Formation of massive black holes in rapidly growing pre–galactic gas clouds

John H. Wise1*, John A. Regan2, Brian W. O'Shea3,4, Michael L. Norman5,6, Turlough P. Downes2 & Hao Xu5,6,7

The origin of the supermassive black holes that inhabit the centres of massive galaxies remains unclear1,2. Direct-collapse black holes—remnants of supermassive stars, with masses around 10,000 times that of the Sun—are ideal seed candidates3–6. However, their very existence and their formation environment in the early Universe are still under debate, and their supposed rarity makes modelling their formation difficult7,8. Models have shown that rapid collapse of pre–galactic gas (with a mass infall rate above some critical value) in metal-free haloes is a requirement for the formation of a protostellar core that will then form a supermassive star9,10. Here we report a radiation hydrodynamics simulation of early galaxy formation11,12 that produces metal-free haloes massive enough and with sufficiently high mass infall rates to form supermassive stars. We find that pre–galactic haloes and their associated gas clouds that are exposed to a Lyman–Werner intensity roughly three times the intensity of the background radiation and that undergo at least one period of rapid mass growth early in their evolution are ideal environments for the formation of supermassive stars. The rapid growth induces substantial dynamical heating13,14, amplifying the Lyman–Werner suppression that originates from a group of young galaxies 20 kiloparsecs away. Our results strongly indicate that the dynamics of structure formation, rather than a critical Lyman–Werner flux, is the main driver of the formation of massive black holes in the early Universe. We find that the seeds of massive black holes may be much more common than previously considered in overdense regions of the early Universe, with a co-moving number density up to $10^{-3}$ per cubic megaparsec.

Fig. 1 | Thermal and chemical evolution of the immediate pre–galactic environment. a–h. Projections of the temperature (orange), metallicity (blue; $Z_\odot$ is the metallicity of the Sun) and gas density (black) of a region 40 kpc across and with a depth of 8 kpc centred on the MMH (a–d) and the LWH (e–h). The MMH and LWH are indicated by arrows. The heated and metal-enriched volumes around early galaxies and population III stars grow from $z = 18$ to $z = 15$ (62 Myr). The dotted, dash-dotted, dashed and solid contours indicate where the average Lyman–Werner flux is $1J_{21}$, $3J_{21}$, $10J_{21}$ and $30J_{21}$. Both candidate haloes, which host the formation of massive black holes, have $3J_{21}$, are just outside of the cosmological $H\text{ II}$ region and are still unaffected by any external metal-rich winds.

1Center for Relativistic Astrophysics, School of Physics, Georgia Institute of Technology, Atlanta, GA, USA. 2Centre for Astrophysics and Relativity, School of Mathematical Sciences, Dublin City University, Dublin, Ireland. 3Department of Computational Mathematics, Science and Engineering, Michigan State University, East Lansing, MI, USA. 4Department of Physics and Astronomy, Michigan State University, East Lansing, MI, USA. 5Center for Astrophysics and Space Sciences, University of California, San Diego, CA, USA. 6San Diego Supercomputer Center, San Diego, CA, USA. 7IBM, Poughkeepsie, NY, USA. *e-mail: jwise@gatech.edu
The flux is increasing from the nearby, growing group of young galaxies at a distance of 10–15 kpc. The Lyman–Werner (LW) radiation flux necessary for SMS formation is higher than previous estimates. This flux is of the order of 6 to 600 times lower than the critical LW intensity needed to form SMSs (and subsequently DCBHs). Out of these ten haloes, we concentrate on two—the most massive halo (MMH) and the halo exposed to the most LW radiation flux (LWH). We resample the mass distributions of these two haloes at $z = 20$ and at a mass resolution higher by a factor of 169, and re-simulate them to study their gravitational collapse in more detail.

Both haloes assemble in a region 10–25 kpc away from a group of young galaxies that have photo-ionized, photo-heated and chemically enriched the surrounding environments. The star-formation rates grow in these young (massive) galaxies, the Lyman–Werner (LW) intensities increase from $J_{\text{LW}} \approx J_{\text{L,18}}$ at $z = 18$ within 5 physical kpc of the galaxies to $J_{\text{LW}} \approx 30J_{\text{L,18}}$ at $z = 15$, where $J_{\text{L,18}}$ is the intensity of the background radiation in units of $10^{-21} \text{ erg cm}^{-2} \text{s}^{-1} \text{Hz}^{-1} \text{sr}^{-1}$. The only other source of Lyman–Werner radiation comes from four nearby haloes that host population III stars, 3–5 kpc from the LWH. Both target haloes are impacted by a Lyman–Werner intensity of $J_{\text{LW}} \approx 3J_{\text{L,18}}$ at $z = 15$ (Fig. 1d, h). This flux is 6 to 600 times lower than previous estimates for the critical Lyman–Werner flux necessary for SMS formation.

The metal-enriched regions around the group of young galaxies extend a distance of only 5 kpc, still far from the target haloes. The heavy elements in these regions originate from both population III progenitors and ongoing star formation in the galaxies. Over the next 60 Myr, the ionizing radiation from the young, growing galaxies will extend the H ii regions to nearly 40 kpc in radius (Fig. 1). This will leave most of the intergalactic medium and associated collapsed haloes chemically pristine, but nonetheless bathed in Lyman–Werner radiation, which will help to prevent population III star formation.

During the process of halo assembly (Fig. 2a), the Lyman–Werner intensity increases from $0.3J_{\text{L,18}}$ to $3J_{\text{L,18}}$ at $z = 15$ (Fig. 2b), corresponding to a minimum halo mass of $M_{\text{crit}} \approx 3 \times 10^6 M_\odot$ that can support H ii cooling and primordial star formation. However, the MMH (LWH) gravitationally collapses only after it reaches the atomic-cooling limit at $z = 16.4$ ($z = 15.3$), when it has a mass of $2.6 \times 10^9 M_\odot$ ($5.8 \times 10^9 M_\odot$) — an order of magnitude above $M_{\text{crit}}$. Upon closer inspection, we find that both target haloes experience a period of rapid mass growth (Fig. 2a). The MMH grows by a factor of 30 over 30 Myr ($z = 21–19$) as it virializes. The LWH experiences two rapid growth events. It first increases from $2 \times 10^7 M_\odot$ to $3 \times 10^7 M_\odot$, between $z = 19$ and $z = 18$ (15 Myr), at which point its mass fluctuates just above $M_{\text{crit}}$. Then at $z = 18.5$, it grows markedly, by a factor of nine within 10 Myr. Most of the accreted matter originates from the parent filament, a major merger and several minor halo mergers. This rapid convergence of matter below the atomic-cooling limit is a prediction of the standard cold dark-matter paradigm, and in conflict with cosmologies that suppress power below the atomic-cooling limit. Nevertheless, rapid convergence is rare, occurring in only about 0.03% of haloes (Methods) with similar masses and that exist in an large-scale overdense environment.

Gas within these growing haloes is dynamically heated as it evolves to virial equilibrium, with a heating rate that is linearly proportional to the mass growth rate of the halo. Dynamical heating is important only when gas cooling is inefficient, particularly in rapidly growing low-mass haloes. In combination with Lyman–Werner negative feedback, it can further suppress gravitational collapse. Both target haloes sustain substantial dynamical heating during their rapid growth events, driven primarily by major mergers. We find that major mergers are the dominant mechanism for preventing population III star formation in these haloes.

The simulations follow the evolution of the target haloes until they reach a density of $10^{-15} \text{ g cm}^{-3}$, at which point it is certain that a collapsed object will form (Supplementary Videos 1 and 2). Both haloes form a gravitationally unstable core, which for the MMH (LWH) has a mass of $3 \times 10^6 M_\odot$ ($2 \times 10^6 M_\odot$) and a radius of 3 pc (15 pc). The MMH grows gradually after its rapid growth event, which allows the system to form a rotationally supported disk that is cold (300 K) compared to the surrounding gas (10,000 K). The medium within the cold disk is turbulent, which causes numerous weak shocks (Fig. 3d). The disk then fragments into three clumps (Fig. 3a, b), which all of which proceed to collapse because thermal pressure and rotational forces cannot counteract the
gravitational forces of the clumps (Methods). The morphology of the LWH is completely different from that of the MMH because of a recent major merger. The collision causes a sheet-like overdensity (Fig. 3e) that cools to 300 K, becoming gravitationally unstable to fragmentation. A single clump fragments from the sheet (Fig. 3f) and undergoes catastrophic collapse. All clumps in both target haloes have masses of around 10^3 M⊙.

