On the Evolution of Supermassive Primordial Stars in Cosmological Flows

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ABSTRACT

Primordial supermassive stars (SMSs) formed in atomic-cooling halos at $z \sim 15 - 20$ are leading candidates for the seeds of the first quasars. Past numerical studies of the evolution of SMSs have typically assumed constant accretion rates rather than the highly variable flows in which they form. We model the evolution of SMSs in the cosmological flows that create them using the Kepler stellar evolution and implicit hydrodynamics code. We find that they reach masses of $1 - 2 \times 10^5 M_\odot$ before undergoing direct-collapse to black holes (DCBHs) during or at the end of their main-sequence hydrogen burning, at 1 - 1.5 Myr, regardless of halo mass, spin, or merger history. We also find that realistic, highly-variable accretion histories allow for a much greater diversity of supermassive stellar structures, including in some cases largely thermally relaxed objects, which may provide a significant source of radiative feedback. Our models indicate that the accretion histories predicted for purely atomic-cooling halos may impose a narrow spectrum of masses on the seeds of the first massive quasars, however further studies incorporating realistic feedback will be essential in order to confirm whether or not this holds true in all cases. Our results also indicate that multiple SMSs at disparate stages of evolution can form in these halos, raising the possibility of SMS binaries and supermassive X-ray binaries (SMXBs), as well as DCBH mergers which could be detected by LISA.

Keywords: quasars: general — black hole physics — early universe — dark ages, reionization, first stars — galaxies: formation — galaxies: high-redshift

1. INTRODUCTION

Supermassive stars (SMSs), as the progenitors of direct collapse black holes, are now one of the leading candidates for the seeds of the first massive quasars in the universe. Over 200 such objects have now been confirmed at $z > 6$ (Inayoshi et al. 2019; Bosman 2021), with 8 known quasars at $z > 7$ (e.g., Mortlock et al. 2011; Wu et al. 2015; Banados et al. 2018; Smidt et al. 2018; Matsumura et al. 2019; Wang et al. 2021). In the canonical formation scenario, a primordial halo grows to masses of $10^7 - 10^8 M_\odot$ without ever having formed stars, either because it is immersed in a strong Lyman-Werner background from nearby Population III (Pop III) stars (e.g., Latif et al. 2015; Agarwal et al. 2016), strong dynamical heating resulting from a rapid halo assembly history (Yoshida et al. 2003; Fernandez et al. 2014; Wise et al. 2019), and/or due to supersonic baryon streaming flows (Tanaka & Li 2014; Hirano et al. 2017; Schauer et al. 2017). At these masses, the virial temperature of the halo reaches $\sim 10^4$ K and triggers rapid atomic H
cooling, which causes gas to collapse at rates of up to \( \sim 0.1-1 \, M_\odot \, \text{yr}^{-1} \) (Bromm & Loeb 2003; Wise et al. 2008; Shang et al. 2010; Becerra et al. 2015). These flows flatten into an accretion disk that builds up at least one SMS at its center (e.g. Lodato & Natarajan 2006; Regan & Haehnelt 2009; Latif et al. 2013; Regan & Downes 2018a), although recent simulations suggest binaries or even small multiples of SMSs are possible (Regan et al. 2014; Latif et al. 2020b; Patrick et al. 2020 – for recent reviews, see Valiante et al. 2017; Woods et al. 2019; Smith & Bromm 2019; Inayoshi et al. 2019; Haemmerlé et al. 2020).

Stellar evolution models show that these supermassive objects do not immediately collapse, but survive as core hydrogen-burning stars that can reach masses of several \( 10^5 \, M_\odot \) when accreting rapidly before dying as direct-collapse black holes (DCBHs) via the general relativistic (GR) instability (e.g., Fuller et al. 1986 and references therein; Umeda et al. 2016; Woods et al. 2017; Haemmerlé et al. 2018a,b; Herrington et al. 2021). Model calculations suggest that in some rare circumstances SMSs may explode at the onset of core hydrogen burning in the case of monolithic collapse (see discussion in Woods et al. 2020) or during core helium burning (Johnson et al. 2013; Chen et al. 2014), although see Nagele et al. (2020). Most of the SMS evolution models find that they evolve as cool, red supergiants along the Hayashi track because of \( \text{H}^- \) opacity in their atmospheres (e.g., Hosokawa et al. 2012, 2013), so they are not thought to be bright sources of ionizing UV radiation that could alter accretion onto the star (Ardaneh et al. 2018; Luo et al. 2018), although Ly\( \alpha \) radiation pressure might affect flows on small scales (Smith et al. 2017). Pop III SMS, nevertheless, have extremely large luminosities that could be detected in the near infrared (NIR) by the James Webb Space Telescope (JWST) and large ground-based telescopes in the coming decade (Hosokawa et al. 2013; Surace et al. 2018, 2019; Whalen et al. 2020b).

