Connecting Primordial Star-forming Regions and Second-generation Star Formation in the Phoenix Simulations

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Abstract
We introduce the Phoenix Simulations, a suite of highly resolved cosmological simulations featuring hydrodynamics, primordial gas chemistry, primordial and enriched star formation and feedback, UV radiative transfer, and saved outputs with $\Delta t = 200$ kyr. We observe 73,523 individual primordial stars within 3313 distinct regions forming 2110 second-generation enriched star clusters by $z \geq 12$ within a combined 177.25 Mpc$^3$ volume across three simulations. The regions that lead to enriched star formation can contain $\gtrsim 150$ primordial stars, with 80% of regions having experienced combinations of primordial Type II, hypernovae, and/or pair-instability supernovae. Primordial supernovae enriched 0.8% of the volume, with 2% of enriched gas enriched by later-generation stars. We determine the extent of a primordial stellar region by its metal-rich or ionized hydrogen surrounding cloud; the metal-rich and ionized regions have time-dependent average radii $r \lesssim 3$ kpc. 7 and 17% of regions have $r > 7$ kpc for metal-rich and ionized radii, respectively. We find that the metallicity distribution function of second-generation stars overlaps that of subsequent Population II star formation, spanning metal-deficient ($\sim 7.94 \times 10^{-8} Z_{\odot}$) to supersolar ($\sim 3.71 Z_{\odot}$), and that 30.5% of second-generation stars have $Z > 10^{-2} Z_{\odot}$. We find that the metallicity of second-generation stars depends on progenitor configuration, with metals from pair-instability supernovae contributing to the most metal-rich clusters; these clusters form promptly after the supernova event. Finally, we create an interpretable regression model to predict the radius of the metal-rich influence of Population III star systems within the first 7–18 Myr after the first Population III stars form in the region.

Unified Astronomy Thesaurus concepts: Population III stars (1285); Population II stars (1284); Primordial galaxies (1293); Star forming regions (1565)

1. Introduction
The first galaxies form from gas that has been enriched by an earlier generation of Population III supernovae (SNe). The initial conditions of metallicity in the universe after these first SN events remain a difficult problem to model in astrophysical simulations. Researchers conducting astrophysical simulations have three practical options to determine the initial metallicity field prior to enriched (Population II) star formation: assume a metallicity floor (e.g., Hopkins et al. 2018), assume initial star formation rates (SFRs) that are independent of metallicity (e.g., Vogelsberger et al. 2013, 2014), or explicitly simulate the primordial (Population III) star formation and feedback (Wise et al. 2012a, 2012b; Smith et al. 2015; Xu et al. 2016). Ideally, all researchers would choose the last option; however, the extremely small scale ($\sim$pc$^3$) of primordial molecular cloud formation (Abel et al. 2000; Bromm et al. 2002) is at odds with the $\sim$Gpc$^3$ scale necessary to gain useful statistics of the observable universe; any simulation using current computing facilities that can fully resolve Population III star formation is severely limited in volume, with the largest being only $\sim$300 Mpc$^3$ (Xu et al. 2016).

The Phoenix (PHX) suite of simulations is designed to facilitate the exploration of a fourth option to model Population III star formation and feedback: to develop surrogate models based on deep neural networks (DNNs) as a new subgrid method to create a heterogeneous metallicity initial condition that reflects the spatially irregular formation of Population III star formation and feedback. Data from the PHX suite have already been used to train StarFind, a predictive DNN-based surrogate model that identifies Population III star formation sites without resorting to halo finding or parsec-scale resolution (Wells & Norman 2021). Training is enabled by the PHX unique time between outputs, such that any star formation or feedback event is recorded to disk with 200 kyr time resolution.

Although their extreme time resolution was intended to provide a high resolution of star formation and feedback events for training DNNs, the PHX suite also provides a unique opportunity to study the transition between Population III and second-generation (Population II.1$^3$) star formation. Studying low-metallicity stars or damped Ly$\alpha$ systems in observations is currently our only window into the Population III initial mass function (IMF; Cooke et al. 2017; Welsh et al. 2019, 2020), but the uncertainty in the IMF (Nakamura & Umemura 2002; Ishigaki et al. 2018) and metallicity of Population II.1 stars that could form from enriching events makes inferences about the Population III era difficult. Due to the fine time resolution in the PHX suite outputs, we use them to study the formation state of small Population II star clusters, as well as the evolution of

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3 Population II.1 is our designation for the first generation of metal-enriched star formation that occurs in gas enriched exclusively by Population III SNe. Population II stars formed from gas also enriched by earlier Population II stars are referred to as Population II.2.
Population III star-forming regions. This will guide future studies that connect Population III and Population II stars by providing a reference of how many Population III stars can be related to a Population II cluster, as well as the range of metallicities that may be observable in a second-generation star cluster.

The remainder of this paper is organized as follows. Section 2 presents a summary of the simulations and included physical models; Section 3 showcases summary statistics, such as structure formation and galaxy assembly. Projections of the simulations consolidate our results and presents an interpretable regression model that predicts the physical models; Section 3 showcases summary statistics, such as structure formation and galaxy assembly. Projections of the simulations consolidate our results and presents an interpretable regression model that predicts the region of influence for a Population III system, given the stellar masses and birth times within that system. Finally, Section 6 consolidates our results and presents final notes on both this study and future directions.

2. The PHX Simulations

The PHX suite consists of three simulations performed with the ENZO (Bryan et al. 2014; Brummel-Smith et al. 2019) adaptive mesh refinement (AMR) hydrodynamic cosmology code designed to study the time and spatial evolution of early structure formation and galaxy assembly. Projections of the largest (512$^3$ root-grid) simulation are shown in Figure 1. In addition to the simulation shown in Figure 1, two other smaller simulations were also performed, as noted in Table 1. The 512$^3$ simulation (PHX512) has volume (5.21 Mpc)$^3$, and the PHX suite includes two smaller 256$^3$ root-grid simulations with volume (2.61 Mpc)$^3$ each (PHX256-1, 2). Prior efforts have produced simulations with similar redshifts as the target range of the PHX suite (Wise et al. 2012a, 2012b; Xu et al. 2016), however, the saved outputs of these earlier works have a time resolution of $\Delta t \gtrsim 1$–5 Myr, whereas the PHX suite has 200 kyr between all saved outputs for redshifts $30 < z < z_{\text{final}}$.