The radial profiles of the gas density (Fig. 4a) generally follow a power law with a slope of −2, as expected for an isothermal collapse. The density can be integrated with respect to radius to obtain a radial mass coordinate that corresponds to the gas mass enclosed within a given radius (Fig. 4b). Deviations from a power law—seen as spikes around 1 pc for the MMH and an inflection point around 1 pc for the LWH—originate from the two other clumps in the MMH and from the sheet-like structure in the LWH, respectively. The gas inside the Jeans mass (marked with squares in Fig. 4) becomes shielded from the extragalactic Lyman–Werner background, allowing the H_2 fraction to increase to 10^-3, which is sufficient to cool the gas to 300 K (Fig. 4c).

Inside a radial mass coordinate of 10^3 M⊙, adiabatic compression heats the gaseous core to 600–800 K. The key indicator for SMS formation is rapid gas inflow onto the gravitationally unstable core, not the overall Jeans mass. It has been shown that accretion rates of more than about 0.04 M⊙ yr^-1 onto a nascent, central core will result in SMS formation. The weak supermassive star formation has been shown to be caused by the collision of two progenitor haloes, where a single clump collapses after becoming self-gravitating. Within a radius of 0.1 pc in all of the clumps, adiabatic compression heats the gas.
hydrogen-ionizing luminosities of SMGs cannot reverse these strong gas flows\textsuperscript{24,25}. The respective infalling mass fluxes (Fig. 4d) at the Jeans mass at the final time are 0.17M\textsubscript{\odot}yr\textsuperscript{-1} and 2.1M\textsubscript{\odot}yr\textsuperscript{-1} for the MMH and the LWH, above the critical value for SMS formation. This ample supply of inflowing gas provides fuel for the clumps within the central unstable object. The infall rates onto the clumps (Extended Data Fig. 7a) are between 0.03M\textsubscript{\odot}yr\textsuperscript{-1} and 0.08M\textsubscript{\odot}yr\textsuperscript{-1} at the boundaries of the clumps, but increase rapidly to about 0.5M\textsubscript{\odot}yr\textsuperscript{-1} at a radial mass coordinate of 10\textsuperscript{14}M\textsubscript{\odot}. This finding suggests that after the final snapshot of our simulation the cores continue to grow rapidly for 1 Myr, similar to the typical lifetime of a SMS (Extended Data Fig. 7b). We therefore conclude that within 1 Myr the two target haloes will host SMS formation and subsequently a DCBH with an initial seed mass of at least 10\textsuperscript{6}M\textsubscript{\odot} and perhaps up to 10\textsuperscript{7}M\textsubscript{\odot}.

Using the formation requirements discussed above, we estimate (Methods) the formation rate of DCBHs per co-moving volume to be 1.1\textsuperscript{+10\textsuperscript{+1}−10\textsuperscript{−1}} Mpc\textsuperscript{−3} (68% confidence interval) for each SMS that forms through this new formation scenario in overdense regions of the Universe. Given that overdense regions make up only 0.01%–0.1% of the Universe, the global number density of DCBH formation is predicted to be 10\textsuperscript{−2}–10\textsuperscript{−6} Mpc\textsuperscript{−3} (co-moving), 100–1,000 times higher than previous estimates\textsuperscript{26}.

SMGs and therefore DCBHs that form in rapidly growing haloes, as proposed here, will be tens of kiloparsecs away from the large-scale overdensity. They will take hundreds of millions of years—a substantial fraction of the age of the Universe at z ∼ 6—to fall into the nearby group of galaxies. We predict that these DCBHs will evolve to form the population of faint quasars observed\textsuperscript{27,28} at z ∼ 6. This population will be within the reach of the James Webb Space Telescope, which will be able to provide stringent constraints on their number densities that will be directly comparable to our results.

Online content
Any methods, additional references, Nature Research reporting summaries, source data, statements of data availability and associated accession codes are available at https://doi.org/10.1038/s41586-019-0873-4.

Received: 21 February 2018; Accepted: 30 November 2018;
Published online 23 January 2019.

1. Volonteri, M. The formation and evolution of massive black holes. Science 337, 544–547 (2012).
2. Greif, T. H. The numerical frontier of the high-redshift Universe. Comput. Astrophys. Cosmol. 2, 3 (2015).
3. Omukai, K. Primordial star formation under far-ultraviolet radiation. Astrophys. J. 546, 635–651 (2001).
4. Begelman, M. C., Volonteri, M. & Rees, M. J. Formation of supermassive black holes by direct collapse in pre-galactic haloes. Mon. Not. R. Astron. Soc. 370, 289–298 (2006).
5. Hosokawa, T., Omukai, K. & Yorke, H. W. Rapidly accreting supergiant protostars: embryos of supermassive black holes? Astrophys. J. 756, 93 (2012).
6. Ardanuh, K. et al. Direct collapse to supermassive black hole seeds with radiation transfer: cosmological haloes. Mon. Not. R. Astron. Soc. 479, 2277–2293 (2018).
7. Habouzit, M., Volonteri, M., Latif, M., Dubois, Y. & Peirani, S. On the number density of direct collapse black hole seeds. Mon. Not. R. Astron. Soc. 463, 529–540 (2016).
8. Chon, S., Hosokawa, T. & Yoshida, N. Radiation hydrodynamics simulations of the formation of direct-collapse supermassive stellar systems. Mon. Not. R. Astron. Soc. 475, 4104–4121 (2018).
9. Hosokawa, T., Yorke, H. W., Inayoshi, K., Omukai, K. & Yoshida, N. Formation of primordial supermassive stars by rapid mass accretion. Astrophys. J. 770, 178 (2013).
10. Umeda, H., Hosokawa, T., Omukai, K. & Yoshida, N. The final rates of accreting supermassive stars. Astrophys. J. 830, L34 (2016).
11. O’Shea, B. W., Wise, J. H., Xu, H. & Norman, M. L. Probing the ultraviolet luminosity function of the earliest galaxies with the renaissance simulations. Astrophys. J. 807, L12 (2015).
12. Xu, H., Wise, J. H., Norman, M. L., Ahn, K. & O’Shea, B. W. Galaxy properties and UV escape fractions during the epoch of reionization: results from the Renaissance simulations. Astrophys. J. 833, 84 (2016).
13. Yoshida, N., Abel, T., Hernquist, L. & Sugiyama, N. Simulations of early structure formation: primordial gas clouds. Astrophys. J. 592, 645–663 (2003).
14. Fernandez, R., Bryan, G. L., Haiman, Z. & Li, M. H2 suppression with shocking inflows: testing a pathway for supermassive black hole formation. Mon. Not. R. Astron. Soc. 439, 3798–3807 (2014).

15. Mortlock, D. J. et al. A luminous quasar at a redshift of z = 7.085. Nature 474, 616–619 (2011).
16. Bañados, E. et al. An 800-million-solar-mass black hole in a significantly neutral Universe at a redshift of 7.5. Nature 553, 473–476 (2018).
17. Bryan, G. L. et al. ENZO: an adaptive mesh refinement code for astrophysics. Astrophys. J. Suppl. Ser. 211, 19 (2014).
18. Wise, J. H. & Abel, T. ENZO+MORAY: radiation hydrodynamics adaptive mesh refinement simulations with adaptive ray tracing. Mon. Not. R. Astron. Soc. 414, 3458–3491 (2011).
19. Shang, C., Bryan, G. L. & Haiman, Z. Supermassive black hole formation by direct collapse: keeping protogalactic gas H2 free in dark matter haloes with virial temperatures T\textsubscript{\text{vir}} ≥ 10\textsuperscript{5} K. Mon. Not. R. Astron. Soc. 402, 1249–1262 (2010).
20. Agarwal, B., Smith, B., Glover, S., Natarajan, P. & Khochfar, S. New constraints on direct collapse black hole formation in the early Universe. Mon. Not. R. Astron. Soc. 459, 4209–4217 (2016).
21. Glover, S. C. O. Simulating the formation of massive seed black holes in the early Universe – I. An improved chemical model. Mon. Not. R. Astron. Soc. 451, 2082–2096 (2015).
22. Machacek, M. E., Bryan, G. L. & Abel, T. Simulations of pre-galactic structure formation with radiative feedback. Astrophys. J. 548, 509–521 (2001).
23. Schleicher, D. R. G., Paila, F., Ferrara, A., Galli, D. & Latif, M. Massive black hole factories: supermassive and quasi-star formation in primordial halos. Astron. Astrophys. 558, A59 (2013).
24. Hosokawa, T. et al. Formation of massive primordial stars: intermittent UV feedback with episodic mass accretion. Astrophys. J. 824, 119 (2016).
25. Sakurai, Y., Hosokawa, T., Yoshida, N. & Yorke, H. W. Formation of primordial supermassive stars by burst accretion. Mon. Not. R. Astron. Soc. 452, 755–764 (2015).
26. Hirano, S., Hosokawa, T., Yoshida, N. & Kujir, S. Supersonic gas streams enhance the formation of massive black holes in the early universe. Science 357, 1375–1378 (2017).
27. Onoue, M. et al. Minor contribution of quasars to ionizing photon budget at z ∼ 6: update on quasar luminosity function at the faint end with Subaru/ Suprime-Cam. Astrophys. J. 847, L15 (2017).
28. Kim, Y. et al. The Infrared Medium-depth Survey. IV. The Low Eddington ratio of a faint quasar at z ∼ 6: not every supermassive black hole is growing fast in the early Universe. Astrophys. J. 855, 138 (2018).
29. Turk, M. J. et al. yt: a multi-code analysis toolkit for astrophysical simulation data. Astrophys. J. Suppl. Ser. 192, 9 (2011).
METHODS