Most studies of Pop III SMS to date, however have only considered constant accretion rates, not the rapidly varying flows in which the stars actually evolve. Sakurai et al. (2015) examined the evolution of Pop III SMS in idealized, bursty accretion that approximated dense clumps in the disk due to fragmentation, and found that the star could exhibit temporary blue, hot phases before settling down onto cooler, redder evolutionary tracks. These hotter episodes occurred when quiescent times between bursts were longer than \( \sim 1,000 \, \text{yr} \) and the accretion rates between bursts were low because they gave the star’s outer layers time to thermally relax into more compact states. Sakurai et al. (2015) followed up this study with accretion rates taken from idealized two-dimensional (2D) primordial disk simulations. They found that in practice accreting protostars will remain cool and red allowing them to reach the supermassive regime (Sakurai et al. 2016).

New cosmological simulations have followed the evolution of atomically-cooling halos over the times required for an SMS to form and then collapse to a DCBH (e.g., Patrick et al. 2020). They show that the accretion disk of the star can be highly turbulent and is prone to episodes of fragmentation, in which large clumps frequently collide with the star. These accretion rates are quite different than those considered in any SMS model so far (see also Becerra et al. 2015, 2018). How Pop III SMS evolve in the turbulent, clumpy flows that create them is crucial to understanding their temperatures, luminosities, actual growth rates and masses at collapse. Intermittent, high surface temperatures could reduce accretion rates onto the star, prolonging its life and reducing its final mass. These processes in turn determine the prospects for the detection of the star and the BH it will ultimately form, and therefore the first quasars at birth. Semi-analytic models indicate any massive clumps formed from fragmentation in the disk will coalesce and merge before entering the main sequence as ionizing sources (Inayoshi & Haiman 2014); however, if turbulence and quiescent accretion lead to extended periods in which the SMS itself is a strong source of ionizing UV photons, then radiation-hydrodynamical models that are fully coupled to stellar evolution models may be required to capture the true properties of the star and its mass at death. In the present work, we have evolved Pop III SMS in their natal cosmological flows. These flows were taken from a sample of simulated atomic-cooling halos that span the likely range of assembly histories (Patrick et al. 2020). In Section 2, we discuss our cosmological models, their accretion rates, and our stellar evolution models.

In Section 3, we examine SMS evolution in these flows and analyze their properties. As new cosmological simulations have revealed the possibility of supermassive binaries, we conclude in Section 4 with a brief discussion of the prospects for interactions between SMSs in the early Universe.

2. NUMERICAL METHOD

We draw accretion rates for the first disk to form at the centers of the eight halos examined in the \textsc{enzo} adaptive mesh refinement (AMR) cosmology code as given by Patrick et al. (2020). These rates were then used to evolve Pop III SMS in the \textsc{kepler} stellar evolution code, as described below.
2.1. Enzo Simulations

The eight halos for which we tallied central accretion rates were simulated in $1.5\ h^{-1}\ Mpc$ boxes in ENZO (Bryan et al. 2014), which self-consistently evolves gas, dark matter, and nonequilibrium primordial gas chemistry and cooling. Each run had a $(256)^3$ root grid with three nested grids centered on the halo and up to 15 levels of refinement for a maximum resolution of 0.014 pc. To simulate the classic SMS formation scenario of isothermal collapse in high Lyman-Werner UV backgrounds, these simulations were limited to six primordial gas species ($\text{H}, \text{H}^+, \text{He}, \text{He}^+, \text{He}^{++}$, and $e^-$) with no $\text{H}_2$ chemistry (though see Regan et al. 2020; Sakura et al. 2020, for recent works investigating the cases of only a very modest Lyman-Werner background and with local UV feedback from the SMS itself, respectively). Cooling due to collisional excitation and ionization of $\text{H}$ and $\text{He}$, bremsstrahlung, and inverse Compton cooling by the cosmic microwave background were all included.

Each halo was evolved for 2 - 3 Myr after the onset of collapse due to atomic cooling, which occurred at redshifts $z = 13.9 - 20.4$ at masses of $1.2 \times 10^7\ \text{M}_\odot - 8.5 \times 10^7\ \text{M}_\odot$. These halos were chosen to bracket their likely range of spin parameters, $\lambda$, where