All simulations share identical cosmological parameters with $\{\Omega_m = 0.3111, \quad \Omega_b = 0.048975, \quad \Omega_{\Lambda} = 0, \quad \Omega_{\gamma} = 0.6889, \quad H_0 = 0.6766, \quad \sigma_8 = 0.811, \quad n = 0.965\}$ (Ade et al. 2014). The cosmological initial conditions are generated at $z = 99$ using MUSIC (Hahn & Abel 2011), where each simulation uses a unique random seed to generate an initial state that is consistent with the given cosmological parameters. All simulations have identical mass and spatial resolution and the same refinement criteria as the Renaissance Simulations (Xu et al. 2013), with dark matter particle mass $M_{DM} = 2.34 \times 10^4 M_{\odot}$ and initial average baryon mass per cell $M_{b,i} = 1.17 \times 10^3 M_{\odot}$. The root grid can be refined up to nine levels of AMR, where refinement occurs on dark matter density, baryon density, and regions surrounding Population III star particles such that the SN radius (10 pc) is resolved by at least four cells or is at the maximum AMR level. Refinement on densities is super-Lagrangian; cells are flagged for refinement at level $l$, where the cell mass $M_l \geq M_{l-1} \times 2^{-0.4 l}$, where $M_l$ refers to $M_{DM}$ or $M_{b,i}$ for refinement on dark matter or baryon density, respectively. With these resolution parameters, and assuming $\sim 100$ dark matter particles for a resolved dark matter halo, the least massive resolved halos have virial masses $2.34 \times 10^6 M_{\odot}$, while the most massive halos ($\sim 10^9 M_{\odot}$) are limited by the total mass within the volume: $3.93 \times 10^{11}$ and $3.14 \times 10^{12} M_{\odot}$ for 256$^3$ and 512$^2$ root grids, respectively. The finest spatial resolution achieved on level 9 subgrids is 19.53 comoving pc, providing $<2$ proper pc resolution for $z \gtrsim 9$.

For hydrodynamic and chemical evolution, each simulation includes nine species of nonequilibrium chemistry for primordial gas species H, H$^+$, H, H$_2$, H$^+_2$, He, He$^+$, He$^+_2$, and e$^-$; radiative heating, cooling, and metal-line cooling as in Smith et al. (2008); and hydrodynamics evolved using the piecewise parabolic method (Colella & Woodward 1984). Radiation interactions are included via a uniform, redshift-dependent Lyman–Werner H$_2$ dissociating radiation background as documented in Xu et al. (2016), as well as photodissociating and ionizing radiation from point sources using the rates and MORAY ray-tracing solver method in Wise & Abel (2011). The radiation is coupled to chemistry through heating and ionization rates and to hydrodynamic evolution via momentum coupling from photons to the gas.

Each simulation includes two types of star formation events, individual Population III stars and Population II star clusters, each tracked with a star particle. Feedback (SNe, stellar winds) from each type of star particle contributes to a unique metal density field so that the contributions from Population III and Population II stars can be tracked independently. The star formation and feedback algorithms used in the PHX suite are well documented and described in several prior works (Wise & Cen 2009; Wise et al. 2012a, 2012b; Xu et al. 2013; Hicks et al. 2021), so the following is restricted to a high-level overview that includes the specific parameters used in the PHX suite. At each time step, every grid cell is evaluated for Population III star formation according to the following criteria: (1) baryon number density $n_b > 100$ cm$^{-3}$, (2) H$_2$ fraction $n_{H_2}/n_b > 10^{-4}$, (3) metallicity$^5 Z < Z_*$ for $Z_*= -5.5$, (4) the AMR grid level that is most refined for that point in space, (5) a cooling time that is less than the freefall time, and (6) converging gas flow ($\nabla \cdot \mathbf{v} < 0$). If a cell qualifies for Population III star formation, a particle representing a single star is formed centered on the host cell with mass taken from a modified Salpeter IMF,

$$f (\log M) dM = M^{1.3} \exp \left[ - \left( \frac{M_{\text{char}}}{M} \right)^{1.6} \right] dM, \quad (1)$$

with characteristic mass $M_{\text{char}} = 20 M_{\odot}$, with masses in the range $1 \leq M_\star/M_{\odot} \leq 300$. The final mass contributing to the star formation is taken from the grid in a sphere containing twice the mass of the star.

Population II star cluster formation involves similar criteria: (1) baryon overdensity relative to the simulation volume $\rho/\bar{\rho} > 100$, (2) $Z > Z_*$, (3) the AMR grid level that is most refined for that point in space, (4) a cooling time that is less than the freefall time, and (5) converging gas flow ($\nabla \cdot \mathbf{v} < 0$). At each time step after the initial particle formation, the mass of the cluster is accreted from the surrounding cold gas mass, $M_{\text{cold}}$, estimated as 7% of the gas mass in a sphere with a mean gas number density $n_b > 10^3$ cm$^{-3}$ until $M_{b,i} > 1000 M_{\odot}$, as described in Wise & Cen (2009). If after one dynamical time, the particle has not accreted 1000 $M_{\odot}$, a low-mass particle is formed with the current mass to prevent loss of the ionizing radiation due to lower-mass star clusters. The metallicity of the formed star is taken as the mass-averaged metallicity of the

$^4$ https://enzo.readthedocs.io/en/latest/

$^5$ With metal mass $M_\star$ and cell baryon mass $M_{\star,i}$, metallicity is given by $Z = \log (M_{\star,i}/M_{\odot}) - \log (M_{\star,i}/M_{\odot})$. 
cells that contributed to its formation; therefore, the final metallicity may be lower or higher than the cell that initially qualified for cluster formation.

Stellar feedback for Population III stars is included in two forms: SNe of varying mass and point-source radiative feedback. The SN channel includes Type II SNe ($11 < M_\text{SN}/M_\odot < 20$), hypernovae (HNe; $20 \leq M_\text{SN}/M_\odot < 40$), and pair-instability SNe (PISNe; $140 < M_\text{SN}/M_\odot < 260$). For SNe, the ejecta mass, energy, and metal yields are taken from Nomoto et al. (2006); HNe event energy and metal yields are linearly interpolated from these values. The PISNe have ejecta mass, metal yield, and energy taken from Heger & Woosley (2002). For each type of SN, the resulting mass, metal yield, and energy are deposited to the grid in a sphere of 10 pc, or a cube of $3^3$ cell widths if 10 pc is unresolved.