Cosmological simulation of early galaxy formation. The Renaissance simulations were carried out using the open-source adaptive mesh-refinement code Enzo17—a physics-rich, highly adaptive code that has been tuned for high-redshift structureformation simulations1,2,10–32. The Renaissance simulations have been detailed previously11,12,20–32; here we summarize the simulation characteristics relevant to this study. All of the Renaissance simulations were carried out in a co-moving volume of 40 Mpc × 40 Mpc × 40 Mpc. We set the cosmological parameters using the 7-year WMAP ΛCDM model very close to the best fit: Ωm = 0.266, ΩΛ = 0.734, Ωh = 0.0449, h = 0.71, σ8 = 0.81 and n = 0.963. Here h is the Hubble parameter in units of 100 km s⁻¹ Mpc⁻¹; Ωm, ΩΛ and Ωh are the fractions of critical energy density of vacuum energy, total matter and baryons, respectively; σ8 is the root-mean-square density fluctuation inside a sphere of radius 8h Mpc; and n is the slope of the primordial scalar power spectrum. The simulations were initially run until a redshift of z = 6 at relatively coarse resolution with 512³ particles, each with a mass of 1.7 × 10¹⁰ M⊙. Three regions of interest were then selected for re-simulation with much higher refinement: a rare-peak region, a normal region and a void region. The rare-peak region has a co-moving volume of 133.6 Mpc³, whereas the normal and void regions each have co-moving volumes of 220.5 Mpc³.

In this study, we focus on the rare-peak simulation, which was selected by extracting the Lagrangian region centred on two 3 × 10¹⁰ M⊙ haloes at z = 6, the most massive at that time. The dimensions of the rare-peak region were set at 5.2 Mpc × 7.0 Mpc × 8.3 Mpc. The simulation was re-initialized using MUSIC9, with a further three nested grids centred on the rare-peak region. This led to an effective resolution of 4.096⁶ and a dark-matter particle resolution of 2.9 × 10⁶ M⊙ within the region of highest refinement. During the course of the simulation, further adaptive refinement is allowed within the refinement zone (the Lagrangian region of the rare-peak) up to a maximum level of 12, leading to a maximum spatial resolution of 19 co-moving pc (1.2 proper pc at z = 15). The simulation was halted at a final redshift z = 15 owing to the high computational expense. The mass function of the halo is well resolved down to 2 × 10¹⁰ M⊙, with 70 particles per halo11, and at the final redshift the simulations contained 822 galaxies with at least 1,000 particles (M₂₀₀, ≈ 2.9 × 10⁹ M⊙). We follow the ionization states of hydrogen and helium with a nine-species primordial non-equilibrium chemistry and cooling network, supplemented by metal-dependent cooling tables45. Dark-matter particle and halo catalogues and the associated merger trees were created with Rockstar12 and consistent-trees43, respectively.

Star formation and feedback. The Renaissance simulations include both self-consistent population III and metal-enriched star formation at the maximum refinement level. The simulation captures star formation in haloes as small as 3 × 10⁷ M⊙. Population III star formation occurs when a cell meets all of the following criteria: (1) an overdensity with respect to the mean density of the Universe of 5 × 10⁴ (about 10⁵ cm⁻³ at z = 10); (2) converging gas flow (∇ × v < 0); and (3) a gas fraction of fgasm > 5 × 10⁻³. These physical conditions are typical of collapsing metal-free molecular clouds located at redshift ≳ 10 Myr before the birth of a population III main-sequence star13. In this scenario, each star particle within the simulation represents a single star. Population III star formation occurs if the metallicity is less than 10⁻⁴ of the solar fraction in the highest-density cell, with metal-enriched star formation proceeding otherwise. Population III star formation further requires that n_H2 > 5 × 10³ cm⁻³. This takes into account the fact that star formation should not proceed in the presence of a strong Lyman–Werner (LW) radiation field. The functional form of the initial mass function (IMF) and supernovae feedback are calibrated44 against high-resolution population III star-formation simulations, stellar evolution models, and observations and models of star formation in local molecular clouds. Stellar feedback uses the Moray radiative transport framework45 for ionizing photons. LW radiation that dissociates H₂ is modeled using an optically thin, inverse-square profile, centred on all star particles. We do not include any H₂ self-shielding, which is important only at high densities. In particular, DCBH host halo candidates shield themselves from the background only at scales46 below 3 pc, which is close to our resolution limit. A LW background radiation field is also included to model radiation from stars outside the simulation volume47 that is added to the spatially varying LW radiation field created by stars inside the volume. In the high-density region of the rare-peak simulation, the LW radiation from stars dominates the background. Although we cannot follow population III star formation in haloes below 3 × 10⁵ M⊙, it is suppressed by the LW background in such haloes46,47. Baryonic streaming velocities in certain regions46,49. Therefore, we are confident that our simulation follows the complete star formation history of all collapsed structure, and thus the metal-enrichment history of pre-galactic gas that is vital to determining the conditions for DCBH formation.

Direct Jeans mass scales. The star formation and feedback models do not include a DCBH formation model but consider the appropriate astrophysical processes to ascertain the chemical and thermal state of all collapsed objects resolved by the simulation, essential for searching for candidate DCBH formation sites. Also critical to any DCBH formation scenario is the inclusion of population III star formation and its supernova feedback that generally enriches typical pre-galactic material with heavy elements. The emergence of a DCBH/SMS environment is therefore a robust prediction of the Renaissance simulations. The dark-matter resolution in the original Renaissance simulations is not sufficient to follow the detailed collapse of these objects48; however, the re-simulations (see next section) of the target haloes have an ultimate mass and spatial resolution of 10³⁵ M⊙ and 60 au; allowing us to accurately follow the dynamics of the collapsing halo and determine whether its gas infall rate is large enough to support SMS and thus DCBH formation.

High-resolution simulations of target haloes. After identifying the candidate haloes in the Renaissance simulations, we re-simulate the two target haloes at higher mass and spatial resolution, starting at z = 20. We first identify the dark-matter particles within three virial radii of the target haloes at the final redshift, z = 15. Using their unique particle identifiers, we determine their positions at z = 20 and split their mass equally into 13 particles. Twelve of the child particles are placed at the 12 vertices of a hexagonal close-packed array, and the remaining particle is placed at the original particle position. We recursively split the particles twice, decreasing the dark-matter particle mass by a factor of 13² to 10³⁵ M⊙ in the Lagrangian region of the target haloes. This method of particle splitting is widely used in high-resolution cosmological simulations49,51–53; however, it may induce artificial smoothing of the density field43 and does not add additional small-scale power to the matter distribution.

The Renaissance simulations show that the target haloes remain metal-free and are not exposed to any ionizing radiation. Their thermodynamic evolution and collapse are therefore primarily controlled by the growth history of the halo and the impinging LW flux. With these priors, we can safely neglect star formation and feedback, focusing on the dynamics of collapse. We impose a uniform LW radiation background that is time-dependent and is taken from the flux measured at the centre of the most massive progenitor halo in the original simulation (see Fig. 2b). Spatial deviations from this value are less than a few per cent within the Lagrangian region and do not affect the thermodynamics of the gas.