$$\lambda = \frac{|J|}{\sqrt{2GMR}},$$

and $J$, $R$, and $M$ are the angular momentum, virial radius and virial mass of the halo, respectively. They were also chosen to include a range of assembly histories ranging from growth primarily by accretion to growth by major mergers. We refer the reader to Patrick et al. (2020) for further details regarding the halo selection criteria. Our ensemble thus yields SMS accretion rates for a variety of primordial environments. We extracted these rates at 10 kyr intervals from the onset of disk formation for all eight halos. Accretion rates onto the central objects were found by summing the total mass flux through a sphere $0.134\text{pc}$ in radius (resolved with at least 20 zones), centred within the disk. At times, the accretion rate as modelled in ENZO can become negative if turbulence drives gas out of the center of the disk. When this happens, we assume that accretion onto any central object formed is halted, i.e., the innermost accretion disk is emptied. We set the accretion rate to zero for our Kepler simulation during such intervals. The resulting input accretion histories are plotted in Figure 1. It is important to clarify here that fragmentation on smaller scales unresolved by our simulation could in principle produce smaller stars and lower mean accretion rates, as found in e.g., Regan et al. (2020); we may note, however, that in contrast to either halo explored in their work, the halo simulations in this study are all implicitly assumed to be embedded in a very strong Lyman-Werner background, and that disk fragmentation in such an environment on scales $\lesssim 10^{-2}\ \text{pc}$ is expected to produce fragments which will merge with the central object before reaching the zero-age main sequence (Inayoshi & Haiman 2014).

Accretion begins with an initial surge, ranging from 0.3 - 1 $\text{M}_\odot\ \text{yr}^{-1}$, that lasts for 200 - 300 kyr. The surge coincides with the formation of the disk, which has an initial diameter of $\sim 0.5\ \text{pc}$. Accretion thereafter can then be relatively smooth (as in Halo 10 in the upper left panel of Figure 2), highly turbulent (as in Halo 20 in the upper right panel of Figure 2) or clumpy because of the fragmentation of the disk (as in Halo 12 in the lower left panel of Figure 2). The large jumps in accretion rate at intermediate times are generally due to the fragmentation of the disk and subsequent collision of the clumps with its center, as at 0.7 Myr in Halo 02. The large peak at 1.0 Myr in Halo 01 (and at 1.4 Myr in Halo 19) is due to the collision of a satellite disk that also hosts an SMS with the main disk, as shown in the lower right panel of Figure 2.

2.2. Kepler Models

We evolve each star in the one-dimensional Lagrangian stellar evolution and hydrodynamics code Kepler (Weaver et al. 1978; Woosley et al. 2002) using the post-Newtonian approximation implemented by Fuller et al. (1986). Specifically, Kepler solves the angular momentum and energy equations with first-order (post-Newtonian) GR corrections to gravity:

$$\frac{dv}{dt} = 4\pi r^2 \frac{\partial P}{\partial m_r} + \frac{4\pi}{r} \frac{\partial Q}{\partial m_r} - \frac{G_{\text{rel}} m_r}{r^2}$$

$$\frac{du}{dt} = -4\pi P \frac{\partial}{\partial m_r} (rv^2) + 4\pi Q \frac{\partial}{\partial m_r} \left(\frac{v}{r}\right) - \frac{\partial L}{\partial m_r} + \epsilon$$

The terms on the right-hand side of Equation 2 are the acceleration due to pressure gradients, viscous drag and gravity, respectively, while those on the right-hand side of Equation 3 are the energy flux due to work, viscous dissipation, radiative flux, and nuclear burning. The post-Newtonian correction to gravity is implemented by modifying the gravitational constant:

$$G_{\text{rel}} = G \left(1 + \frac{P}{\rho c^2} + \frac{4\pi P r^3}{m_r c^2} \left(1 - \frac{2Gm_r}{rc^2}\right)^{-1}\right)$$

The factor $Q$ in the viscous term is

$$Q = \frac{4}{3} \eta_r r^4 \frac{\partial}{\partial r} \left(\frac{v}{r}\right).$$
Figure 1. SMS accretion rates from Patrick et al. (2020). The blue vertical lines indicate the times when the stars collapse in our Kepler runs (see Section 3). Only the main disk in each halo is considered here.
where $\eta_\nu$ is the dynamic viscosity from Weaver et al. (1978), defined as:

$$\eta_\nu = \eta_R + \frac{3}{4} l_1 \rho c_s + \frac{3}{4} l_2^2 \max(0, -\nabla \cdot \mathbf{v})$$

which includes the real ($\eta_R$) and artificial viscosity, with the latter used to dampen acoustic oscillations during quiescent phases of the evolution of a star. Here we choose the canonical values $l_1 = 0.1 \Delta r$ and $l_2 = 2 \Delta r$ for Kepler simulations, where $\Delta r$ is the local width of a zone.

Nuclear-burning is evolved with an adaptive network that is implicitly coupled to the hydrodynamics (Woosley et al. 2004). We use a Helmholtz-like equation of state that includes electron-positron pair production, relativistic and non-relativistic degenerate and non-degenerate electrons, and radiation (Timmes & Swesty 2000). Time-dependent convection as described in Weaver et al. (1978) is included in our runs, as is convective heat transport when a zone satisfies the Ledoux criterion.