Population II stars, modeled as coeval clusters of stars, use a continuous injection model of energy, mass, and metal deposition that represents both SNe and stellar winds. At each time step during the 20 Myr lifetime of the cluster, mass is returned to the computational grid as

$$m_{\text{ej}} = \frac{0.25 \Delta t \times M_\text{SN}/M_\odot}{16 \text{ Myr}},$$

where $\Delta t$ is the grid time step. The ejecta has a metallicity fraction matching solar metallicity ($Z_\odot = 0.01295$). The ejecta has energy $1.12 \times 10^{59}$ erg $M_\odot^{-1}$, which is coupled to the grid as thermal energy along with mass and metal ejecta in a 10 pc sphere surrounding the source particle, again depositing to a $3^3$ cube if 10 pc is unresolved.

### 3. General Observations from the PHX Suite

Halo finding was performed using ROCKSTAR (Behroozi et al. 2013), requiring 50 dark matter particles per identified

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**Table 1**

| Designation | $D$ (Mpc) | $V$ (Mpc$^3$) | $z_{\text{final}}$ |
|-------------|-----------|---------------|-------------------|
| PHX512      | 512       | 141.8         | 14.04             |
| PHX256-1    | 256       | 17.7          | 12.45             |
| PHX256-2    | 256       | 17.7          | 13.27             |

**Note.** Each simulation includes the root-grid dimension ($D$), volume ($V$), and final redshift ($z_{\text{final}}$), which is completely determined by run time. All parameters aside from $D$ and $V$ between the three simulations are identical; see Section 2 for details.
halos that contain Population II stellar mass, in underresolved halos. $M_{\text{III SN}}$ remnants of any type. At the active Population III stars, and in halos with simulations. The fraction of halos with mass $M_{\text{vir}}>10^6 M_\odot$ hosts active Population III stars at various redshifts, including data from all simulations. Halos with $M_{\text{vir}} \sim 5 \times 10^5 M_\odot$ are the primary hosts of Population III stars, and the highest-mass halo with Population III stars is $M_{\text{vir}} = 3 \times 10^8 M_\odot$.

Figure 2. Halo counts at the final redshift of each simulation, with simulation and redshift annotated within each panel. Here $M_{\text{vir}}$ counts all halos, $M_\star$ counts halos that contain Population II stellar mass, $N_{\text{III}} > 0$ counts halos that contain active Population III stars, and $N_{\text{rem}} > 0$ counts halos that contain Population III SN remnants of any type. At the final redshift, halos with mass $M_{\text{vir}}>2 \times 10^7 M_\odot$ all contain remnants, while some halos above $M_{\text{vir}} = 2 \times 10^7 M_\odot$ still host active Population III stars. Population III stars found in halos with $M_{\text{vir}} < 2 \times 10^8$ indicate that Population III formation does occur in underresolved halos.

The fact that Population III stars still exist in halos forming Population II stars begs the question: is there a redshift dependence on the mass of the halo that will contain Population III stars? Figure 3 displays the fraction of halos hosting active Population III stars at various redshifts, including data from all simulations. The fraction of halos with mass $\sim 10^6-7 M_\odot$ hosting Population III stars is notably higher at higher redshift. Higher fractions of halos hosting Population III stars with $M_{\text{vir}}>5 \times 10^7 M_\odot$ are visible at lower redshift, e.g., $z \lesssim 17$. However, this observation is also likely due to the fact that higher-mass halos occur with more frequency at lower redshift. The fraction of halos hosting Population III stars is highest for halos with $3 \times 10^6 M_\odot \leq M_{\text{vir}} \lesssim 2 \times 10^7 M_\odot$; it is likely that halos with higher mass have generally been enriched by Population III stars earlier in their assembly history and no longer host high-density reservoirs of pristine gas to fuel primordial star formation. The visible outlier case is that of a high-mass, high-redshift halo with $M_{\text{vir}} \sim 2 \times 10^8 M_\odot$ at $z=18$ with active Population III stars. These result from a lower-mass ($M_{\text{vir}} = 7.8 \times 10^7 M_\odot$) halo with a low-mass Population III star merging into a larger halo; the Population III star did not form in the larger, $M_{\text{vir}} > 10^8 M_\odot$ halo. There are only two halos in this mass bracket at $z=18$, and the above scenario happened in one of them to result in the high fraction observed in the plot.

Figure 4 shows the fraction of volume with gas enriched above a varying redshift $Z$ looking back from $z=14.04$. Less than 0.1% of the volume has been enriched to $Z_e$ required for Population II star formation.
of the volume is fully ionized and not begun to any substantial degree. Population II sources at the final redshift, emphasizing the importance of Population III chemical enrichment at high redshifts.

The fraction of the volume that is ionized to varying degrees in PHX512 is shown in Figure 5. The ionized fraction is presented as \( f_{\text{ion}} = n_{\text{H}^+}/(n_{\text{H}^1} + n_{\text{H}^1}) \); less than 0.5% of the volume is ionized to \( f_{\text{ion}} > 0.5 \) at the final redshift, indicating that the point-source radiation feedback from ionizing sources has not yet escaped the dense clumps of halo or galactic gas. The highest levels of ionized gas, \( f_{\text{ion}} > 0.9 \), likely result from ionizing radiation from Population III stars at these redshifts, with subsequent drops in \( f_{\text{ion}} \) resulting from recombination after the Population III main-sequence phase. Lower-to-middling values, \( f_{\text{ion}} \leq 0.5 \), reflect the increasing volume affected by hydrodynamic shock heating from infalling gas and evolved Population III SN remnant gas, as seen in the halo zoom-in temperature panel of Figure 1.

Star formation statistics are presented in Figure 6. The SFR densities (SFRDs) before \( z \approx 22 \) are similar for Population II and Population III; however, the SFRD of Population II eclipses that of Population III stars by \( z = 22 \). This is also the point at which the total mass in Population II stars surpasses that of the cumulative formed Population III mass. The Population II SFRD is fit by \( SFR_{\text{fit}} = 0.65 \exp(-z/2.45) \, M_\odot \, \text{yr}^{-1} \, \text{Mpc}^{-3} \), shown on the figure. The \( z \lesssim 18 \) Population III SFRD approaches a relatively constant \( 10^{-3} \, M_\odot \, \text{yr}^{-1} \, \text{Mpc}^{-3} \), representing the contribution from both newly collapsing halos in pristine gas and pristine regions of partially enriched halos; since so little of the volume has been enriched, this will continue until more IGM gas has been enriched and the newly collapsed halos are enriched prior to their formation (Hicks et al. 2021).