In addition to the increased mass resolution, we increase the spatial resolution by resolving the local Jeans length by at least 16 cells, whereas the original simulation did not have enough mass resolution to enforce such a refinement criterion. We use this initial re-simulation to identify the time of collapse. We then restart the simulations a free-fall time (approximately 20 Myr) before the collapse time, further increasing the spatial resolution so that the Jeans length is resolved by at least 64 cells. Computational limitations restrict us from running at such high resolution for the entirety of the re-simulation; therefore, we increase the resolution only during the final stages of the collapse. We also include H₂ self-shielding of the LW radiation field during this final re-simulation38 and compute the primordial cooling rates with the software library Grackle50. We enforce a maximum refinement level of 24, corresponding to a co-moving (physical at z = 15) resolution of 960 au (60 au). We stop the re-simulations once they reach this maximum refinement level. We smooth the dark-matter density field at scales below 9.5 co-moving pc (0.6 physical pc at z = 15; refinement level 13). At these scales, the gas density dominates the matter density, and by smoothing the dark-matter density we remove any artefacts associated with the discrete representation of the dark-matter mass distribution51.

Dynamical heating. For a halo to potentially host a SMS or DCBH, it must grow to the atomic-cooling limit without forming stars or being chemically enriched; any efficient cooling must therefore be suppressed. LW radiation can suppress H₂ formation and dynamical heating can counteract any H₂ cooling in low-mass haloes. The dynamical heating rate13 is

\[ \dot{I}_{\gamma} = \gamma M_{\text{halo}} \frac{dM_{\text{halo}}}{dt} \frac{\Delta M_{\text{halo}}}{\gamma - 1} \]

where \( \alpha \) is a coefficient37 relating the virial mass and temperature of the halo \( \gamma_{\text{halo}} = \alpha M_{\text{halo}} \cdot M_{\text{halo}} \) is the total halo mass, \( k \) is the Boltzmann constant and \( T_{\gamma} \approx 5 \) is the adiabatic index. This process is relevant only when the radiative cooling rates \( \dot{I}_{\gamma} \) for hydrogen atom have similar values. Below the atomic-cooling limit, chemically primordial haloes rely on the inefficient coolant H₂ to collapse and form stars. Radiative cooling will thus be suppressed when \( \dot{I}_{\gamma} > n_{\Lambda} \), where \( n_{\Lambda} \) is the hydrogen number density. This inequality sets a critical halo growth rate13

\[ \left( \frac{dM_{\text{halo}}}{dt} \right)_{\text{crit}} = \frac{2\alpha}{3} \frac{\gamma - 1}{n_{\Lambda}} \frac{M_{\text{halo}}}{\Delta M_{\text{halo}}} \]
shown as the dashed vertical line for $f_{\text{H}_2} = 1/\zeta$, the intensity at both target haloes when they have such a mass. Atomic-hydrogen cooling becomes dominant over molecular cooling at $T \approx 7,000\, K$ (corresponding to a halo mass of $6 \times 10^9\, M_\odot$ at $z = 15$; indicated by the sharp rise in the critical curves), above which dynamical heating becomes unimportant in the target haloes. In any chemically pristine halo unaffected by ionization, gravitational collapse ensues above this mass within a free-fall timescale. Models of SMS formation require infall rates above about $0.04\, M_\odot\, \text{yr}^{-1}$ that are driven only by deep gravitational potentials of atomic-cooling haloes, the mass of which are shown as the dotted vertical line at $2.2 \times 10^7\, M_\odot / (1 + z/16)^{3/2}$.

The MMH and LWH both assemble rapidly as they virialize, initially growing at a rate per unit redshift of $-dM/dz = (1-3) \times 10^9\, M_\odot$ when they have a mass $M \leq 10^9\, M_\odot$. Although $H_2$ formation is photo-suppressed at these low masses, dynamical heating is present in these early rapid periods of growth and have lasting effects on the halo gas. The infalling gas shocks near the halo centre, heating the halo to the virial temperature. Only after a sound-crossing time does the halo come into virial equilibrium. This takes $30\, \text{Myr}$ for a $3 \times 10^8\, M_\odot$ halo (150 pc radius) and a sound speed of $10\, \text{km}\, \text{s}^{-1}$.

As the haloes equilibrate they continue to grow, at a reduced rate but still above the critical $f_{\text{H}_2} = 10^{-6}$ curve until a mass of $6 \times 10^9\, M_\odot$. The MMH accretes at a nearly constant rate per unit redshift of $3 \times 10^9\, M_\odot$, with a peak rate at recent unit redshift of $7 \times 10^9\, M_\odot$. The growth rate per unit redshift of the LWH fluctuates between $10^7\, M_\odot$ and $10^9\, M_\odot$. When atomic cooling becomes efficient, catastrophic collapse occurs within a free-fall timescale $t_{\text{ff}} = 3\sqrt{3\pi}/32G\rho$ (where $G$ is the gravitational constant) that is equal to $20\, \text{Myr}$ for a density of $\rho = 10^{-23}\, \text{g}\, \text{cm}^{-3}$, typical of haloes that are compressed adiabatically.

As shown in Fig. 2, the MMH undergoes one rapid growth event, starting at $2 \times 10^9\, M_\odot$ to $2 \times 21$ as it virializes and occurring before $H_2$ cooling becomes efficient (and hence before the local LW flux becomes important). The rapid infall creates a shock near its centre, heating the halo gas over a sound-crossing time of $30\, \text{Myr}$. The halo gas stabilizes after this event and then collapses on a free-fall timescale of $t_{\text{ff}} \approx 20\, \text{Myr}$, when $\rho \approx 10^{-23}\, \text{g}\, \text{cm}^{-3}$ is the maximum gas density before collapse. After the rapid growth halts, the halo must grow to the atomic-cooling limit within $50\, \text{Myr}$, the sum of the sound-crossing and free-fall times. Otherwise, it will collapse when atomic cooling is not efficient, and it will cool through $H_2$ and fragment into more typical population III star formation. It collapses at a reduced rate when the mass is just above the atomic-cooling limit. There are 75 Myr between these two redshifts, leaving $25\, \text{Myr}$ for early rapid growth. Given that halo masses increase exponentially, $dM/dz \propto M(z) \propto e^{\alpha z}$, we can estimate a critical growth rate in those first $25\, \text{Myr}$ (left thick grey line in Extended Data Fig. 1) using the mass difference between $z = 21$ and $z = 19.21$ (25 Myr), when it grows to $3 \times 10^9\, M_\odot$. The LWL experiences two rapid growth episodes, the first of which is similar to that of the MMH. Afterwards, its mass hovers just above the critical value $M_{\text{crit}}$ for efficient $H_2$ cooling. The later growth spur occurs just before it starts to cool atomically, as seen by the increase in $-dM/dz$ to greater than $3 \times 10^9\, M_\odot$. The associated dynamical heating delays the collapse of the LWL until its mass is $5.8 \times 10^8\, M_\odot$, twice the atomic-cooling limit.

In general, for dynamical heating to suppress metal-free star formation, halo growth must be rapid from the $H_2$-cooling limit to the atomic-cooling limit. More specifically, it must happen faster than a free-fall time (20 Myr). This sets another, more general, critical growth rate between these two halo mass regions, using the same approach as before. This rate is shown as the thick grey line in Extended Data Fig. 1 between the green $f_{\text{H}_2} = 10^{-6}$ critical curve and the atomic-cooling limit.

Any halo that grows faster than this rate will have its gravitational potential deepen faster than it can collapse, making it more likely to support strong radial inflows, conducive for SMS formation. The MMH, the core of the halo first becomes unstable with an enclosed mass approximately $3 \times 10^6\, M_\odot$. (orange circle). As the halo grows in mass, the region grows to almost $10^9\, M_\odot$ by the end of the simulation, which is gravitationally unstable and in principal also subject to fragmentation. The LWL first crosses into a region of instability with an enclosed mass of greater than $10^9\, M_\odot$, and by the end of the simulation the central region of almost $10^9\, M_\odot$ has become unstable to gravitational collapse.

**Support within the collapsing core.** As the core regions of both haloes start to undergo gravitational collapse, as outlined above, thermal, turbulent and rotational support will act to counteract the gravitational collapse. If there is sufficient gas support, the gravitational collapse can be suppressed even though the Jeans mass has been exceeded. Extended Data Fig. 3 shows the thermal and turbulent sound speeds as functions of enclosed mass. The thermal sound speed $c_s$ is calculated as

$$c_s = \sqrt{\frac{\kappa G T}{\mu m_H}}$$

where $\gamma$ is the adiabatic index, $k_B$ is the Boltzmann constant, $T$ is the temperature, $\mu$ is the mean molecular weight and $m_H$ is the hydrogen mass. In calculating the total pressure support of the gas, the impact of the turbulent velocity field must also be considered. We calculate the root-mean-square turbulent velocities of the gas by subtracting the bulk gas velocity from the velocity field. We compute the bulk velocity as the velocity of the native computational cells averaged over a spherical $32^3$ grid that has cell widths much coarser than the simulation data. This grid has an outer radius equal to the virial radius, equally spaced angular bins and equally logarithmically spaced radial bins. We then approximate the bulk velocity of each native cell with the value of the spherical grid cell that contains the native cell centre.

