Beyond the First Light: Novel Simulations of Pop III Stars with PeakPatch-GIZMO Pipeline

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CITA ICAT Canadian Institute for Theoretical Astrophysics L'institut Canadien d'astrophysique théorique

JWST's Early-Universe Challenges

High-z ($z \gtrsim 10$) SMBH observations challenging formation models[1,2]

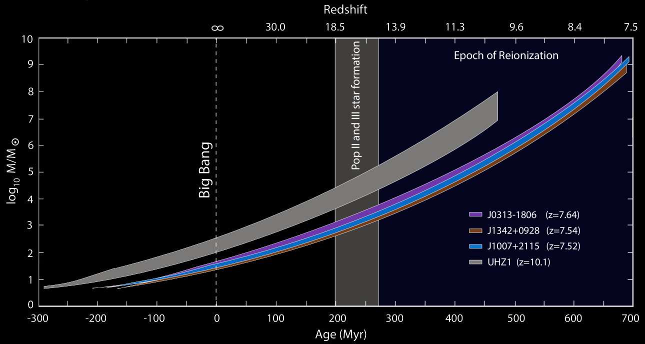

Figure 1. Theoretical Eddington accretion by earliest observed AGN[3]

[1] Wang et al. 2024.

[2] Goulding et al. 2023.

[3] Melia 2024.

Massive Seeds Solution: Pop III Stars?

Potential SMBH seeding mechanisms for $30 \gtrsim z \gtrsim 15$:

- Direct collapse IMBH formation?[1]
- Pop III (first-generation) stars?[2,3]

[1] Latif and Ferrara 2016.

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PopIII 101

- First-generation objects in the Universe
- Formation time: end of dark ages $\rightarrow$ beginning of reionization
- Formed from primordial H/He gas
- Became the first sources of heavier resources

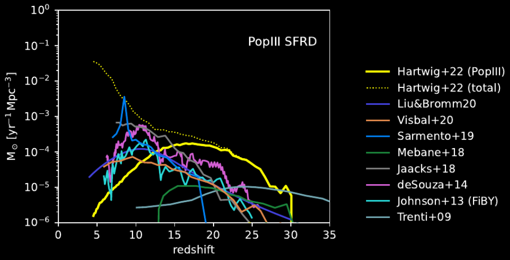

Figure 2. Formation of Pop III stars vs redshift in different simulations[a]

[a] Klessen and Glover 2023.

Simulating Pop III stars

Traditional approach:

- Idealized initial conditions[1,2]
- Isolated collapse models

[1] Jaura et al. 2022.

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Great, BUT: Missing LSS environment effects; Unrealistic ICs

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Study of Pop III formation environment, LSS effects

$\downarrow$

Cosmological Simulations

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$\downarrow$

Cosmological Simulations

(Of the largest halos at high-z)

Study of Pop III formation environment, LSS effects

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Cosmological Simulations

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High-σ events require <u>large high-resolution boxes</u>

High-z Halo Finding: HMF Sampling

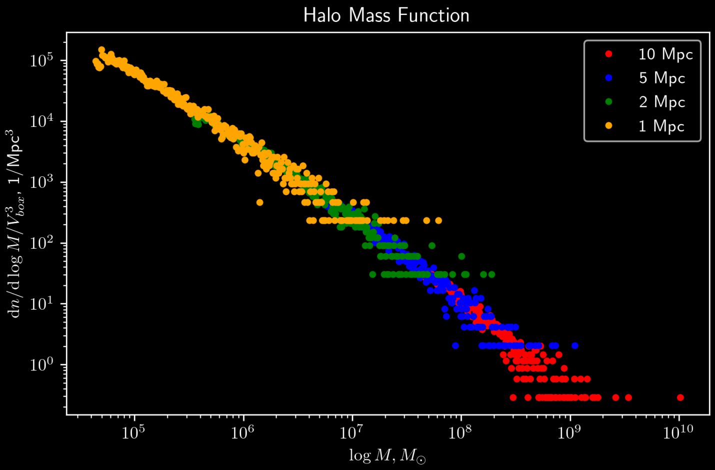

Figure 3. Halo Mass Function (HMF) for $z = 15$ (different box sizes)