The stellar mass-weighted metallicity distribution function (MDF) for Population II stars across all PHX simulations is presented in Figure 7. The MDF of all Population II stars shows a large range of possible metallicities, with the most metal-deficient cluster having \( Z = -7.1 \). Although the simulation parameter for Population II cluster creation requires \( Z > -5.5 \) at the cell hosting cluster formation, the mass-averaged metallicity of the gas that contributed to star formation allows these low-Z clusters to exist. The highest-Z cluster has \( Z = 0.57 \); the mean metallicity of all Population II stars is \( \langle Z \rangle = -1.89 \). The open blue line shows only Population II stars.
II.1 stars, with mean $(Z) = -2.46$. For an observational reference point, we include the distribution retrieved from the JINA database (Abohalima & Frebel 2018), shown in orange. The overlap between the JINA observations and Population II stars is reassuring; however, we also note that our Population II.1 stars can, in general, have metallicities above the JINA observations. This comparison implies that a great many Population II.1 stars may go unrecognized due to the a priori assumption that Population II.1 stars necessarily have low metallicity. Indeed, the MDF of Population II.1 and Population II.2 stars is completely overlapping, suggesting that while cases of stars with low metallicity may indicate very old Population II.1 stars, many more may have high, even supersolar, metallicity. Having these high-metallicity cases excluded from studies that attempt to reconstruct the Population III IMF will make it much more difficult to decipher the full range of Population III masses and their relative frequency.

4. Analysis: The First Stars and the Second Generation

To study the origin of Population II.1 star formation, we take two primary frames of reference: (1) we analyze Population III star-forming regions, studying the evolution of the region as it leads to Population II star formation, and (2) we examine the region about the Population II.1 cluster immediately after formation to study the events that immediately contributed to its formation. Each frame of reference uses separate analyses of the simulations.

4.1. Method: Population III Frame

Population III star formation within the PHX suite is clustered, which is not unexpected (e.g., Stacy et al. 2010). If we follow a single Population III star-forming region as defined in this section, we find that there can be $\lesssim 200$ individual Population III stars per region. Although clustered, there are not generally enough individual stars to qualify as a star cluster in the canonical sense; we will therefore refer to them as PIII associations to avoid ambiguity with modern or Population II star clusters but in analogy to modern O–B associations.

To examine the simulations from the perspective of Population III stars and define the extent of a PIII association, we iterate each output of the simulation to find new Population III star particles that formed within 200 kyr by iterating dark matter halos and searching for new particles within 3$R_{\text{vir}}$ of the center of the halo. When found, and if that star is only accompanied by coeval Population III star formation (i.e., other new Population III stars only formed within 200 kyr, with no SN remnants, black holes, or Population II stars within the radius), we form a sphere to measure mean metallicity from new Population III stars ($Z_{\text{III}}$) and the H$^+$ fraction ($f_{\text{H}^+}$) using the analysis software yt (Turk et al. 2011). Starting from a smaller radius than expected for either metal-rich bubbles or ionized regions, $R = 250$ pc, the average value for a field, $\bar{X}$, is measured. If $\bar{X}$ is not less than some critical value, $R$ is increased to $R_{\text{crit}} = 1.1R$, and a new average is taken. This procedure is repeated until the value of $\bar{X}$ is below our chosen critical values: $Z_{\text{III}} < -5.5$ and $f_{\text{H}^+} < 0.05$. The “edge” of the region is then defined by this final radius. The final product of this analysis is an effective radius as a function of time for the $Z_{\text{III}}$ and $f_{\text{H}^+}$ variables.

4.2. Method: Population II.1 Frame

From the perspective of Population II clusters, we again iterate through simulation outputs to identify Population II star formation events. When a new Population II star particle is formed, and it occurs in gas enriched by only Population III stars, i.e., the metallicity from Population II stars, $Z_2$, meets the criterion $Z_2 < -6$ in the cell hosting star cluster formation, we evaluate a sphere centered on that star with $r = 200$ comoving kpc. This initial radius assumption stems from the analysis of Section 4.1; greater than 95% of Population III star-forming regions are contained within 8 proper kpc, corresponding to $<200$ comoving kpc at $z = 20$. Within this sphere, we connect any Population III SN remnant to the Population II cluster via a ray. We then verify that the ray has $Z > Z_2$ for all cells it intersects and require that the distance between particles, $d$, satisfies $d \leq vt$ for a $v = 100$ km s$^{-1}$ SN remnant expansion speed and $t$, the time between SN and Population II formation; $d \leq vt$ implies that metals from the Population III star could feasibly have reached the forming star cluster and acts as a filter for overlapping metal clouds from separate PIII associations. If these criteria are satisfied, then that Population III event is “connected” to the Population II formation and considered to be part of the same “metal system.” The extremely fine time resolution between outputs ensures that Population III events connected to the formed Population II cluster were connected at the time of formation ($\lesssim 200$ kyr prior).

4.3. The Population III Frame

The time evolution of the metal and ionized radii of the PIII associations including all PHX simulations is presented in Figure 8 using B-spline quantile regression fits to the $q = \{0.2, 0.5, 0.95\}$ quantiles. After the initial formation, both radii take on small starting values, reflecting that $Z_{\text{III}}$ is sourced from SNe that have not occurred yet, and that H ionization requires time to first ionize the dense cloud that the particle formed within. The average radius for $Z_{\text{III}} (R_{\text{III}})$ is maximum at $9–12$ Myr after the first formation; this is the time frame expected for most Population III stars to have reached their main-sequence end point if we are considering a coeval system of stars formed at $t = 0$. The reduction in $R_{\text{III}}$ likely reflects gravitational collapse, with the radius supported at later times by increased temperatures and the feedback from Population II stars. The radius of H ionization, $R_{\text{H}^+}$, increases quickly to a maximum average within 10 Myr. The reduction beyond this point reflects recombination after the most massive and ionizing Population III sources of radiation have extinguished. Since the quantiles represent fits, they do not exactly bound the annotated quantile of observed data; 7% of $R_{\text{III}}$ fall above the 0.95 quantile fit, while 17% of $R_{\text{H}^+}$ fall above.