The turbulent and thermal components act together to support the gas against collapse and create an effective sound speed, $c_{\text{eff}} = c_s + v_{\text{rms}}$. In Extended Data Fig. 3, we see that the infall speed always exceeds the effective sound speed at some enclosed mass, indicating that, at this scale, the thermal and turbulent support cannot suppress the gas against gravitational collapse. For the MMH, the infall speed exceeds the effective sound speed at approximately $10^9\, M_\odot$. This is similar to the scale at which the gas also becomes Jeans-unstable, and so we define the radius of the collapsing core to be equal to this scale. For the LWL, the gas provides no thermal or turbulent support, and the gas is free to collapse on approximately the free-fall timescale.

Interestingly, in both cases, the radial inflow becomes transonic at scales between $10^8\, M_\odot$ and $10^9\, M_\odot$. This indicates that at mass scales greater than approximately $10^9\, M_\odot$ any fragments are thermally and/or turbulenty supported, and we do not expect fragmentation of the gas cloud below this scale. Any protostars forming within these clouds would have most of the gas contained in the fragment available for accretion. We examine more closely the possible fragmentation of the outer core into gas clouds in the next section.

Extended Data Fig. 4 shows the rotational support provided by the gas against gravitational collapse. The rotational velocity of the gas is calculated as $j/\mu\alpha$, the ratio of the specific angular momentum $j$ of the gas and the largest eigenvalue $\alpha$ of the inertia tensor, corresponding to the largest axis of the system. The centre of these profiles are taken to be the maximum gas density, consistent with the rest of our analysis. We compare this rotational velocity against the Keplerian velocity $v_{\text{Kep}} = \sqrt{GM/r}$. The regions where the rotational velocity exceeds the Keplerian velocity are shaded and indicate regions of rotational support. The rotationally supported region in the MMH extends from $2 \times 10^9\, M_\odot$ to $3.3 \times 10^9\, M_\odot$. For the LWL, the region of rotational support is much smaller, spanning only from $7 \times 10^8\, M_\odot$ to $6 \times 10^9\, M_\odot$. The rotational velocities within $100\, M_\odot$ are not well defined because the separation between the densest gas parcel and the rotation centre becomes comparable to the radius ($0.02\, \text{pc}$) enclosing $100\, M_\odot$. We therefore do not consider them to be rotationally supported from this analysis. The (disk-like) regions of rotational support are nonetheless unstable to fragmentation, and fragmentation of the disk does occur in the MMH.

**Fragmentation of the collapsing core into gas clouds.** As the cloud collapses, cooling instabilities can cause the gas to fragment into self-gravitating clumps. Such fragmentation can be stabilized by thermal pressure or centrifugal forces that can be quantified by the Toomre parameter:

$$Q = \frac{c_s}{\pi G \Sigma}$$

The system is stable if $Q > 1$. Here $\Sigma$ is the gas surface density, and the epicyclic frequency $\kappa$ is calculated directly from the data as

$$\kappa^2 = \frac{2\Omega^2(r + d_2)}{r}$$

where $\Omega = v_{\text{circ}}/r$ is the angular velocity and $r$ is the radius in cylindrical coordinates, with the $z$ axis aligned with the total angular momentum vector of the Jeans-unstable
gas cloud. These expressions assume an axisymmetric object. However, the collapsed objects in both haloes have non-ideal geometries. It is therefore beneficial to consider a local measure of stability\(^{20}\).

\[ Q_{\text{local}} \approx \frac{\Omega^2}{\pi G \rho} \]  

(2)

that can identify unstable regions with arbitrary geometries. Extended Data Fig. 5 shows \(Q_{\text{local}}\) for both haloes in fields of view of 20 pc and 4 pc. In the MMH, the disk-like object is marginally stable in the spiral overdensities (Extended Data Fig. 5a). Within these arms, there are three clumps that have fragmented (Extended Data Fig. 5b) and started to collapse. In the LWH, the overdense sheet-like object, which is induced by a major merger, is unstable to fragmentation in many regions and marginally stable in the remainder of the object. However, their collapse times are spread out, resulting in only one (the first) clump to fragment out of the overdense sheet by the end of the simulation.

Extended Data Fig. 6a shows \(Q\) as a function of \(r\), where we have aligned the cylindrical \(z\) axis with the total angular momentum vector of the inner 10 pc. We compare \(Q\) with the effective \(Q\) \(Q_{\text{eff}}\), where we substitute \(c_{\text{crit}}\) by \(c_{\text{crit}}\) to include any turbulent-pressure support in the stability analysis. When considering only rotational support as a counterbalance to gravitational collapse, the MMH and LWH are unstable \((Q < 1)\) within a radius of 3 pc and 8 pc, respectively. As we have shown, turbulent pressures are comparable to thermal pressures, and this additional support stabilizes the rotating system against fragmentation \((Q > 1)\) outside 0.8 pc and 1 pc in the MMH and LWH, respectively. The LWH is also susceptible to fragmentation at radii of 0.8 pc and 2 pc, where \(Q_{\text{eff}}\) becomes slightly less than unity.

From the dispersion relation

\[ w^2 = \kappa^2 + k^2 v_{\text{tot}}^2 - 2\pi G \rho \Sigma \]

that is used to calculate the growth perturbations in a gaseous disk, the associated maximum growth rate\(^{21}\) of a perturbation, which occurs at \(K = Q_{\text{eff}}\), is

\[ \left| w_{\text{max}} \right| = \frac{\kappa (1 + Q_{\text{eff}})^{1/2}}{Q_{\text{eff}}} \]

Here \(k\) is the wavenumber and \(w\) is the growth rate. We define the growth time \(t_{\text{grow}} = 1/w_{\text{max}}\), where \(Q < 1\) (Extended Data Fig. 6b). For such a perturbation to form before the system collapses, the growth time must be smaller than a free-fall time (Extended Data Fig. 6c), \(t_{\text{grow}}/t_{\text{ff}} < 1\). For the MMH, this condition is valid for radii less than 0.03 pc, corresponding to 100\(M_{\odot}\) of enclosed gas mass. Between this radius and 1 pc, the system is unstable to fragmentation, but it is collapsing faster than it can fragment. This analysis is centred on the densest point, contained in one of the clumps. This indicates that any fragmentation at small scales will be surrounded by a monolithic rapid collapse, most probably suppressing further fragmentation as this matter falls inward. The two other clumps in the MMH form about 1 pc away. Because we compute these quantities within cylindrical shells, the clumps with small \(Q_{\text{local}}\) (see Extended Data Fig. 5) are averaged out. Once they fragment, they begin to gravitationally collapse. In the LWH, fragmentation as this matter falls inward. The two other clumps in the MMH form in one of the clumps. This indicates that any fragmentation at small scales will be suppressed as the system is closer to the rotation centre.

\[ \dot{m}_{\text{infall}} = \frac{\kappa (1 + Q_{\text{eff}})^{1/2}}{Q_{\text{eff}}} \]

Lastly, there is a peculiar case when the SMS has a mass of around 5.5

\[ \text{M}_{\odot} \], the timescale for each clump is approximately 10 kyr. The Kelvin–Helmholtz timescale for massive stars (up to about 100\(M_{\odot}\)) is less than 100 kyr. The stars that form within these gas clouds will therefore reach the main sequence while still accreting, as is the case for SMS formation. Given the timescales shown here, the infall rates suggest that the (super)massive protostars will reach masses of at least 100\(M_{\odot}\) before reaching the main sequence\(^{24}\). If the accretion onto the central protostar is fast enough, full gravitational contraction will be avoided (so-called ‘hot accretion’ flows) and the stellar envelope will remain bloated, leading to SMS formation in this context\(^{3,5,8-6,6}\). After its formation, SMS lifetimes are around 1 Myr, suggesting that the whole gas cloud could be accreted before the star exhausts its hydrogen supply. SMSs with accretion rates below 0.1\(M_{\odot}\) yr\(^{-1}\) experience a general relativistic instability, creating a massive black hole with a mass similar to that of its progenitor, when its nuclear fuel is exhausted. For higher accretion rates, the collapse occurs when the star is still burning hydrogen or helium\(^{25}\), producing black holes with masses between 2 \(\times 10^5\) \(M_{\odot}\) and 8 \(\times 10^5\) \(M_{\odot}\). Lastly, there is a peculiar case when the SMS has a mass of around 5.5 \(\times 10^4\) \(M_{\odot}\) that produces an extremely energetic supernova\(^{26}\).