High-z Halo Finding: HMF Evolution

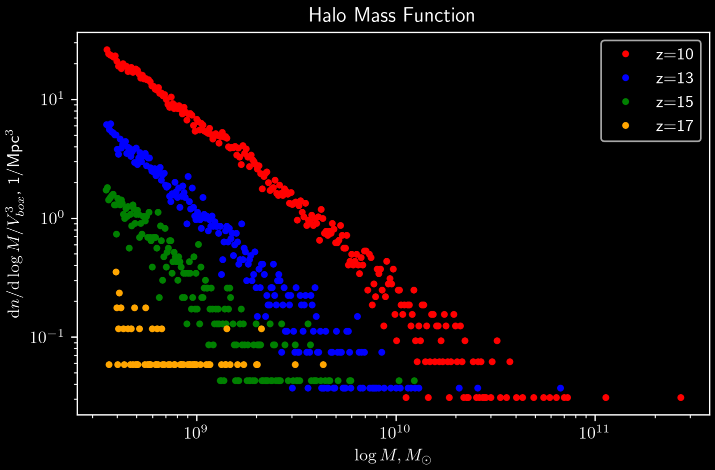

Figure 4. HMF evolution with redshift (20 Mpc box)

Our Cosmological Approach

Pipeline used by FORGE'd in FIRE collaboration [1]

[1] FIRE Wiki

[2] Hahn and Abel 2011.

[3] Hopkins et al. 2018.

[4] Grudić et al. 2021.

Our Cosmological Approach

MUSIC (low-res) → GIZMO (DM Only) → Halo Finding → MUSIC (high-res) → GIZMO (FIRE) → GIZMO (STARFORGE)

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- **MUSIC**: MUlti-Scale Initial Conditions (ICs)[2]

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- **STARFORGE**: Stellar-scale phyiscs GIZMO extension[4]

Running STARFORGE in cosmological box will require particle splitting!

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Our Cosmological Approach

Our Cosmological Approach

Speedup from ≈ 30 hrs to < 1 hr with PeakPatch!

PeakPatch – semi-analytic halo finder code that solves *ellipsoidal collapse*[1]

[1] Stein, Alvarez, and Bond 2018.

PeakPatch-MUSIC Validation: High z

- Boxsize = 10 cMpc
- Successful halo identification at z=17
- Maximum halo mass: $\sim 10^8$ $M_\odot$
- Hydro (GIZMO) zoom-in ICs creation and successful run

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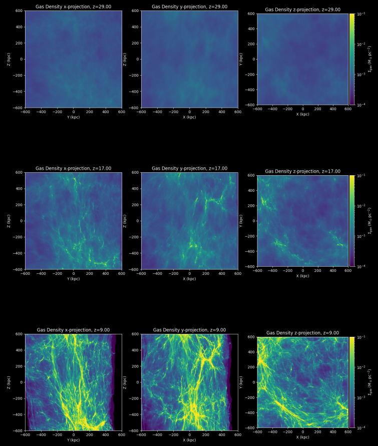
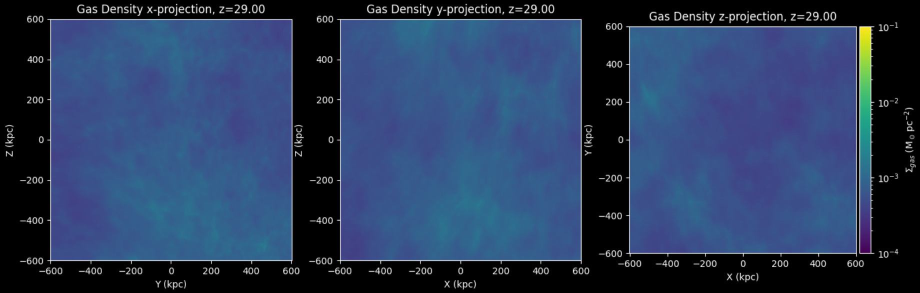


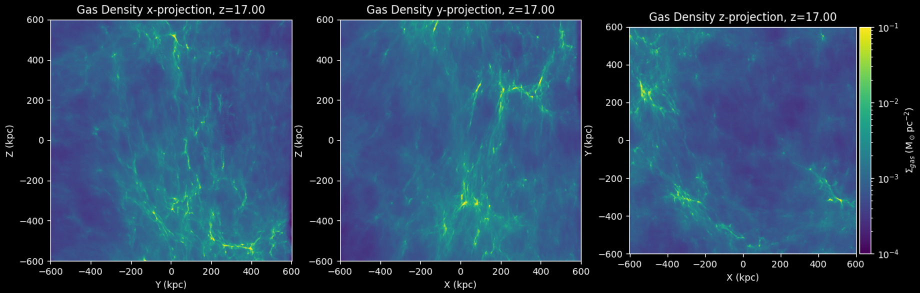
Figure 5. z=29 vs z=17 vs z=9 baryon density fields