In Figure 9 (left panels), we present quantile fits to the SFR of 3313 distinct primordial star-forming regions considering regions from all PHX simulations. The SFR at these early times is roughly constant for Population III stars; i.e., regions that are creating stars are doing so at similar rates, regardless of time. In

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6 The JINA database does not quote mass-abundance metallicity, as it is tracked in Enzo. Assuming solar metal abundance mass ratios with fixed H abundances, $[\text{Fe/H}] = \log(M_{\text{Fe}}/M_{\odot}) - \log(M_{\text{H}}/M_{\odot}) = \log(Z/\overline{Z})$. Despite that this approximation will not always be true, e.g., carbon-enhanced metal-poor stars common at low metallicity (Frebel & Norris 2015), we quote the values as presented in the database to provide a point of comparison against the simulated metallicities.

7 Using the python patsy package, https://patsy.readthedocs.io.
contrast, the Population II SFR is increasing in time, with $q = 0.5$ approaching $10^{-3} M_{\odot} \text{yr}^{-1}$ by 50 Myr. In the $q = 0.95$ fit, 5.05% and 5.07% of regions fall above the 0.95 quantile fit for Population III and Population II SFRs, respectively. In the right panel, we show the fraction of regions that are forming stars at each time. Within the first 50 Myr, the Population II SFR is sporadic, with $>87.5\%$ of regions having zero SFR at any time, including several intervals where no region is forming Population II stars. The Population III SFR is similarly sporadic, with $<85\%$ of regions forming stars at any given time. The Population III SFR is surprisingly constant throughout the 50 Myr period for regions that are forming Population III stars; however, we do observe that the average Population II SFR ($q = 0.5$) increases with the region age. The early nonzero Population II SFR results from prompt star formation around the earliest and most massive Population III stars.

4.4. The Population II.1 Frame

Generated using Section 4.2, we present the statistics of Population II.1 star clusters including all PHX simulations immediately after the cluster’s formation in Table 2. The region surrounding the Population II.1 star particle is categorized based on the type of Population III progenitors it contains: SNe, HNe, PISNe, or any combination of the three. There are several immediate observations worth noting. For single progenitor type regions, there is an inverse correlation between the distance between the progenitor and Population II.1 star, $R_f$, and the SN energy of the progenitor, while the metallicity of the resulting Population II.1 cluster is correlated to the energy. The mass of the Population III stars that contributed to formation is highly variable. Finally, 14.4\% of Population II.1 stars were enriched by an average of $N_{\text{III}} = 1.1$ PISNe, while other Population II.1 stars are enriched by $N_{\text{II}} > 2$ Population III progenitors. The average distance from progenitor to Population II.1 cluster is maximized if all types of Population III progenitors are present and connected to the Population II.1 star; in fact, we find a generally higher $R_f$ for the more complicated regions with high $N_{\text{III}}$ and many progenitor types. Outside the single type of progenitor cases of the SNe and HNe, the average Population II.1 star is connected to $M_{\text{III}} > 200 M_{\odot}$ of Population III progenitors, with some Population II.1 stars connecting to $M_{\text{III}} > 1000 M_{\odot}$ of Population III SN-generating stars. Interestingly, the mean metallicity of the Population II.1 clusters enriched by PISNe is above the observed metallicity in, e.g., the JINA database samples presented in Figure 7, suggesting that observational campaigns seeking Population II.1 stars by their low metallicity will miss a very large fraction of these Population II.1 stars. In fact, the metallicity of regions with PISN, HN–PISN, and SN–HN–PISN progenitors all have a mean metallicity falling above the selection effect cutoff of the JINA database ($Z > 2.5$).

We do note that $M_{\text{III}}$ and $N_{\text{III}}$ are both highly dependent on the chosen IMF, and this influence will definitely have an impact on $R_f$. We also note that the lack of correlation between cluster metallicity and progenitor configuration may be an
artifact of the star formation algorithm; since the Population II clusters take on the mass-averaged metallicity of the cold gas that formed them, we lose the ability to track extreme cases that may occur with higher resolution and modeling Population II stars as single stars. That said, within the framework of the model designed to predict the range of influence of PIII associations. Using data generated via the method of Section 4.1, we create a model to learn the extent of primordial metals from a PIII association based on the composition of SN events and the duration we wish to model, \( t_{\text{final}} \). The modeled duration includes all SN and formation events from the first star to form in the region to \( t_{\text{final}} \); any formation or SN events after \( t_{\text{final}} \) are excluded. To translate the continuum of available Population III masses and creation times, we transform the stellar information into a simple series of features as binned mass and creation times. The mass features \( \{X_M\} \) are defined by edges \{1, 11, 20, 40, 100, 140, 200, 260, 300\} \( M_\odot \), and the creation time bins \( \{X_t\} \) have edges \{0, \( \Delta t \), \( 2\Delta t \), \ldots, \( n\Delta t \)\} Myr, where \( \Delta t = \text{floor}(t_{\text{final}}/\Delta t) \Delta t \). As a concrete example of mass and creation time features, consider a region with five stars. They have masses \{14, 12, 86, 94, 210\} \( M_\odot \), with creation times \{4, 4, 3, 0, 7\} Myr, as measured from the first star created. With this hypothetical sample, \( X_M = \{0, 2, 0, 2, 0, 0, 1, 0\} \), if we take \( \Delta t = 6\) Myr with \( t_{\text{final}} = 16\) Myr, the time feature bins are \{0, 6, 12\} Myr, so that \( X_t = \{4, 1, 0\} \). This idea is motivated by a method commonly known as tokenization; we use it here to create an input that can accommodate regions with any number of stars without altering the model. We split samples in a spatial sense to prevent information leaking between training and testing splits; if the center of the region (\( r \)) at the first star’s formation is \( r > \{0.4, 0.4, 0.5\} \times L_{\text{box}} \) relative to the simulation volume, then the sample is assigned to the test split and \( r < \{0.6, 0.6, 0.5\} \times L_{\text{box}} \) is assigned to validation, while all others are assigned to training. This splitting of data yields 2273 training, 722 validation, and 318 testing samples.