We initialize our models as $10 \, M_\odot$, $n = 3$ polytropes with primordial compositions, and with central densities $\rho_c = 10^{-3} \, \text{g cm}^{-3}$ and temperatures $T_c = 1.2 \times 10^6$ K, which are capable of sustaining deuterium burning. Varying the initial mass and entropy significantly does not have a substantive impact on the subsequent evolution of the SMS, so long as it is small relative to the final SMS mass, given that the core quickly becomes convective; see discussion in Woods et al. (2017) and Haemmerlé et al. (2018b). The accretion flow onto the star is also primordial in composition. We match its entropy to that of the surface of the star, which neglects the luminosity due to the accretion shock, but at $1 \, M_\odot \, \text{yr}^{-1}$ this luminosity is on the order of $10^4 \, L_\odot$, which is negligible in comparison to that of the star. Studies that include this luminosity at the base of the photosphere of the SMS find little change in its evolution above a few thousand $M_\odot$ (e.g., Hosokawa et al. 2013). We also do not include the accretion of angular momentum, restricting our attention to non-rotating models (though see Haemmerlé et al. 2018a; Haemmerlé & Meynet 2019, for more on rotating SMSs). Additional details on our treatment of accretion can be found in Woosley et al. (2004) and Woods et al. (2017).

Kepler partitions each star into a large number of zones (here, up to $8,000$) with especially high mass resolution near its center ($\sim 10^{30}$ g/zone) and outer layers ($\sim 10^{26}$ g/zone). In each model, the code makes an arbitrarily large initial guess for each time step, and then iterates to identify the largest step the code can take without exceeding preset limits on the change in fractional radius, temperature, luminosity, or density anywhere on the grid, and while still following the emergence of shocks. This approach enables us to follow the long-term evolution of the star over thermal and nuclear timescales, dropping to short time steps to resolve hydrodynamic timescales only when instabilities appear. This includes the onset of the post-Newtonian or GR instability (Chandrasekhar 1964). Recently, Haemmerlé (2020) confirmed that Kepler predicts collapse at masses that are consistent with those expected from careful analytic estimates. We ignore mass loss due to winds, which are thought to be negligible in primordial stars (Vink et al. 2001) and in any event could not overcome the ram pressure of infall. We also do not consider pulsations and pulsational mass losses here (Baraffe et al. 2001).

3. RESULTS

The evolution of the star in the main disk in each halo, along with its total mass and energy generation and transport within the star, are shown in the Kippenhahn diagrams in Figure 3. We discuss the salient features of each model in Section 3.1 and infer general aspects of SMS formation and their connection to the properties of their host halos in Section 3.2.

3.1. Individual Halos
Figure 3. Kippenhahn diagrams illustrating energy generation, energy transport, and stellar structure as a function of time and mass coordinate for the stars in our study. Figure captions: “conv” (green single-line hashing) denotes convective regions, “semi” (red ‘x’ cross-hashing) denotes semi-convective regions, and “neut” (light blue ‘x’ cross-hashing) denotes neutral regions. The specific energy generation rate (blue shading) at each mass coordinate in the star is indicated by the color axis (see, e.g., the description in Woods et al. 2017).
In Halo 01, the initial surge in accretion rate due to the formation of the disk peaks at $\sim 0.4 \, M_\odot \, yr^{-1}$ in the first 100 kyr, before subsiding somewhat. Consequently, the SMS initially develops a large, high-entropy radiative envelope surrounding its convective, nuclear-burning core, much as it would in the constant accretion rate case (e.g., Hosokawa et al. 2013). This outer radiative envelope is only very marginally stable against convection, and indeed, small transient convective cells do form within the upper envelope, as also seen in e.g., Umeda et al. (2016) and Woods et al. (2017). Accretion then nearly halts before three later dramatic bursts that are separated by long quiescent phases. During each pause, the star thermally relaxes, and convective cells formed in the outer envelope in each accretion burst eventually merge with the central region as the star becomes almost wholly convective.

The last of these bursts corresponds to the collision of the main accretion disk with a smaller, satellite disk that likely hosts another SMS. Our ENZO simulations lack the resolution to determine if these two stars merge, so we simply include the collision of the smaller disk in the accretion rate of the main disk in our KEPHER runs. In this halo, we find that the star reaches $\sim 170 \, kM_\odot$ at $\sim 1.2$ Myr, at which point it collapses due to the GR instability while still burning hydrogen, with a central hydrogen fraction of $X_c \approx 0.29$. We stress, however, that this merger event should be examined in greater detail, using e.g., a detailed three-dimensional smoothed particle hydrodynamical simulation to follow the trajectories of the stars and their subsequent interaction. We will study such systems in future work. Notably, however, we can confirm that the two massive stars in Halo 01 will interact while both are on the main sequence, ultimately colliding in a supermassive stellar merger or forming a supermassive binary.