z=30 Results



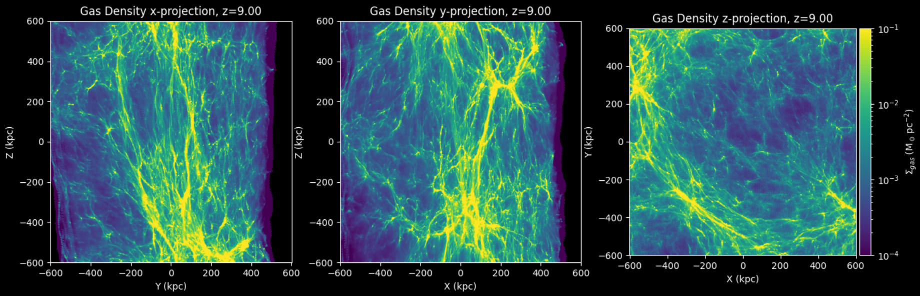
Earliest time of *possible* PopIII star formation (SF)
Max zoom-in region size: 800 kpc (box)

z=17 Results



Expected time of SF in our simulation.
No actual SF happened

z=9 Results



Actual time of SF in our simulation.
FIRE-3 physics, FIRE-2 results were reproduced (SF beginning at z $9-10$).
No primordial physics introduced here, thus no PopIII production.

PeakPatch-MUSIC Validation: Ultra-High z Soon...

- Boxsize = 2 cMpc
- Successful halo identification at z=30
- Maximum halo mass: $\sim 10^5$ $M_\odot$

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Figure 5. No figure :(

(But the pipeline is working!)

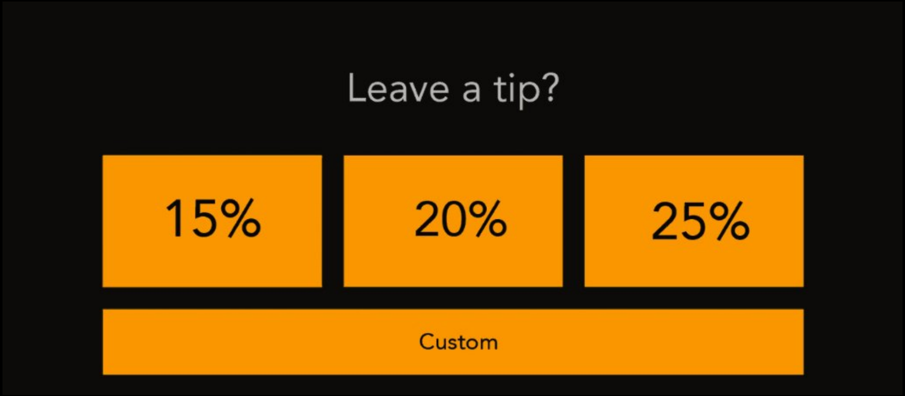
Key Advances

- Novel pipeline enables:
  - Cosmological Pop III simulations with a large sample size
  - BLAZINGLY FAST halo identification
- First validation complete:
  - PeakPatch-MUSIC interface working
  - Initial hydro runs confirm FIRE-2 results
  - PeakPatch tested in regime never tested before

What's next?

1. Forming stars with FIRE at high-z
2. Achieving $z = 30$ ICs generation (MUSIC MPI rewrite)
3. Particle splitting implementation
4. STARFORGE integration to obtain IMF

Thank you!

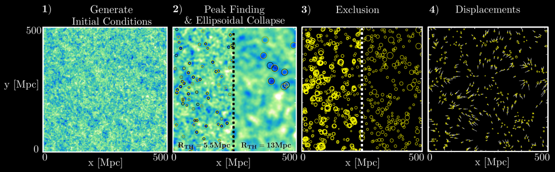


Website:

What is PeakPatch?