In Extended Data Fig. 8, we plot the fractional support against collapse, similarly to Extended Data Fig. 3. We do this by again comparing the thermal, turbulent and infall velocities of the clumps. Extended Data Fig. 8a shows the velocities of the clump found for the LWH. Extended Data Fig. 8b–d shows the clump velocities of each of the three clumps found for the MMH. We find that in all cases the clumps are thermally supported and stable against further gravitational collapse. The radial inflows are subsonic for all four clumps, although the clump in the LWH contains transonic flows between 100\(M_{\odot}\) and 1,000\(M_{\odot}\). The thermal-pressure support is strongly dominant over the turbulent-pressure support in all four clumps. This is in contrast to the Jeans-unstable parent cloud, where the turbulent pressures are dominant.

\[ \dot{m}_{\text{infall}} = \frac{\kappa (1 + Q_{\text{eff}})^{1/2}}{Q_{\text{eff}}} \]

Estimating the number density of SMS/DCBH formation sites. We estimate the co-moving number density \(n_{\text{DCBH}}\) of DCBH formation sites as\(^{27}\)

\[ n_{\text{DCBH}} = \frac{n_{\text{AACH}}}{f_{\text{rapid}} f_{\text{cool}}} \]

Here, \(n_{\text{AACH}} = 5.0 \pm 0.19\) per co-moving \(\text{Mpc}^3\) is the co-moving number density of atomic-cooling haloes at redshift \(z = 15\) (haloes above the mass threshold where cooling via atomic hydrogen is effective), \(f_{\text{cool}} = 0.015 \pm 0.0045\) is the fraction of those haloes that are of primordial composition, \(f_{\text{rapid}} = 0.1 \pm 0.05\) is the fraction of the atomic-cooling haloes that are in regions where \(f_{\text{infall}} \geq 3 f_{\text{cool}}\) (the fraction of the simulation volume above that flux threshold), and \(f_{\text{rapid}} = 0.20 \pm 0.14\) is the fraction of the primordial atomic-cooling haloes that are
growing above the critical threshold where accretion heating is greater than cooling. On the basis of the quantities found in the rare-region of our simulation, we estimated these values and their variance, which are given in the main article. We then perform a Monte Carlo sampling of the parameter space. Extended Data Fig. 9 shows the cumulative probability of the expected DCBH number density in different large-scale environments. They steeply decrease above 10−5, 10−6 and 10−7 DCBHs per co-moving Mpc3 in the rare-peak, normal and void regions of the Renaissance simulations, respectively. The rare-peak has a median value of n_{DCBH} = 1.1 \times 10^{-3} h\text{halos per co-moving Mpc}^3, a 68% confidence interval of 1.9 \times 10^{-4}–2.8 \times 10^{-3} h\text{halos per co-moving Mpc}^3 and a 95% confidence interval of 0–5.2 \times 10^{-3} h\text{halos per co-moving Mpc}^3.

When the same quantities are extracted from the normal and void simulation regions at z = 15, the median number density of DCBH haloes is expected to be about 10^{-3} h\text{halos per co-moving Mpc}^3 and 0 haloes per co-moving Mpc3, respectively, owing to the lack of atomic-cooling haloes of primordial composition and to a lack of atomic-cooling haloes that grow rapidly. The rare-peak region has a volume of 133.6 co-moving Mpc3 (equivalent to a sphere of approximately 2.25/h co-moving Mpc in radius) and an average density of 1.65 times the cosmic mean. At z = 15, regions of that size and overdensity are expected to be formed in approximately 0.01%–0.1% of the volume of the Universe, implying that a more realistic estimate of the global number density of DCBH candidates forming through this mechanism is in the range 10^{-2}–10^{-3} h\text{halos per co-moving Mpc}^3, consistent with our estimate in the normal region. This estimate is nonetheless approximately 100–1000 times greater than the observed z ≈ 6 quasar number density27. Our results suggest that faint quasars at these high redshifts should be strongly clustered and associated with large overdensities, providing an observational test of our proposed seeding mechanism. Furthermore, we find that DCBHs forming in this scenario have the same number density as the observed number density63,70 of present-day supermassive black holes above 10^6 M\odot. This abundance matching suggests that such central black holes in most elliptical galaxies have a common origin, beginning their lives as SMSs.

The strength of rapidly growing atomic-cooling haloes. We compute an additional check on the fraction of rapidly growing haloes with the semi-analytic galaxy-formation code Galaxia13. Most of the rare-peak region collapses into a halo with a mass of 8.5 × 10^{11} M\odot at z = 5. We calculate 50 merger trees of equivalent z = 5 haloes that follow progenitor haloes as small as 3 × 10^10 M\odot. Each merger tree has approximately 4 × 10^4 progenitor haloes at z = 15, totalling 2 × 10^5 progenitors in all of the calculated merger trees at this epoch. We find that 0.03% of haloes around the atomic-cooling threshold, M_{\text{coo}}> = (3–6) \times 10^9 M\odot, grow more than a factor of six between z = 16 and z = 15 (about 20 Myr). Using the halo descendant at a much later time, we can incorporate the effects of being in an overdense environment that lead to higher halo mass growth rates. This leads to a more accurate estimate when compared to randomly sampling atomic-cooling haloes at z = 15. These merger trees of which would be unlikely to be representative of our target haloes.

The metal-free haloes found in the Renaissance simulations. We searched and reported on the final output at z = 15 of the rare-peak region in the Renaissance simulation that satisfies the following criteria: (1) an atomic-cooling halo (M_{\text{coo}}> = 4.9 \times 10^9 M\odot at z = 15); (2) contains only high-resolution dark-matter particles; (3) does not support metal or dust radiative cooling (Z < 10^{-2}); and (4) has no prior star formation. We consider the last criterion because some population III stars collapse directly into a stellar-mass black hole, producing no metals; however, because we randomly sample from an IMF, it is just as likely that the same population III star particle in question could have chemically enriched its host halo. Of 670 atomic-cooling haloes, ten fit these conditions (Extended Data Table 1). We also searched the normal and void regions and found no haloes matching the same criteria at z = 15. This suggests that SMS formation through this channel is much more likely in overdense regions of the early Universe. This crowded high-redshift environment lends itself to a high LW radiation field from more nearby galaxies and haloes with very high growth rates, existing in a medium with a higher average mass density. This null detection agrees with our statistical expectations. We note that the accretion rates given here are for a single snapshot, and the average accretion rate will vary as haloes undergo quiescent and intensive periods of cosmological accretion.

Data availability. The numerical experiments presented here were run with a hybrid OpenMP+MPI fork of the Enzo code, which is available from https://bitbucket.org/jwise77/ openmp, using the changeset bcb436949d16. The data are publicly available from the Renaissance Simulation Laboratory at http://girder.rensimlab.xyz.