The SMS in Halo 02 initially only accretes at an average rate of about $0.07 \, M_\odot \, yr^{-1}$ for the first 500 kyr. This leads to a (relatively) shallow radiative envelope (in keeping with previous calculations, e.g., Woods et al. 2017; Haemmerlé et al. 2018b). Then the disk fragments, and accretion thereafter proceeds in an extremely clumpy manner, with the first accretion spike at $\sim 500$ kyr leading to the emergence of a deep high-entropy radiative envelope, which then largely relaxes over the subsequent, relatively quiescent $\sim 0.3$ Myr before the next accretion spike. During this spike, the supermassive star rapidly accretes $40 \, kM_\odot$ over $\sim 100$ kyr in a marginally-convective, superadiabatic envelope before accretion nearly halts. Over the next 200 kyr the star largely thermally relaxes again, notably with a strong gradient between the inner convective core and the outermost envelope, before collapsing while still burning hydrogen ($X_c \approx 0.34$) at the onset of a third accretion burst at 1.46 Myr at a final mass of $\sim 155 \, kM_\odot$. This is extremely close to the upper boundary mass for avoiding direct collapse for fully thermally relaxed SMSs (Woods et al. 2020).

In Halo 08, after a brief initial burst that peaks at $0.37 \, M_\odot \, yr^{-1}$, accretion proceeds at rates of $0.1 - 0.3 \, M_\odot \, yr^{-1}$ for the first $\sim 700$ kyr of the star’s evolution. During this time, the SMS very closely resembles stars accreting at uniform rates with similar average values (e.g., Hosokawa et al. 2013; Woods et al. 2017; Haemmerlé et al. 2018b). This is only somewhat interrupted by a minor accretion episode at $\sim 0.7 - 0.8$ Myr, which peaks at just below $0.5 \, M_\odot \, yr^{-1}$ before subsiding. Although convective cells form in the outer envelope, the supermassive star remains far from being thermally relaxed up to its collapse at 0.954 Myr and $\sim 186 \, kM_\odot$, when it is still burning hydrogen ($X_c \approx 0.38$).

The SMS in Halo 10 grows by nearly $0.4 \, M_\odot \, yr^{-1}$ for the first 100 kyr of evolution, with the accreted mass mostly remaining in the high-entropy envelope. Accretion then begins to slow, allowing the star to thermally relax somewhat and the central, nuclear-burning convective region to grow both in absolute mass and in total mass fraction of the star. The star continues to grow at a more modest pace over the next 1.6 Myr, which allows its convective hydrogen- and helium-burning “core” mass fraction to grow as it continues to thermally relax. The mean accretion rate over the life of the SMS is $\sim 0.07 \, M_\odot \, yr^{-1}$. During this latter accretion phase, transient convective regions within the high-entropy envelope arise and disappear or merge with the central convective region before accretion nearly halts at 1.7 Myr. A little over 100 kyr later, the star is almost fully convective. Shortly after the onset of a final accretion burst at $\sim 1.9$ Myr, the SMS collapses near the end of central hydrogen-burning ($X_c \approx 0.06$) at a final mass of $132 \, kM_\odot$.

As in halos 01 and 02, the disk in Halo 12 is strongly turbulent and begins to fragment soon after formation, which leads to large accretion bursts at the beginning of our KEPHER run and at 0.5 Myr and 0.65 Myr. Unlike those in the other halos, the SMS in Halo 12 produces somewhat more substantial, transient semi-convective regions at the interface between the convective core and the high-entropy envelope, the reason for which remains unclear. Ultimately, the precise treatment of convection in extremely radiation-dominated SMSs remains highly uncertain, with potential repercussions for the stellar structure, the response to variable accretion, and the dredge up and mixing of metal-enriched matter in the
stellar envelope; however, a full exploration of 3-D convective motions in SMS envelopes is beyond the scope of the present work. We find that the star collapses at 1.22 Myr at a final mass of 178 kM⊙ while burning hydrogen (Xc ≈ 0.31). At collapse, the star has not been able to fully thermally relax because of persistent rapid accretion and is therefore not quite fully convective.

The accretion history in Halo 16 is somewhat of an outlier in our sample because the initial peak associated with the formation of the disk is particularly strong and persistent, depositing nearly 80 kM⊙ onto the star in its first 200 kyr. Accretion then almost entirely halts before resuming at ~700 kyr. Infall rates at the center of the disk fall to low values because Halo 16 collides with three other halos just before cooling and collapsing. These mergers spin gas up at the center of the halo and make the disk very rotationally supported, reducing accretion onto the star. The initial accretion peak produces an enormous, high-entropy envelope surrounding the convective hydrogen-burning region of the star. The latter grows in mass much more slowly, following the thermal relaxation of the SMS, only nearly catching up with the total mass of the star at ~400 kyr, well after the initial accretion burst has ended. After accretion resumes at 0.7 Myr, the SMS slowly accumulates another 30 kM⊙ before collapsing at a mass of 110 kM⊙ at 1.68 Myr. This is the only star in our sample that reaches core hydrogen exhaustion (Xc ≈ 5 × 10⁻¹², with a central helium fraction of ≈ 100%). Coincidentally, this is also roughly when a second disk forms in Halo 16, raising the possibility of interactions between a second SMS and the DCBH of the first star. Such interactions could result in a tidal disruption event that could be highly luminous in the NIR today (Kashiyama & Inayoshi 2016) or a long-lived, interacting supermassive X-ray binary. We will investigate the evolution of the companion disk in Halo 16, and the possibilities for interaction with the DCBH, in future studies.

