraction is $7.22 \times 10^{-12}$, well below the threshold for star formation.

For TestB, the shielding length is $l_{\text{sh,D}} = 0.151 \text{ pc}$, and $N_{\text{H}_2} = 4.68 \times 10^{16} \text{ cm}^{-3}$ at the density maximum (green dotted line in Fig. 4). The corresponding shielding factor is small (0.0192), but $N_{\text{H}_2}$ just increases temporarily. Around the density maximum, we can see spikes in $N_{\text{H}_2}$ with a height of six orders of magnitude and a width of $\sim 3 \times 10^{-2} \text{ pc}$ (green curve in Fig. 4e). The sound crossing time of the spikes is $l_{\text{sc}} \sim 1 \text{ kyr}$ for the temperature 300 K, shorter than the dynamical time $\sim 10 \text{ kyr}$. This indicates that the spikes are dumped very quickly. The small-scale noise is generated by the sensitivity of the length $l_{\text{H}_2,D}$ to the turbulent motion (convergent flow) of the gas. In the D-type front, the column density is $\sim 10^{15} \text{ cm}^{-3}$ on average, which corresponds to $f_{\text{sh}} \sim 1$. Therefore, nearly all of the $\text{H}_2$ molecules are destroyed by LW photons, and further star formation does not occur in the D-type front.

For TestC, the shielding length is $l_{\text{sh},C} = 0.0392 \text{ pc}$, and the column density is $N_{\text{H}_2} = 1.74 \times 10^{16} \text{ cm}^{-3}$. As in Section 3.3, we compare column densities calculated with the three different methods, using a snapshot for TestC at the time $t_{\text{SF}} = 36.7 \text{ kyr}$ (Fig. 5). The column density is overestimated with respect to $4.12 \times 10^{15} \text{ cm}^{-3}$ for the direct integration by a factor of four. The shielding factor is $f_{\text{sh}} = 5.44 \times 10^{-8}$ and $k_{\text{LW}}$ in the D-type front is small ($2.70 \times 10^{-12} \text{ s}^{-1}$). As a result, the criterion for star formation is satisfied, and the secondary stars form in this test.

### 3.5 Effect of the primary stellar mass

For M40, the result is the same as M10: no additional stars form for TestA and TestB while 8 additional stars form in a D-type front for TestC (Table 2). Fig. 6 shows the radial profiles of the physical values just before the secondary star formation for TestC. For TestC, the $\text{H}_2$ fraction is $9.25 \times 10^{-3}$ at the density maximum, which is by six orders of magnitude larger than $4.29 \times 10^{-9}$ for TestA (Fig. 6d). This is because the column density is significantly overestimated to be $8.83 \times 10^{21} \text{ cm}^{-2}$, compared to the value $5.92 \times 10^{14} \text{ cm}^{-2}$ for TestA (Fig. 6e). Since the shielding factor is underestimated, the flux of dissociation photons is smaller for TestC (Fig. 6f).

For TestB, the result is the same as M10, but the shielding factor is moderately underestimated at the density maximum, opposite to M10. For M40, the $\text{H}_2$-ring (purple hatched regions in Fig. 6) overlaps with the D-type front (orange hatched regions), because the structures are radially contracted more due to the stronger thermal pressure in the H II region than for TestA. At the density maximum, the $\text{H}_2$ abundance also reaches the maximum value $8.84 \times 10^{-5}$ (Fig. 6d). Then, $N_{\text{H}_2}$ is overestimated (Fig. 6e), resulting in smaller $k_{\text{LW}}$ (Fig. 6f). The $\text{H}_2$ fraction is still smaller than the threshold for star formation, and thus secondary star formation does not occur for TestB.

### 4 Discussion

#### 4.1 Computational time

We carry out the simulations with 448 cores on the Frontier supercomputer system at Texas Advanced Computing Center. Table 3 shows the computational time $t_{\text{comp}}$ for the different approximate methods and threshold densities $n_{\text{H},\text{th}}$ for M10. The computational time is generally longer for n8 than for n6 by a factor of $\sim 10$. Because the gas density increases up to $10^6 \text{ cm}^{-3}$ in n8, it takes additional computation to solve hydrodynamics, chemistry and radiative transfer in the region with densities $\sim 10^6 < n_{\text{H}_2} < 10^8$.

For n6, $t_{\text{comp}}$ is shorter at 6.35 hours for TestB than the 15.5 hours taken for TestA by a factor of 2.5. The local approximation can reduce the numerical cost, compared to solving the radiative transfer equation of LW photons. We
estimate the fraction $f_{\text{RT}}$ of computational time for radiative transfer calculation that includes the ionizing photons and, for $\text{TestA}$, the LW photons (fourth column of Table 3). For $\text{TestB}$, $f_{\text{RT}} = 46.1\%$, smaller than 86.9\% for $\text{TestA}$. For $\text{TestC}$, $t_{\text{comp}}$ is similar to $\text{TestA}$.