Semi-analytic halo finder based on peak patches

- Key features:
  - Fast $\rightarrow$ enables large parameter surveys
  - Works at any redshift (in theory)
  - Lightcones!
- Main steps of the code:
  - Looks at different filter scales
  - Resolves homogeneous ellipsoidal collapse
  - Excludes overlapping halos
  - Performs lagrangian displacements after peaks were found

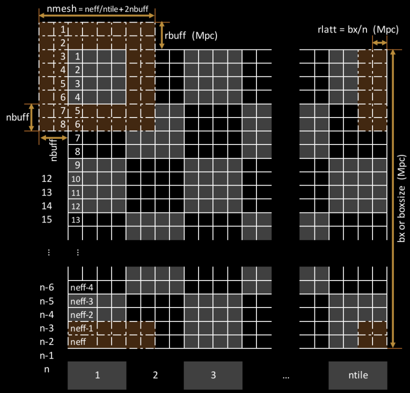


PeakPatch algorithm overview. Credit: Stein et al., 2018

PeakPatch Tiling Strategy

Domain decomposition into tiles

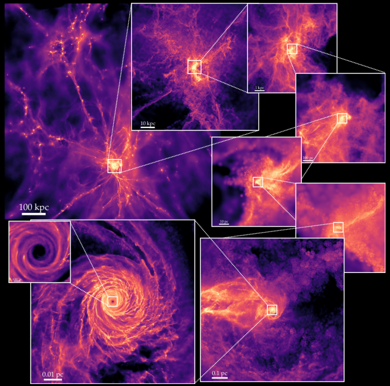
- Each tile has:
  - Core region
  - Buffer zones ($n_{\rm buff}$ layers)
- $R^{\rm max}_{\rm smooth}$ sets maximum halo radius → should be less than $n_{\rm buff}$
- Buffer size ensures boundary independence



PeakPatch tile structure with buffer zones

Zoom-in Simulations: Why We Need Them

- Cosmic variance/gas accretion for star formation → Need large volumes
- But resolve Pop III physics → High resolution
- Solution: Hierarchical zoom-in
    - Large parent box (100 Mpc/h?)
    - Initial progressive refinement to ∼ kpc scales
    - Particle splitting to go to ∼ pc scales



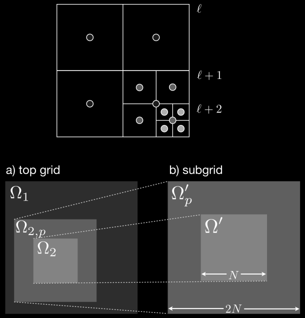
STARFORGE + FIRE Zoom-in.

Credit: 2309.13115

Multi-Scale Initial Conditions (MUSIC)

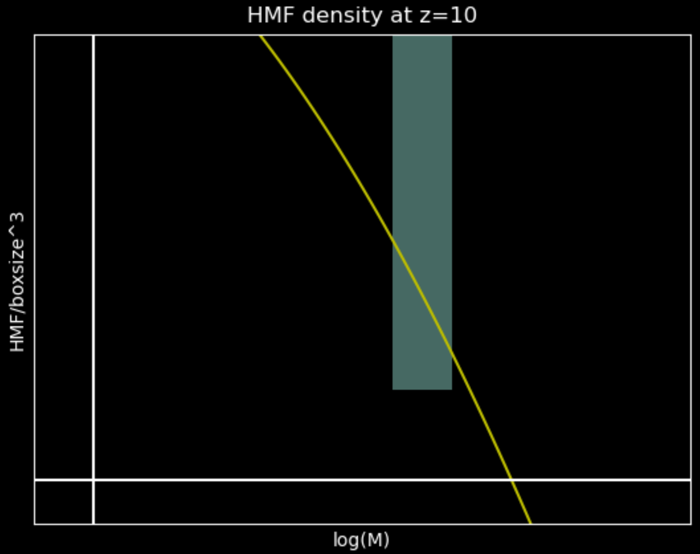
Steps for zoom-in ICs refinement with MUSIC:

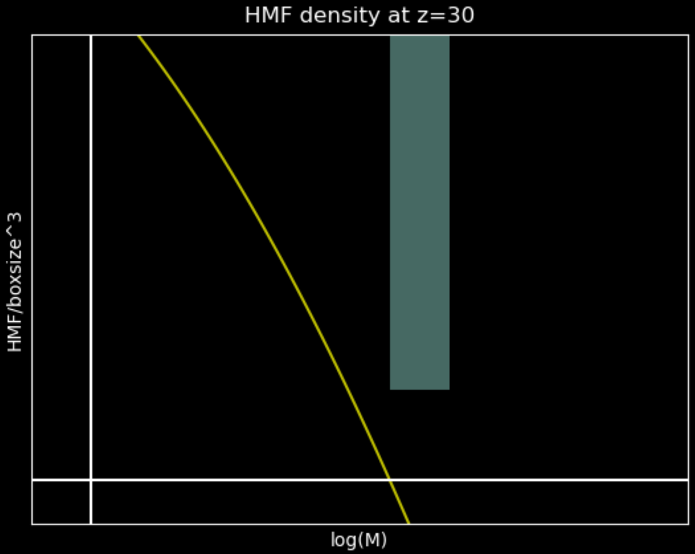
- Set up lowest-res grid
- Pick a region of interest for further refinement (for us, based on generated halo tables)
- Increase particle density by a factor of 2 for evey next region
- Generate density field and convolve it with previous level
- Baryons are only placed in the highest-resolution region