5.1. Data

Figure 10 shows \( \log(R_{\text{III}}) \) (with \( R_{\text{III}} \) measured in kiloparsecs) according to the number of Population III stars \( N_e \) within the region for the training examples at \( t_{\text{final}} = 16\) Myr. The side histogram shows a probability density function (PDF) of \( \log(R_{\text{III}}) \) as measured in kiloparsecs; the distribution of \( \log(R_{\text{III}}) \) is distinctly more evenly distributed about the peak (\( \log(R_{\text{III}}) \approx 0.3 \)) than without the logarithm. We therefore make our predictions on \( \log(R_{\text{III}}) \), as regression is more successful at modeling scatter from a mean than long tails of asymmetric distributions. We also observe significant variation in the number of Population III stars contained within \( R_{\text{III}} \); regions contain \( 1 < N_e \leq 155 \) within that radius. For each \( t_{\text{final}} \), we define \( N_e = \mu(N_e) + \sigma_e \cdot (\log(N_e)) \), then, for 16 Myr, \( N_e = 1.337 \) and \( \sigma_e = 0.374 \). In addition, while we observe a general trend that increasing \( N_e \) increases \( R_{\text{III}} \), this

---

### Table 2

| Configuration | \( N_{\text{II}} \) | \( f_\beta \) | \( \langle Z \rangle \) \( \pm \) \( \langle R_f \rangle \) (pc) | \( N_{\text{III}} \) | \( M_{\text{III}} \) (\( M_\odot \)) |
|---------------|-------------------|---------------|--------------------------|-------------------|------------------|
| SN            | 17                | 0.011         | \(-3.27 \pm 1.15\)       | 95.38 \pm 101.56  | 2.3 \pm 1.1      | 35.0 \pm 6.0     |
| HN            | 188               | 0.045         | \(-2.79 \pm 0.64\)       | 67.19 \pm 102.57  | 2.3 \pm 1.9      | 73.6 \pm 54.4   |
| PISN          | 618               | 0.144         | \(-1.54 \pm 0.57\)       | 27.55 \pm 17.88   | 1.1 \pm 0.3      | 201.3 \pm 71.6  |
| SN–HN         | 356               | 0.266         | \(-2.77 \pm 0.85\)       | 225.41 \pm 404.98 | 12.0 \pm 8.1     | 286.4 \pm 204.4 |
| SN–PSN        | 11                | 0.008         | \(-2.75 \pm 1.71\)       | 162.64 \pm 146.85 | 3.2 \pm 1.5      | 223.8 \pm 54.8  |
| HN–PISN       | 133               | 0.032         | \(-2.06 \pm 0.83\)       | 92.92 \pm 153.19  | 5.1 \pm 3.7      | 352.6 \pm 171.9 |
| SN–HN–PISN    | 787               | 0.494         | \(-2.27 \pm 0.94\)       | 558.50 \pm 815.70 | 21.9 \pm 15.6    | 829.8 \pm 504.8 |

**Note.** Characteristics of 2110 Population II.1 star clusters from all PHX simulations given the connected Population III events within the region. We categorize each region containing a new Population II star by the type of Population III SN it contains: SN, HN, PISN, or combinations thereof. For each configuration, we present the number of Population II.1 stars formed \( (N_{\text{II}}) \), the fraction of Population II.1 stellar mass generated \( (f_\beta) \), the mean metallicity \( \langle Z \rangle \), the mean radius from progenitor to forming cluster \( \langle R_f \rangle \), the mean number of progenitors in the region \( (N_{\text{III}}) \), and the mean total progenitor mass \( (M_{\text{III}}) \). Note that 61.0% (by mass) of Population II.1 stars have progenitors of multiple types.
relationship is by no means linear in \( N_\ast \) and is not single-valued; i.e., \( N_\ast = 10 \) could lead to many values in the range \(-0.5 < \log(R_{\text{fl}}) < 0.8 \). Here \( \bar{N}_\ast \) and \( \sigma_\ast \) have a very small dependence on \( t_{\text{final}} \); when fit with a simple polynomial, we find that they are fit with a \( \leq 1\% \) error by

\[
\bar{N}_\ast(t_{\text{final}}) \approx 1.197 + 0.0195t_{\text{final}} - 6.57 \times 10^{-4}t_{\text{final}}^2, \tag{3}
\]

\[
\sigma_\ast(t_{\text{final}}) \approx 0.314 + 7.25 \times 10^{-3}t_{\text{final}} - 2.87 \times 10^{-4}t_{\text{final}}^2. \tag{4}
\]

### 5.2. Model and Hyperparameters

To generate an interpretable model, we use a simple linear regression model, where we wish to minimize the error

\[
L = \frac{1}{2}(Y - \hat{Y})^2, \tag{5}
\]

with ground-truth radii \( Y \) and predicted radii \( \hat{Y} \) represented as vectors. The prediction is simply solved by \( \hat{Y} = X \cdot w \). The learnable weights are denoted by \( w \), and \( X \) is composed of mass and creation time features with a bias feature, \( X = \{ 1, X_M^1, X_M^2, \ldots, X_M^8, X_\text{C}^1, X_\text{C}^2, \ldots, X_\text{C}^\text{final} \} \), with, e.g., \( X_M^n \) referring to the \( n \)th feature in the \( X_M \) vector. Since Equation (5) is convex, the solution we seek is \( dL/dw = 0 \), which is solved by

\[
w = (XX^T)^{-1}X^TY. \tag{6}
\]

This regression only admits linear behavior, which, as outlined in Section 5.1, is not a reasonable expectation in this case. The nonlinearity is not only influenced by \( N_\ast \) but also by the varying lifetimes, explosion energies, metal yields, birth times, and SN times. Instead of abandoning the linear model for a less interpretable deep-learning architecture, we split the training samples into subsets based on \( N_\ast \) and apply the linear model to each subset. We use the samples \( X_n \) to train only the model \( M_n \) according to

\[
M_n = \begin{cases} 
M_0, & X|\log N_\ast < \bar{N}_\ast - \sigma_\ast \\
M_1, & X|\bar{N}_\ast - \sigma_\ast < \log N_\ast < \bar{N}_\ast \\
M_2, & X|\bar{N}_\ast < \log N_\ast < \bar{N}_\ast + \sigma_\ast \\
M_3, & X|\log N_\ast > \bar{N}_\ast + \sigma_\ast.
\end{cases} \tag{7}
\]

In this way, we have piecewise defined models specifically for small systems with few stars, average systems, and highly populated systems.