In Mpc-scale cosmological simulations, hundreds of Pop III stars form by a redshift $\sim 10$ (Skinner & Wise 2020; Jeon, Besla, & Bromm 2021; Schauer et al. 2021). It is costly to solve the radiative transfer equation of LW photons for all the stars, because LW photons reach longer distance than ionizing photons by two orders of magnitude (see Fig. 2). The density gradient approach can reduce the computational time by a factor of 2.5, reproducing the star formation history although it fails to include the contribution of the H$_2$-ring to the column density and thus underestimates the column density.

4.2 Feedback effects

We have studied that the approximation methods of LW radiative transfer and their effects on the multiplicity of Pop III stars in a MH. This may significantly affect the efficiency of radiative and SN feedback. In this section, we discuss the impact from the different numerical setups in a quantitative manner.

4.2.1 Ionization feedback

The emission rates of UV photons is roughly proportional to the number of massive Pop III stars. In Fig. 7a, we compare the radial profiles of the H$^+$ and He$^+$ abundances at the time $t_{\text{SF}} = 0.1$ Myr for the three approximation methods for n6. We define the radius of the I-front as the distance where $y(\text{H}^+) = 0.01$, which is comparable to the radius of the I-front for He. The I-front reaches 31.3 comoving pc for $\text{TestC}$, which is larger than $\sim 5$ pc for the other runs, because multiple radiation sources form.
In this work, we terminate the simulations at $t_{SF} = 0.1$ Myr, but we can predict whether the H ii region will eventually expand beyond the virial radius. Chiaki et al. (2018) estimated the critical halo mass, below which the radiation energy exceeds the binding energy of a MH, to be

$$M_{\text{halo,cr}} = 5.64 \times 10^6 M_\odot \left( \frac{v_D}{10 \text{ km s}^{-1}} \right)^{3/4} \left( \frac{t_{\text{life}}}{10 \text{ Myr}} \right)^{3/4} \times \left( \frac{Q(\text{H})}{5 \times 10^{49} \text{ s}^{-1}} \right)^{3/4} \left( \frac{1 + z}{26} \right)^{-3/2},$$

where $v_D$ is the expansion velocity of a D-type front, and $t_{\text{life}}$ is the stellar lifetime. A Pop III star with a mass $10.4 M_\odot$ emits ionizing photons at a rate $5.42 \times 10^{57} \text{ s}^{-1}$ (Table 2). In models where a single star forms (TestA and B), the critical halo mass is $1.89 \times 10^6 M_\odot$. Since the mass of the host halo $3.39 \times 10^6 M_\odot$ exceeds the critical mass, we can predict that the H ii region does not expand beyond the virial radius. For TestC, the total emission rate is $3.88 \times 10^{49}$ and $6.53 \times 10^{49} \text{ s}^{-1}$ for n6 and n8, respectively. Since the halo mass is below the critical mass ($4.60 \times 10^6$ and $6.89 \times 10^6 M_\odot$, respectively), we can predict that ionizing photons can reach IGM. This indicates that the different models can affect the initial stage of cosmic reionization.

4.2.2 LW feedback

LW radiation can suppress star formation in neighboring clouds by dissociating H$_2$ (O'Shea & Norman 2008; Hirano et al. 2015) or sometimes trigger the formation of supermassive stars and black holes (Omukai 2001; Wise et al. 2019; Regan et al. 2020). We compare the LW intensity

$$J_{\text{LW}} = \frac{f_{\text{sh}} E_{\text{LW}} Q(\text{LW})}{4\pi \Delta v_{\text{LW}} D^2},$$

where $D$ is the distance from a star (cluster), and $\Delta v_{\text{LW}} = 5.80 \times 10^{23} \text{ Hz}$ is the width of the LW band. Hereafter we use

$$M_{\text{PopIII,1}} = 10.4 M_\odot \quad n_{\text{H,th}} = 10^8 \text{ cm}^{-3} \quad t_{\text{SF}} = 36.694 \text{ kyr}$$

the LW intensity $J_{\text{LW}}$ in units of $10^{-21} \text{ erg s}^{-1} \text{ cm}^{-2} \text{ Hz}^{-1} \text{ sr}^{-1}$.