Accretion in Halo 19 is similar to that in Halo 01: after the initial peak, accretion falls to modest rates with occasional and brief bursts prior to the appearance of a large burst due to the merger of the main disk with a satellite disk, in this case at 1.4 Myr. Here again, although the satellite disk may also host an SMS we make no attempt to model its mass or follow its merger with the star in the main disk. Because of the lower infall rates up to 1.4 Myr the SMS in the main disk has mostly thermally relaxed and become almost fully convective by the time the disks collide, and it remains largely convective during the collision. Given its relatively modest prior accretion rate, the SMS within the most massive disk in Halo 19 is largely thermally relaxed and almost fully convective by the time of the merger, remaining largely convective as it survives the resulting burst of accretion. After another much smaller spike in accretion at ~1.6 Myr, the star finally collapses at 1.79 Myr at a mass of 177 kM⊙ while still burning hydrogen (Xc ≈ 0.19).

The formation of the central disk in Halo 20 is accompanied by a particularly strong accretion peak, similar to that in Halo 16. In Halo 20, however, accretion never subsides, in spite of the formation of another disk that soon rivals the original in mass. A close encounter with this companion disk at 1.36 Myr produces a second powerful surge in accretion (see Patrick et al. 2020, for more details). After this burst, accretion falls off and the SMS collapses at 1.48 Myr at a final mass of 178 kM⊙ while still burning hydrogen (Xc ≈ 0.14).

3.2. General Properties

Comparing the results in Figure 3 with the classic, constant accretion rate case examined previously (see e.g., Hosokawa et al. 2012, 2013; Woods et al. 2017; Haemmerlé et al. 2018b), it is immediately apparent that a major consequence of the significant variations seen in more realistic accretion histories is a much wider diversity of stellar structures throughout the evolution of SMSs. In some cases, we find SMSs almost wholly thermally relaxed, in particularly sharp contrast to the now-standard picture of a deep, radiative, high-entropy envelope surrounding a convective core (Begelman 2010). In principle, this invites the possibility that the SMS may become a significant source of photoionizing emission, and thus provide a significant source of feedback in the halo which may impede its further growth (Sakurai et al. 2015, 2016). If so, this would indicate that the evolution of atomic cooling halos and SMSs is strongly coupled, and a careful consideration of the accretion history must be made in evaluating the reliability of any such halo simulation (see also Latif et al. 2020a).

Two limitations prevent us from making a more definite statement in this regard: first, radiative feedback is not included in the original calculations of Patrick et al. (2020); second, the photospheric temperatures of accreting SMSs are generally found to be systematically hotter in Kepler simulations than found in other studies (e.g., Hosokawa et al. 2013; Haemmerlé et al. 2018b), for reasons which remain uncertain but which may relate to problems with resolution near the surface. For a detailed discussion of benchmarking efforts, see Woods et al. 2019. We note that the effective temperatures of SMSs modelled here never exceed ~2–5 × 10⁴ K during their lifetimes, such that only the Wien tail of their emission would provide significant ionizing photons; this
together with the particularly dense gas flows seen in the halos we consider suggests feedback may remain ineffective in these particular cases (see also Sakurai et al. 2020), however we do not speculate further for the reasons outlined above.

In many other aspects, however, these objects do resemble the standard evolution of SMSs. We find that the object at the center of the disk in each halo survives initial thermal contraction and reaches pp-chain hydrogen-burning without first collapsing to a BH. Eventually, the central temperature exceeds $T_c \sim 10^8$ K, permitting the onset of of the triple-alpha reaction, quickly producing the CNO abundances needed to reach sufficient hydrogen-burning to stabilizing the star against further contraction, and producing a long-lived SMS. The subsequent evolution of the star depends on the halo’s accretion and merger history but a number of general trends are evident.