30. Abel, T., Bryan, G. L. & Norman, M. L. The formation of the first star in the universe. Science 295, 93–98 (2002).
31. O’Shea, B. W. & Norman, M. L. Population III star formation in a JCDM universe. I. The effects of atomic cooling and heavy element environment on protostellar accretion rate. Astrophys. J. 654, 66–92 (2007).
32. Turk, M. J., Abel, T. & O’Shea, B. The formation of population III binaries from cosmological initial conditions. Science 325, 601–605 (2009).
33. Xu, H., Wise, J. H. & Norman, M. L. Star formation on the high-mass end of the hierarchy. ApJ 737, 110 (2014).
34. Xu, H., Ahn, K., Wise, J. H., Norman, M. L. & O’Shea, B. W. Heating the intergalactic medium by X-rays from population III binaries in high-redshift galaxies. ApJ 773, 83 (2013).
35. Chen, P., Wise, J. H., Norman, M. L., Xu, H. & O’Shea, B. W. Scaling relations for galaxies prior to reionization. Astrophys. J. 795, 144 (2014).
36. Ahn, K., Xu, H., Norman, M. L., Alvarez, M. A. & Wise, J. H. Spatially extended 21 cm signal from strongly clustered UV and X-ray sources in the early Universe. Astrophys. J. 802, 8 (2015).
37. Xu, H., Norman, M. L., O’Shea, B. W. & Wise, J. H. Late pop III star formation during the epoch of reionization: results from the Renaissance simulations. ApJ 763, 140 (2016).
38. Komatsu, E. et al. Seven-year Wilkinson Microwave Anisotropy Probe (WMAP) observations: cosmological interpretation. Astrophys. J. Suppl. Ser. 192, 18 (2011).
39. O’Shea, B. W. & Abel, T. Multi-scale initial conditions for cosmological simulations. Mon. Not. R. Astron. Soc. 415, 2101–2121 (2011).
40. Abel, T., Anninos, P., Zhang, Y. & Norman, M. L. Modeling primordial gas in numerical cosmology. New Astron. 2, 181–207 (1997).
41. Springel, V., Turk, M. J., Sijacki, D., Mihos, J. C., Dekel, A. & White, S. D. G. Simulations of the formation of high-redshift galaxies. Astrophys. J. 691, 441–451 (2009).
42. Behroozi, P. S., Wechsler, R. H. & Wu, H.-Y. The ROCKSTAR phase-space temporal halo finder and the velocity offsets of cluster cores. Astrophys. J. 769, 102 (2013).
43. Behroozi, P. S. et al. Gravitationally consistent halo catalogs and merger trees for precision cosmology. Astrophys. J. 763, 18 (2013).
44. Wise, J. H., Turk, M. J., Norman, M. L. & Abel, T. The birth of a galaxy: primordial metal enrichment and stellar populations. Astrophys. J. 745, 50 (2012).
45. Regan, J. A., Johansson, P. H. & Wise, J. H. Forming super-massive black hole seeds under the influence of a nearby anisotropic multi-frequency source. Mon. Not. R. Astron. Soc. 459, 3377–3394 (2016).
46. Wise, J. H. & Abel, T. Suppression of H2 cooling in the ultraviolet background. Astrophys. J. 671, 1559–1567 (2007).
47. O’Shea, B. W. & Norman, M. L. Population III star formation in a ΛCDM universe. II. Effects of a photodissociating background. Astrophys. J. 673, 14–33 (2008).
48. Naoz, S., Yoshida, N. & Gnedin, N. Y. Simulations of early baryonic structure formation with stream velocity. II. The gas fraction. Astrophys. J. 763, 27 (2013).
49. Regan, J. A., Johansson, P. H. & Wise, J. H. The effect of dark matter resolution on the collapse of baryons in high-redshift numerical simulations. Mon. Not. R. Astron. Soc. 449, 3766–3783 (2015).
50. Kitsionas, S. & Whitworth, A. P. Smoothed particle hydrodynamics with particle splitting, applied to self-gravitating collapse. Mon. Not. R. Astron. Soc. 330, 129–136 (2002).
51. Greif, V. & Loeb, A. Formation of the first supermassive black holes. Astrophys. J. 596, 34–46 (2003).
52. Dotti, M., Colpi, M., Haardt, F. & Mayer, L. Supermassive black hole binaries in gaseous and stellar circumnuclear discs: orbital dynamics and gas accretion. Mon. Not. R. Astron. Soc. 379, 956–962 (2007).
53. Hirano, S. et al. One hundred first stars: protostellar evolution and the final masses. Astrophys. J. 781, 60 (2014).
54. Chiaki, G. & Yoshida, N. Particle splitting in smoothed particle hydrodynamics based on Voronoi diagram. *Mon. Not. R. Astron. Soc.* **451**, 3955–3963 (2015).
55. Wolcott-Green, J., Haiman, Z. & Bryan, G. L. Photodissociation of $\text{H}_2$ in protogalaxies: modelling self-shielding in three-dimensional simulations. *Mon. Not. R. Astron. Soc.* **418**, 838–852 (2011).
56. Smith, B. D. et al. GRACKLE: a chemistry and cooling library for astrophysics. *Mon. Not. R. Astron. Soc.* **466**, 2217–2234 (2017).
57. Barkana, R. & Loeb, A. In the beginning: the first sources of light and the reionization of the Universe. *Phys. Rep.* **349**, 125–238 (2001).
58. Wise, J. H. & Abel, T. Resolving the formation of protogalaxies. I. Virialization. *Astrophys. J.* **665**, 899–910 (2007).
59. Wechsler, R. H., Bullock, J. S., Primack, J. R., Kravtsov, A. V. & Dekel, A. Concentrations of dark halos from their assembly histories. *Astrophys. J.* **568**, 52–70 (2002).
60. Regan, J. A. & Haehnelt, M. G. The formation of compact massive self-gravitating discs in metal-free haloes with virial temperatures of 13000-30000K. *Mon. Not. R. Astron. Soc.* **393**, 858–871 (2009).
61. Wang, B. & Silk, J. Gravitational instability and disk star formation. *Astrophys. J.* **427**, 759–769 (1994).
62. Hartwig, T., Agarwal, B. & Regan, J. A. Gravitational wave signals from the first massive black hole seeds. *Mon. Not. R. Astron. Soc.* **479**, L23–L27 (2018).
63. Shu, F. H. Self-similar collapse of isothermal spheres and star formation. *Astrophys. J.* **214**, 488–497 (1977).
64. Bonnell, I. A., Bate, M. R. & Zinnecker, H. On the formation of massive stars. *Mon. Not. R. Astron. Soc.* **298**, 93–102 (1998).
65. Hosokawa, T., Yorke, H. W. & Omukai, K. Evolution of massive protostars via disk accretion. *Astrophys. J.* **721**, 478–492 (2010).
66. Woods, T. E., Heger, A., Whalen, D. J., Haemmerlé, L. & Klessen, R. S. On the maximum mass of accreting primordial supermassive stars. *Astrophys. J.* **842**, L6 (2017).
67. Chen, K.-J., Heger, A., Woosley, S., Almgren, A. & Whalen, D. J. Pair instability supernovae of very massive population III stars. *Astrophys. J.* **792**, 44 (2014).
68. Ota, K. et al. Large-scale environment of a $z = 6.61$ luminous quasar probed by Ly$\alpha$ emitters and Lyman break galaxies. *Astrophys. J.* **856**, 109 (2018).
69. Shankar, F. The demography of supermassive black holes: growing monsters at the heart of galaxies. *New Astron. Rev.* **53**, 57–77 (2009).
70. Terrazas, B. A. et al. Quiescence correlates strongly with directly measured black hole mass in central galaxies. *Astrophys. J.* **830**, L12 (2016).
71. Benson, A. J. GALACTICUS; a semi-analytic model of galaxy formation. *New Astron.* **17**, 175–197 (2012).
72. Heger, A., Fryer, C. L., Woosley, S. E., Langer, N. & Hartmann, D. H. How massive single stars end their life. *Astrophys. J.* **591**, 289–300 (2003).
73. Chatzopoulos, E. & Wheeler, J. C. Effects of rotation on the minimum mass of primordial progenitors of pair-instability supernovae. *Astrophys. J.* **748**, 42 (2012).
74. Visbal, E., Haiman, Z. & Bryan, G. L. A no-go theorem for direct collapse black holes without a strong ultraviolet background. *Mon. Not. R. Astron. Soc.* **442**, L100–L104 (2014).
Extended Data Fig. 1 | Simulated and critical halo mass growth rates for SMS formation. A halo conducive for SMS formation must grow to the atomic-cooling limit ($2.2 \times 10^7 M_\odot$ at $z = 15$; orange dotted line) without hosting star formation or being chemically enriched from nearby galaxies. Haloes with masses below minimum mass $M_{\text{min,LW}}$ (dashed green line) are suppressed by an external LW radiation field. Above this mass, haloes with sufficient dynamical heating to suppress radiative cooling grow above a critical rate (equation (1)), shown for H$_2$ number fractions $f_{\text{H}_2}$ of $10^{-4}$ (blue solid line), $10^{-5}$ (orange solid line) and $10^{-6}$ (green solid line). The simulated growth rates of the MMH (circles) and LWH (triangles) are above the $10^{-6}$ rate once the halo masses pass $M_{\text{min,LW}}$. Above a halo mass of $8 \times 10^6 M_\odot$ (a virial temperature of 8,000 K at $z = 15$), dynamical heating will not suppress cooling because the atomic-radiative cooling rates are several orders of magnitude higher than the molecular ones. Both haloes grow rapidly to $M_{\text{min,LW}}$, causing dynamical heating and preventing collapse for a sound-crossing time. The LWH grows from $8 \times 10^6 M_\odot$ to the atomic-cooling limit within a dynamical time of the central core. Both conditions set a critical growth rate (thick solid grey lines). All other atomic-cooling haloes (grey points) have similar growth rates between halo masses of $M_{\text{min,LW}}$ and $8 \times 10^6 M_\odot$ but far short of the critical growth rate. Nearly all of these haloes cool and form stars before reaching the atomic-cooling limit.
Extended Data Fig. 2 | Gravitational instability of the growing core. The ratio of the enclosed gas mass $M_{\text{enc}}$ and the Jeans mass $M_{\text{Jeans}}$ as a function of enclosed gas mass is shown for the MMH (solid lines) and the LWH (dashed lines) when each halo first becomes gravitationally unstable (thick black lines), that is, when $M_{\text{enc}}/M_{\text{Jeans}} \geq 1$ (shaded region), and in the final simulation state (thin blue lines). The orange circles and red squares indicate the mass scale of the collapsing gas cloud that is co-located with the centre of the host halo.
Extended Data Fig. 3 | Thermal and turbulent support of the collapsing core. a, b, Gravitational forces dominate over thermal and turbulent internal pressures within the collapsing core in the MMH (a) and the LWH (b). The thermal sound speed (blue dotted lines) and turbulent root-mean-square velocity (orange dash-dotted line) both contribute to the effective sound speed (black solid line) that provides partial resistance to a catastrophic collapse. The radial infall speed (green dashed line) shows that the flow becomes supersonic at the Jeans mass scale and then transitions to a subsonic flow at smaller mass scales. In the LWH, the radial inflow becomes transonic at a mass scale of $10^3 M_\odot$. 