Fig. 7b shows the LW intensity as a function of the distance from the primary star at the time $t_{\text{SF}} = 0.1$ Myr. At distances $D \lesssim 0.01$ pc (comoving), the intensity is largest for TestC because of multiple Pop III star formation. At $0.01 \lesssim D/\text{pc} \lesssim 1$, the intensity for TestC is smaller than in the optically thin case, where the intensity declines as $\propto D^{-2}$ due to geometrical dilution. This indicates that dense clumps absorb LW photons, and additional star formation may occur in the self-shielded regions for TestC. At $D > 1$ kpc, the intensity roughly follows a profile $\propto D^{-2}$ for all the tests, but the intensity is the largest for TestC. LW radiation can quench star formation in low-mass MHs with intensities $J_{\text{LW}} \gtrsim 0.1$ (O'Shea & Norman 2008). J$_{\text{LW}}$ exceeds this value in larger region of 3.84 kpc in TestC. Star formation may be delayed for $\sim$ Myr in neighboring MHs due to strong LW emission from the star cluster.

At $D \sim 10$ kpc, the intensity rapidly declines for TestA, because the gas is optically thick in the LW band. For TestB, the gas remains optically thin, and the profile follows $\propto D^{-2}$. The local approximation with density gradient can safely estimate the column density in the D-front, but it fails to estimate the column density at larger distances $D \gtrsim 30$ kpc. Fortunately, at these distances, J$_{\text{LW}}$ is not so strong ($\sim 10^{-2}$), and thus star formation may not be significantly affected by this overestimate of J$_{\text{LW}}$.

4.2.3 SN feedback

Massive Pop III stars will undergo SN explosions at the end of their lives and release the first metals into ISM and IGM. Chiaki et al. (2018) found that there are two modes of metal enrichment: internal enrichment (IE) and external enrichment (EE). The latter occurs if the emission rate of ionizing photons is sufficiently large before SN explosions occur. If an H ii region expands beyond the virial radius of a host halo, SN shocks can propagate through the rarefied region without energy loss by radiative cooling. Therefore, EE occurs for a halo with masses below the critical value of Eq. (14).

For TestA and B, we can predict that, since the H ii region will be bound in the MH, IE will occur. The ejected metal mass is $M_{\text{ej,1}} \sim 1 M_\odot$ for a progenitor mass $M_{\text{PopIII}} \sim 10 M_\odot$ (Nomoto, Kobayashi, & Tominaga 2013). If the metal...
als are uniformly mixed with the pristine gas with a mass $M_{\text{gas}} = 5 \times 10^4 \, M_{\odot}$ in the MH, the metallicity is estimated to be

$$Z_{\text{IE}} = \frac{M_{\text{met}}}{M_{\text{gas}}} = 10^{-3} \, Z_{\odot} \left( \frac{M_{\text{met}}}{1 \, M_{\odot}} \right) \left( \frac{M_{\text{gas}}}{5 \times 10^4 \, M_{\odot}} \right)^{-1}$$

as confirmed by earlier numerical studies (Ritter et al. 2012, 2015; Sluder et al. 2016; Chiaki & Wise 2019). For TestC, since the halo mass is below the critical mass, the cloud will be disrupted by multiple SN explosions. SN ejecta will reach neighboring halos. However, only a small fraction of ejecta can reach the center of the halos because of the pressure gradient force of gas clumps. Therefore, EE is expected to be less effective than IE. The resulting metallicity will be $Z_{\text{EE}} \lesssim 10^{-5} \, Z_{\odot}$ in the neighboring halos (Smith et al. 2015; Chen et al. 2017; Chiaki et al. 2018).

**4.3 Applicability to other astrophysical problems**

We have found that the Sobolev approach is the most accurate approximation in the triggered star formation scenario. There are other astrophysical problems which can be affected by the different approximation methods of LW transfer. In this section, we discuss that our finding can be applied to other problems.

When the first Pop III stars form, H$_2$ line cooling plays a crucial role in the fragmentation of primordial collapsing clouds (Bromm et al. 1999; Abel et al. 2002; Yoshida et al. 2003). Greif (2014) studied the escape fraction of photons in the transition lines, comparing a full ray tracing model and the Sobolev approximation. They ran high-resolution simulations which can resolve small-scale turbulence. They found that the escape fraction is overestimated with the Sobolev approximation, because the length scale $l_{h,v}$ of velocity fluctuations is too small compared to the bulk inflow velocity.

Direct collapse is one of the possible pathways to SMBH formation (Inayoshi et al. 2020, for a review). If a primor-
cooling (e.g., H2015). The mass loss rate can be suppressed by molecular fragmentation. LW transfer is crucial to determine the fate changes at length scales comparable to or less than the Sobolev length of $10^{-13}$ cm. In their atmospheres, the velocity gradient changes at length scales comparable to or less than the Sobolev length of $\sim 1$–10 times planet radius (Yoshida et al. 2022). Therefore, the Sobolev approximation cannot be applied to this problem.