All of the stars in our sample undergo collapse at some point during the hydrogen-burning main sequence with the nominal exception of the SMS in Halo 16, which collapses at the exhaustion of its central hydrogen. This is in keeping with the large masses deposited onto these SMSs by rapid accretion, which in almost all cases bring the SMS up to the post-Newtonian limit and the onset of the GR instability before the end of their main sequence lifetimes (as also found in, e.g., Woods et al. 2017; Haemmerlé et al. 2018a). The SMS in Halo 16 accretes almost all its mass in its first 200,000 yr and then lives for very nearly the main sequence lifetime predicted for an Eddington-limited star, before collapsing at the age expected for a wholly thermally-relaxed SMS (Woods et al. 2020). Note that some stars, like those in Halos 10 and 19, live somewhat longer than the Eddington-limited main sequence lifetime because of the ingestion of additional hydrogen at later times in their accretion histories.

The properties of each SMS and its host halo are listed in Table 1. Note that these eight halos were chosen by Patrick et al. (2020) to span their likely range of spin parameters and assembly histories, i.e., growth primarily by accretion, by major mergers, or both. Here, a major merger is defined to be the collision of two halos with mass ratios of 1/5 or more. We show scatter plots of mean accretion rate and final stellar mass, core hydrogen fraction and age versus halo mass, collapse redshift, spin parameter and number of major mergers prior to collapse in Figure 4. Although our sample is small, it is clear that some properties of SMS populations at high redshift can be inferred from those of the halos in which they form.

First, a history of major mergers limits the maximum mass of the SMS and therefore produces the least massive DCBHs. These halos form the smallest and most rotationally-supported disks, and thus have the lowest accretion rates. Lower rates create more thermally-relaxed, compact SMSs with less opportunity for growth before significant nuclear evolution, as in Halo 16 where the star collapses after reaching the end of the main sequence. Second, if we exclude the two halos with major mergers prior to collapse, we see that there is also a tentative correlation between redshift and accretion rate, and thus an anti-correlation between redshift and SMS lifetime, because more rapidly-accreting SMS have shorter lives (Woods et al. 2017). In the six halos that grew primarily by accretion, we also see a tentative anti-correlation between halo mass and final SMS mass, suggesting that more massive halos may produce less massive quasar seeds, however this is primarily motivated by the extreme case of Halo 2, which has about 3 times the mass of the other halos in our sample. Therefore, we defer further discussion of this trend to future studies with larger samples, as we cannot presently exclude some stochastic variation due to a random outlier.

Table 1. Properties of the halos at collapse (redshifts, masses, spin parameters, and number N of major mergers prior to collapse) and their stars (final masses and central hydrogen fractions, times at which they reach the post-Newtonian instability, and average accretion rates).

| Halo | $z_{col}$ | $M_{halo}$ | spin | N | $M_{SMS}$ | $X_c$ | $t_{GR}$ | $\dot{M}_{avg}$ |
|-----|----------|-----------|------|---|----------|------|--------|-------------|
| 1   | 16.7     | 3.68      | 0.0389 | 0 | 1.73     | 0.29 | 1.17   | 0.15        |
| 2   | 14.5     | 8.47      | 0.0388 | 0 | 1.55     | 0.34 | 1.46   | 0.11        |
| 8   | 20.4     | 1.15      | 0.0321 | 0 | 1.86     | 0.38 | 0.95   | 0.19        |
| 10  | 17.3     | 2.60      | 0.0500 | 1 | 1.32     | 0.06 | 1.95   | 0.07        |
| 12  | 16.8     | 1.93      | 0.0471 | 0 | 1.78     | 0.31 | 1.22   | 0.15        |
| 16  | 16.5     | 2.91      | 0.0258 | 3 | 1.10     | 0.00 | 1.68   | 0.06        |
| 19  | 13.9     | 2.12      | 0.0072 | 0 | 1.77     | 0.19 | 1.79   | 0.10        |
| 20  | 17.7     | 3.56      | 0.0199 | 0 | 1.78     | 0.14 | 1.48   | 0.12        |
Perhaps the most striking feature with regard to the final mass, however, is the only modest deviations found given even highly variable accretion. In particular, taking the mean accretion rate over the lifetime of the star in each halo, and interpolating the final mass expected from previous constant accretion rate models (Woods et al. 2017), we find the final mass in our constant accretion case differs stochastically, but only within a margin of \( \sim 10\% \).

In some respects, Halo 08 is the most extreme object in our sample because it collapses at the highest redshift and produces the most massive but shortest-lived star, although it is only slightly more massive than those in Halo 12, Halo 19, and Halo 20. This means it is also the least-evolved at the time it encounters the GR instability and collapses with a central hydrogen fraction of 0.38. While we do not follow the ensuing collapse in detail because of the limitations of our 1D post-Newtonian approximation, if even a small fraction of nuclear-processed material were to be expelled to the surrounding environment it would provide a profoundly important source of chemical enrichment in the very early Universe, and an unusual one given the hot, hydrogen-rich burning conditions and the enormous mass available. Indeed, such a mechanism is not unlike that suggested to explain the unusual abundances of proton-rich elements observed in globular clusters (Denissenkov & Hartwick 2014). While in the present study we neglect rotation (though see Haemmerlé et al. 2018a), this together with the existing uncertainties in mass loss and the nature of convection in supermassive envelopes, may yet allow for chemical enrichment by SMSs of their surrounding environment, however this is beyond the present scope.