© 2019 Springer Nature Limited. All rights reserved.
Extended Data Fig. 4 | Rotational properties of the target haloes.

a, Radially averaged profiles of circular velocity $v_{\text{Kep}} = \sqrt{GM/r}$ (red lines) and rotational velocity $v_{\text{rot}}$ (blue lines) around the largest principal axis of the MMH (dashed lines) and the LWH (solid lines) at the end of the simulation. b, Radially averaged profiles of the fractional rotational support; a ratio greater than one indicates that rotational velocities are sufficient to prevent gravitational collapse. The shaded regions show where the systems are rotationally supported: $2 \times 10^3 M_\odot - 3.3 \times 10^5 M_\odot$ for the MMH (light shading) and $7 \times 10^3 M_\odot - 6 \times 10^4 M_\odot$ for the LWH (dark shading). Rotation works in tandem with thermal and turbulent pressures to marginally slow the collapse, seen in the lower infall speeds at these mass scales in Extended Data Fig. 3. Inside $100 M_\odot$, this rotational measure becomes ill-defined because the rotation centre and centre-of-mass are not co-located; thus, we do not conclude that the inner portions are rotationally supported even though $v_{\text{rot}}/v_{\text{Kep}} > 1$. © 2019 Springer Nature Limited. All rights reserved.
Extended Data Fig. 5 | Distribution of fragmentation-prone regions. a–d. Density-weighted projections of a local estimate of the Toomre Q parameter (equation (2)) for the MMH (a, b) and the LWH (c, d) in a field of view of 20 pc (left) and 4 pc (right), centred on the densest point and aligned to be perpendicular with the angular momentum vector of the disk. A value greater than one indicates that rotation and internal pressure stabilizes regions against fragmentation into smaller self-gravitating objects. In the MMH, this analysis highlights the clump fragments with the filaments being only marginally stable at $Q \approx 1$. The sheet in the LWH that formed from a preceding major halo merger is apparent in this measure. The bulk of the sheet is only marginally stable, with the edge and collapsing centre containing an environment that is conducive to fragmentation.
Extended Data Fig. 6 | Growth rates for fragmentation. A rotating system will fragment into self-gravitating clumps only when the growth rates of the density perturbations are faster than the collapse timescale. 

a, Cylindrical radial profiles of \( Q \) when considering only thermal support (red) and with thermal and turbulent support (blue), for the MMH (dashed) and the LWH (solid). The shaded region indicates where the system is unstable to fragmentation. 

b, The unstable regions have a characteristic growth rate, defining a growth timescale \( t_{\text{grow}} \), which exhibits an increasing trend with radius for the MMH (orange) and the LWH (green). 

c, If the ratio of \( t_{\text{grow}} \) and the free-fall time \( t_{\text{ff}} \) is less than one, the region can fragment before it gravitationally collapses. In the MMH, this condition is true at radii less than 0.03 pc, indicating that small-scale fragmentation might occur but will subsequently be suppressed by a rapid monolithic collapse. The LWH exhibits this feature inside 0.1 pc but is surrounded by gas that is stable against fragmentation.
Extended Data Fig. 7 | Clump infall rates and timescales. Similar to the results presented in Fig. 4d, the self-gravitating clumps are growing through radial infall. **a**, The infall rates are computed as the mass flux through spherical shells and steadily increase with enclosed mass. The rate in the single clump of the LWH (dotted purple line) is more than a factor three greater than the three major clumps in the MMH. The circles mark the infall rate at the clump mass. **b**, The infall time, the ratio of the mass enclosed and infall rate, is an informative scale that can be used to compare against star-formation timescales. This timescale is constant and approximately 10 kyr within 100M⊙ for all clumps and rises to about 100 kyr for the entire clump, marked by the circles. This rapid infall suggests that sufficient mass will collapse into the supermassive protostar before it reaches main-sequence.
Extended Data Fig. 8 | Thermal and turbulent support of collapsing clumps. a–d, Same as Extended Data Fig. 3, but for the clumps in the LWH (a) and the MMH (b–d). The vertical dotted lines mark the clump mass. The radial inflows are subsonic for all four clumps, but the clump in LWH contains transonic flows between 100$M_\odot$ and 1,000$M_\odot$. Thermal support is dominant inside the clumps, unlike the larger parent Jeans-unstable system, where turbulent effective pressures are comparable to their thermal counterparts (see Extended Data Fig. 3).
Extended Data Fig. 9 | Abundance estimate of DCBHs. The cumulative probability of the co-moving number density of haloes that potentially host supermassive star formation is shown for the rare-peak (red solid line), normal (blue dashed line) and void (black dash-dotted line) regions of the Renaissance simulations. Their respective median number densities are $1.1 \times 10^{-3}$, about $10^{-7}$ and 0 haloes per co-moving Mpc$^3$. Subsequent DCBH formation is most likely to occur in overdense regions of the early Universe, whereas few or no haloes will form in average and underdense regions.
### Extended Data Table 1 | Properties of halo candidates hosting supermassive star formation

| log\(_{10}(M_{\text{halo}})\) [M\(_{\odot}\)] | log\(_{10}\)(mean Growth rate) [M\(_{\odot}\) per unit redshift] | J\(_{\text{LW}}\)/J\(_{21}\) | \(D_{\text{gal}}\) [kpc] | \(T_c\) [K] | Gas infall rate [M\(_{\odot}\)/yr] |
|-------------------------------------------|--------------------------------------------------|-----------------|-----------------|---------|-----------------|
| 7.84*                                     | 7.78                                            | 2.71            | 12.7            | 2250   | 0.275           |
| 7.76†                                     | 7.53                                            | 3.23            | 11.8            | 4390   | 0.171           |
| 7.76                                      | 7.76                                            | 1.91            | 14.7            | 4220   | 0.286           |
| 7.75                                      | 7.65                                            | 0.583           | 35.5            | 1730   | 0.290           |
| 7.75                                      | 7.39                                            | 0.958           | 19.7            | 7570   | 0.0294          |
| 7.74                                      | 7.88                                            | 1.49            | 25.0            | 8670   | 0.0574          |
| 7.73                                      | 7.79                                            | 0.894           | 29.9            | 1760   | 0.396           |
| 7.70                                      | 7.22                                            | 2.62            | 18.3            | 6520   | 0.0292          |
| 7.67                                      | 7.90                                            | 0.16            | 124             | 1080   | 1.05            |
| 7.64                                      | 7.78                                            | 2.14            | 6.20            | 7890   | 0.0356          |

The growth rate is averaged over the last 20 Myr of the simulation. The values of \(J_{\text{LW}}\) and of the gas temperature \(T_c\) are given at the densest point. \(D_{\text{gal}}\) is the distance to the nearest galaxy with at least \(10^6\) M\(_{\odot}\) of stars. The gas infall rate is the mass-averaged value within 100 pc. All data are given at \(z = 15\) from the original Renaissance simulation of the rare-peak region.

*MMH.
†LWH.