What follows is a concrete example of using this model for observed data, as used in the rest of this paper, or for predictions. For this example, we choose \( \delta t = 6 \text{ Myr} \) and \( t_{\text{final}} = 16 \text{ Myr} \). To generate a sample, we statistically estimate the number of stars by sampling a random number described by a lognormal distribution with \( \bar{N}_\ast(16 \text{ Myr}) \) and \( \sigma_\ast(16 \text{ Myr}) \). Given the number of stars in this sample, we then determine the mass of each star by sampling the IMF described in Section 2 and determine the creation time of each star by sampling the SFR of Figure 9(a). Using this information, we can build \( X \) as described above and determine which \( M_n \) to use. Using the weights of the \( M_n \) model, \( w_n \), we can finally predict the radius of the enriched region as \( \log(R_{\text{fl}}) = X \cdot w_n \).

Finally, we can use the weights to gain insight into the relative importance of different features of \( X \). For example, in Table 4, we present the final trained weights of the \( M_n \) models for \( t_{\text{final}} = 16 \text{ Myr} \). By examining the relative values of \( w_1 \) (which multiplies the 1–11 \( M \) feature) with \( w_6 \) and \( w_7 \) (which multiply the 140–200 and 200–260 \( M_\odot \) features, respectively), we observe that \( w_5 \gg w_1 \) and \( w_7 \gg w_4 \), implying that the 140–260 \( M_\odot \) stars have a much stronger effect on the final radius of the metal cloud. This is, of course, intuitively true as well; 140–260 \( M_\odot \) stars generate PISNe, which distribute more metals with more SN energy than any other mechanism in these simulations.

To evaluate the model-predicted radii, we employ two metrics. We use the \( R_2 \) score for \( N \) samples, given by

\[
R_2(Y, \hat{Y}) = 1 - \frac{1}{N} \sum_{i=1}^{N} (y_i - \hat{y}_i)^2, \tag{8}
\]

for \( \bar{y} = 1/N \sum_{i=1}^{N} y_i \) and \( y_i \) are the individual components of \( Y \). The \( R_2 \) score is informative in comparing the quality of the model as compared to simply predicting the mean value of \( Y \); 1 is a perfect \( R_2 \) score, \( R_2 = 0 \) indicates predicting \( \hat{y} = \bar{y} \) for all inputs, and \( R_2 < 0 \) indicates an arbitrarily worse performance. In addition to the individual predictions, we would also like the PDF of the predicted radii to match that of the ground-truth radii. We define the PDF of \( Y \) as \( P_y, \hat{Y} \) as \( P_{\hat{y}}, \) and the Kullback–Leibler divergence \( D(P||Q) = P \log(P/Q) \) for probability distributions \( P \) and \( Q \), to compare the PDFs using the Jensen–Shannon distance given by

\[
J(P, Q) = \sqrt{\frac{D(P||\hat{P}) + D(Q||\hat{P})}{2}}, \tag{9}
\]

where \( \hat{P} \) represents the average of the distribution \( P_\ast \), and \( J = 0 \) represents two identical distributions, with higher values indicating mismatches in the PDFs. Although not used in the initial evaluation of the models, we include reports on the average \( L_1 \) distance as

\[
\bar{L}_1 = 1/N \sum_{i=1}^{N} |y_i - \hat{y}_i|. \tag{10}
\]
This method is generally capable if lines at those early times. Hydrodynamic state of the system are making the modeling task more difficult at those early times.

The only true hyperparameter of this model is $\delta t$, the time width of the $X_C$ bins. We tested several widths and found no significant improvement beyond the inclusion of two time features, early coeval formation and all other formation, so all results here use $\delta t = 6$ Myr. The $J$ and $R_2$ as functions of predicted time in the data sets are shown in Figure 11, while the tabulated quantification of errors is presented in Table 3. All times have $0.12 < J < 0.23$, while $R_2$ has more variation with $0.33 < R_2 < 0.60$. The overall performance is quantified by combining $R_2$ and $J$ as $R_2/(1 + J)$, which will be maximized if $R_2$ is maximized and $J$ is minimized. These results show that while the model may struggle, e.g., with the lowest $R_2$ score at $T = 18$ Myr, to reproduce exact predictions, it does well at reproducing the distribution of possible radii reflected in the relatively low value of $J = 0.167$. Based on Table 3, if we take the “best”-performing model as the one that maximizes $R_2/(1 + J)$, we find that models with $t_{\text{final}} = \{7, 8, 9, 16\}$ Myr are the best performing, while $t_{\text{final}} = \{12, 13, 15\}$ have the worst performance. The remainder of the discussion in this section considers the 8 and 16 Myr models. While 8 Myr is the most performant model according to our recorded metrics, the 16 Myr model is a desirable time frame to evaluate. Given the stellar lifetimes and IMF used in the PHX, we expect any coeval stars formed near $t = 0$ to have reached their respective end points by $t \sim 16$ Myr. We can also observe that the metal radius is maximized around 16 Myr, as seen in Figure 8.

The final weights of the exemplary $t_{\text{final}} = \{8, 16\}$ Myr models are presented in Table 4. These weights represent the entirety of the trained model. Due to their simplicity, erroneous predictions could be traced through the model to find the offending weight and determine why the model made such an error very easily.

### 5.3. Model Results

Exemplary results from the 8 and 16 Myr models are shown in Figure 12. On the left side, we plot the model predictions, color coded by which model made the prediction. While these models score well with $J = 0.189$ and 0.162 for 8 and 16 Myr, respectively, we can still observe mismatches on the tails of the PDFs for low and high $R_{\text{II}}$. However, it is reassuring that there are no erroneous massive predictions given by the validation or testing data set, e.g., predicting $R_{\text{III}} > 50$ kpc. This is largely due to our splitting of the data set among different models. Using a single model for all $N_*$ leads to linear fits that had erroneously high estimates of $R_{\text{III}}$ at high $N_*$; however, the $M_1$ submodel, which models high $N_*$, has a nearly flat slope, reducing the errors from very high $N_*$ systems. Also, a single model struggled to reproduce the low end of the radii from very low-$N_*$ systems, making no predictions of $R_{\text{III}} < 1$ kpc. Restricting $M_0$ to predict low-$N_*$ systems allows the fit to have a high slope that can predict both $R_{\text{III}} < 1$ kpc while still avoiding falsely large regions that may happen if the same model is responsible for predictions in the higher-$N_*$ regime.