Finally, we note that all but one of our stars (the one in Halo 01) collapse before the end of our ENZO simulations, well before the gas in the disk is exhausted. Accretion onto the nascent BH from its natal disk or a companion star will release X-rays that will alter the course of the evolution of the halo by, for example, catalyzing \( \text{H}_2 \) formation and triggering new star formation in the vicinity of the BH (e.g., Akyutalp et al. 2014; Inayoshi & Tanaka 2015). Stellar evolution calculations with accretion rates from cosmological simulations will be required to predict when X-rays are turned on in a halo after the death of its SMS in future studies of its later evolution.

4. CONCLUSION

Stars evolving in cosmological flows taken from numerical simulations of the collapse of atomically-cooling halos become supermassive before collapsing to BHs after 1 - 1.5 Myr. Accounting for the nuclear evolution and the short- and long-term response of SMSs to accretion, we find that all objects within our sample collapse during or at the end of the hydrogen-burning main sequence. In particular, halos that cool purely by atomic cooling produce DCBHs with a narrow range of masses (\( \sim 1 - 2 \times 10^5 \, M_\odot \)) for a wide range of collapse redshifts, spin parameters and merger histories. These masses are similar to the final masses of stars in Woods et al. (2017), whose uniform accretion rates were comparable to our average ones. Future studies incorporating radiative feedback and careful estimates of the SMS’s ionizing photon luminosity will be able to investigate whether extended quiescent accretion phases within the disks formed in some halos may be able to modify this picture in some cases.

Patrick et al. (2020) do not bridge all the spatial scales of accretion onto the star because they are limited to resolutions of \( \sim 0.01 \) pc, so it is possible that fragmentation and less massive stars could appear at smaller scales (e.g., Becerra et al. 2015, 2018). Our SMS masses should therefore be taken to be upper limits. In numerical simulations with higher resolutions, however, small clumps tend to merge over time at these scales. Whether or not one star or many form in purely atomically-cooled halos remains an open question.

Previous studies have shown that Pop III SMSs with masses similar to those in our models would have extremely large luminosities that could be detected in the near infrared (NIR) by the James Webb Space Telescope (\( \text{JWST} \)) and large ground-based telescopes in the coming decade (Hosokawa et al. 2013; Surace et al. 2018, 2019; Whalen et al. 2020b). Their BHs could also be found in the NIR at \( z \sim 15 - 20 \) using \( \text{JWST} \) (with \( \sim 24\text{–}100 \) hr exposures by NIRCam, as shown by Pacucci et al. 2015; Natarajan et al. 2017; Barrow et al. 2018; Whalen et al. 2020a, see therein for details) and at \( z \sim 6 - 8 \) by Euclid and the Roman Space Telescope (although lensing by galaxy clusters and massive galaxies in their wide fields could extend these detections up to \( z \lesssim 10 - 15 \); Vikaeus et al. 2021). DCBHs will only be marginally visible to the Square Kilometre Array or next-generation Very Large Array in the radio at \( z \gtrsim 6 - 8 \) (Whalen et al. 2020b) but would become more luminous after growing to larger masses at later times. They could also be detected out to \( z \sim 10 \) by future X-ray missions such as the Advanced Telescope for High-Energy Astrophysics (\( \text{ATHENA} \)) and Lynx (Aird et al. 2013; The Lynx Team 2018).

Here, we have focused on the first disk to form in each halo, but Patrick et al. (2020) found that other disks can appear and exchange mass or even merge with the
Figure 4. Scatter plots of mean accretion rates and final SMS masses, core hydrogen fractions and ages from our Kepler models vs. key properties of the host halos from Patrick et al. (2020). Individual halos are each identified by a unique colour and shape for all plots, as described in the figure legend.
original disk. Although we do not model such mergers here, we find that they can occur at any time from when the SMS in the main disk is early in its evolution to well after it has collapsed to a black hole. This suggests a number of possible interactions between SMSs and their progeny in the early Universe, from supermassive stellar mergers to stable mass exchange in supermassive X-ray binaries (“SMBXs”) to DCBH–DCBH mergers, the latter being detectable by LISA out to redshifts of $\sim 15–20$ (Hartwig et al. 2018). Such massive and early DCBH mergers would be easily discriminated from the normal build-up of massive BH mergers, which arise only at somewhat lower redshifts in the course of hierarchical structure formation (Sesana et al. 2007). The growing evidence that multiple very massive and supermassive stars may have been common in atomically-cooled halos (see also Chon et al. 2018; Regan & Downes 2018b,c; Regan et al. 2020; Patrick et al. 2021) indicates that these exotic interactions occurred in the early Universe.

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