4.4 Caveats

4.4.1 Multifrequency effects

In our direct integration model, we have not considered the frequency dependence of the photodissociation cross-section. The cross-section has spikes at frequencies corresponding to resonance lines (e.g., Heays et al. 2017), and Doppler shifts of the lines can cause photon escape in a fluid moving relative to a source (Wolcott-Green & Haiman 2011). In the context of Pop III star formation, Greif (2014) evaluated this effect with their multifrequency radiation transport model. They found that the escape probability of H$_2$ lines are underestimated by a factor of two if the Doppler shift is not considered. We can expect that the effect can be important also in the case of triggered star formation. In our simulations, the radial velocity of the H II shell ($\sim 20$ km s$^{-1}$) is larger than the thermal velocity

$$v_{sh} = \left(\frac{kT}{2n_H}\right)^{1/2} = 5 \text{ km s}^{-1} \left(\frac{T}{5000 \text{ K}}\right)^{1/2}.$$  

Thus, a larger fraction of dissociation photons can escape if we had considered the multifrequency effect, possibly leading to secondary star formation being suppressed further.

4.4.2 Updated shielding function

We have used the shielding function $f_{sh}(N_{H_2})$ presented by Wolcott-Green et al. (2011). Wolcott-Green & Haiman (2019) lately updated the shielding function, including the effect of non-local thermal equilibrium (LTE) populations of H$_2$ molecules. In the D-type front, the density, temperature and LW intensity are typically $n_H \sim 10^5$ cm$^{-3}$, $T \sim 5000$ K and $J_{21} \sim 10^3$, respectively, where the non-LTE effect is not negligible. In this regime, we have underestimated the shielding factor. If we use the updated shielding function, $f_{sh}(N_{H_2})$ will be larger, and there will be more chance to suppress secondary star formation. This strengthens our conclusion in the more accurate methods: direct integration and the Sobolev approximation. In any case, we will include the non-LTE effect for more physically-motivated formulation of the shielding function.

4.4.3 HD photodissociation

In this work, we do not consider photodissociation of HD molecules, another important coolant in collapsing gas clouds (Johnson & Bromm 2006; Hirano et al. 2014). HD molecules absorb photons in the LW band but in lines at different frequencies from H$_2$. The gas is generally optically thin in the absorption lines, because the HD abundance is smaller than H$_2$ by five orders of magnitude (Omukai 2012). In our implementation, we assume that each photon package is monochromatic, and we use the shielding function (Eq. 8) averaged over all frequencies in the LW band (Wolcott-Green et al. 2011). HD molecules could receive only a fraction of photons that were not absorbed by H$_2$. To overcome this problem, it is ideal to separate the photon package into...
three energy bins that interact with H$_2$, HD and both. We will improve our model in forthcoming papers.

5 CONCLUSION

Massive stars emit tremendous amounts of ionizing photons, creating an H II region. At the limb of the H II region, a dense shell forms due to internal thermal pressure. This D-type front is a potential star-forming site (triggered star formation; Elmegreen & Lada 1977; Whitworth et al. 1994; Hosokawa & Inutsuka 2005, 2006). In this work, we find that star formation in the D-type front depends on the numerical scheme to solve LW radiation transport. The LW flux depends on the estimate of the H$_2$ column density $N_{H_2}$. We test three cases: the direct integration of H$_2$ density (TestA), local approximation based on the density gradient (TestB) and the Jeans length (TestC).

We compare the number of secondary stars forming in the D-type front. No secondary stars form in TestA while five stars form in TestC. In TestA, dissociating photons are only partially (~0.3) absorbed in a thin H$_2$-ring, and the secondary star formation is suppressed. In Test B, the result is consistent with TestA, but we caution that the local approximation underestimates or overestimates the column density when the primary Pop III stellar mass is 10 and 40 M$_\odot$, respectively. In TestC, the number of forming stars is overestimated because the Jeans length is generally larger than the thickness of the H$_2$-ring.

It is numerically expensive to solve radiation transport of LW photons in numerical simulations because the gas is typically optically thin in the LW band, and photons can reach a large distance (~10 comoving kpc). In large-volume cosmological simulations with a side of ~comoving Mpc, the local approximation is useful to reduce computational costs. We find that the computational time is reduced for the local approximation with the density gradient (TestB) by a factor of 2–3, compared to direct integration of $N_{H_2}$ (TestA). Although the local approximation has limitations, the density gradient approach is balanced strategy to reproduce the star formation history in the early stage of structure formation while keeping computational costs low.

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DATA AVAILABILITY

The versions of ENZO, GRACKE, and VT used in this work are available at https://github.com/genchiaki/enzo-dev/tree/metal-dust. The simulation data will be shared on reasonable request to the authors.

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