In the scatter plots, we can identify that the high predictions stem from the $M_1$ and $M_2$ models; however, even these results are plausible for the radius of the metal bubble. As a final stress test of the model, we generated 3000 samples that match the $N_*$ and mass distribution of the training data set at 16 Myr using creation times derived from the SFRs presented in Figure 9(a). We compare the PDF of the synthetic sample and full data set in Figure 13, where the full data set is in gray and the synthetic data set is in orange. There is no ground truth for the synthetic data set (so there are no $R_2$, $L_1$, and $L_2$ scores), but it produced a PDF that is in agreement with the ground-truth data set, with $J = 0.150$.

### 6. Conclusions

All halos in the PHX suite with $M_{\text{vir}} \geq 2 \times 10^7 M_\odot$ have Population III star remnants within their radii and have some finite mass of stars (either Population III or Population II). However, all three simulations also contain several halos without stellar mass above $M_{\text{vir}} \geq 10^7 M_\odot$; these may be candidates for further study to analyze whether they may be supermassive black hole candidates, as in the analysis of Regan.
et al. (2017). At $z \sim 12$–14, all simulations are dominated by Population II star formation; however, there continue to be pockets of pristine gas that can form more Population III stars. Also, we do not observe large-scale enrichment or ionization of the IGM at these redshifts, with only $\sim 0.8\%$ of the gas being enriched to $Z_e$ and only 2% of that volume being primarily enriched by Population II sources. Both of these findings are in agreement with prior works (Wise et al. 2012b; Xu et al. 2016).

Population III stars in the PHX suite form in PIII associations. These are very diverse, with up to $\sim 155$ individual stars and system Population III stellar masses up to $M_\star \gtrsim 10^3 M_\odot$; $49.4\%$ of Population II.1 stars are connected to at least one progenitor of each SN type (SN–HN–PISN; Table 2). A PIII association’s influence is large but limited, with 5% and 17% of the PIII association radii having $R > 8$ kpc for $Z_{\text{III}}$ and $H^-$, respectively.

Several important observations have been noted regarding Population II.1 stars within the PHX suite. Their MDF is not distinguishable from Population II.2 cluster formation; i.e., we cannot state with any certainty that a star with metallicity $Z < Z_e$ is a Population II.1 star. Future work may be able to track separate PIII associations that led to the PHX formation of molecular gas clouds proceeds at a rate of $M_{\text{SFRD}} = 7.43 \times 10^{-9} M_\odot$ yr$^{-1}$ pc$^{-3}$ within those regions, implying a Population III SFE of $\sim 2\%$.

The data in Table 2 can be compared to prior works and observational campaigns. Welsh et al. (2020) estimated $5^{+13}_{-3}$ progenitor stars per metal-poor enriched star formation. Our presentation of $N_{\text{III}}$ is largely consistent with their estimate and highlights the dependence on the IMF to generate reasonable estimates of the number of enriching events. Average star-forming halos in Hicks et al. (2021) contained $\lesssim 20$ enriching events, with the most massive halo having $> 100$. Table 2 indicates that the average halo contained a few discrete PIII associations that led to the final state of the halo, while the most massive may have had several. Welsh et al. (2019) placed an upper limit of 70 Population III enriching events in a metal-poor damped Lyman-alpha system; our results indicate that such a system would likely have several PIII associations contained within it but is also small enough to be a single system.

Progenitor configurations that lead to Population II.1 star formation are diverse, so it would be difficult to analytically build an accurate metal abundance model for a Population II.1 star. Future work may be able to track separate

### Table 4

| $w(M_\odot, M_1, M_3)$ | $N_{\text{III}}$ | $SFE_{\text{III}}$ |
|----------------------|------------------|------------------|
|                             |                  |                  |

**Note.** These exemplary weights are only for 8 and 16 Myr; however, the data table with full machine precision for all models presented in Table 3 will be available at www.rensimlab.github.io.
metallicity fields from each progenitor type, allowing an estimation of the Population II.1 metal abundances given the composition of progenitors and mixing of the interstellar medium that has occurred. Within the PHX, we find that while PIII associations have an average radius $R_{III} \sim 3$ kpc, the low-mass, high-redshift halos we observe have $R_{vir} \sim 0.4$ kpc. Because the PIII associations tend to be much larger than their host halos, and the halos tend to be clustered together, we find that only 17.5% of PIII associations in the PHX512 simulation encompass a single halo, 64.1% contain $>5$ halos, and 81.2% contain $\leq 10$ halos; the remaining PIII associations cover up to 58 halos. Hence, these PIII associations can serve as an metal-enriching source for many potential protogalaxies, including those hosted by neighboring halos.

The PIII association influence can be modeled reasonably well by piecewise linear regression fits, with our best-performing models having $R^2 \gtrsim 0.5$, and reproducing the PDF of observed radii with $J \approx 0.2$. We also find that these models are dependent on the time since the first stars’ formation. This model has been used to generate a distribution of enrichment radii that agrees well with our observations in the PHX suite while affording both simplicity and interpretability. Given a halo distribution or sites of Population III star formation, this model can be used to estimate the extent of enriched regions from primordial stars, providing a new alternative to generating the metallicity initial conditions of cosmological simulations. A more complicated model with parameters for inferring hidden variables or learning from hydrodynamic inputs may be more successful in the short evolution time frame or able to generate nonspherical metallicity fields that reflect the complexity of the density distribution of a star-forming region.

This research was supported by National Science Foundation CDS&E grants AST-1615848, AST-2108076, and AST2108076 to M.L.N. The simulations were performed on the Frontera supercomputer operated by the Texas Advanced Computing Center (TACC) with LRAC allocation AST20007. Data analysis was performed on the Comet and Expanse supercomputers operated for XSEDE by the San Diego Supercomputer Center. Simulations were performed with Enzo (Bryan et al. 2014; Brummel-Smith et al. 2019) and analysis with YT (Turk et al. 2011), both of which are collaborative open-source codes representing efforts from many independent scientists around the world. The authors thank John Wise for his insight and guidance regarding the Population III and Population II methods in Enzo.

Figure 12. For predicting the metal radii at two time frames, 8 and 16 Myr, we present the training (top), validation (middle), and testing (bottom) performance as plots of the predictions for each model ($M_0$, $M_1$, $M_2$, and $M_3$ in orange, green, purple, and cyan, respectively) according to the number of stars in the system ($N_*$). The left histograms compare the PDF of the true radii (gray) with the model predictions (orange).

Figure 13. The PDF of radii predicted from the synthetic data set (orange) with those from the full ground-truth data set (gray) at $t_{final} = 16$ Myr. The two PDFs agree well, with $J = 0.150.$
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