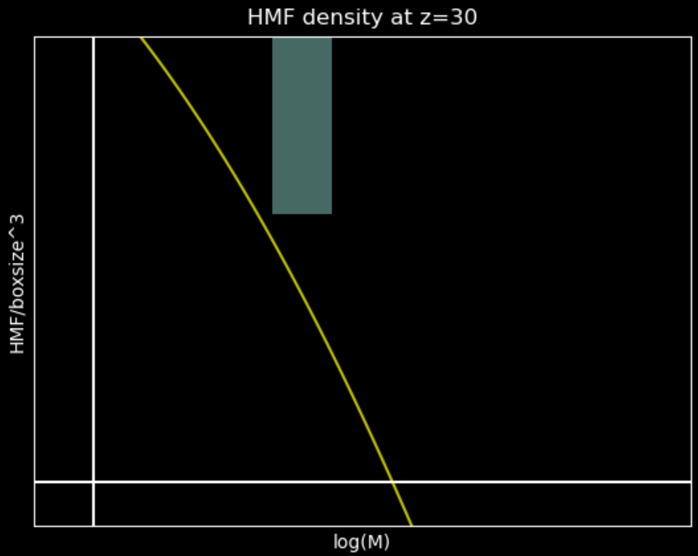


MUSIC zoom-in grid structure.

Credit: Hahn, Abel, 2011


HMF density at z=10
HMF/boxsize^3
log(M)


HMF density at z=30
HMF/boxsize^3
log(M)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References I

[1] P J Alister Seguel et al. "Formation of SMBH seeds in Population III star clusters through collisions: the importance of mass loss". In: *Monthly Notices of the Royal Astronomical Society* 493.2 (2020), pp. 2352–2362. ISSN: 1365-2966. DOI: 10.1093/mnras/staa456. arXiv: 1912.01737. URL: http://dx.doi.org/10.1093/mnras/staa456.

[2] Vieri Cammelli et al. "The formation of supermassive black holes from Population III.1 seeds. III. Galaxy evolution and black hole growth from semi-analytic modelling". Preprint. 2024. arXiv: 2407.09949.

[3] Andy D. Goulding et al. "UNCOVER: The growth of the first massive black holes from JWST/NIRSpec – spectroscopic redshift confirmation of an X-ray luminous AGN at z=10.1". Preprint. 2023. arXiv: 2308.02750.

References II

[4] Michael Y Grudić et al. "STARFORGE: Towards a comprehensive numerical model of star cluster formation and feedback". In: *Monthly Notices of the Royal Astronomical Society* 506.2 (2021), pp. 2199–2231. ISSN: 1365-2966. DOI: 10.1093/mnras/stab1347. arXiv: 2010.11254. URL: http://dx.doi.org/10.1093/mnras/stab1347.

[5] Oliver Hahn and Tom Abel. "Multi-scale initial conditions for cosmological simulations: Multi-scale initial conditions". In: *Monthly Notices of the Royal Astronomical Society* 415.3 (2011), pp. 2101–2121. ISSN: 0035-8711. DOI: 10.1111/j.1365-2966.2011.18820.x. arXiv: 1103.6031. URL: http://dx.doi.org/10.1111/j.1365-2966.2011.18820.x.

References III

[6] Philip F Hopkins et al. “FIRE-2 simulations: physics versus numerics in galaxy formation”. In: *Monthly Notices of the Royal Astronomical Society* 480.1 (2018), pp. 800–863. ISSN: 1365-2966. DOI: 10.1093/mnras/sty1690. arXiv: 1702.06148v2. URL: http://dx.doi.org/10.1093/mnras/sty1690.

[7] Ondrej Jaura et al. “Trapping of H ¡scp¿ii¡/scp¿ regions in Population III star formation”. In: *Monthly Notices of the Royal Astronomical Society* 512.1 (2022), pp. 116–136. ISSN: 1365-2966. DOI: 10.1093/mnras/stac487. arXiv: 2202.09803. URL: http://dx.doi.org/10.1093/mnras/stac487.

[8] Ralf S. Klessen and Simon C. O. Glover. “The first stars: formation, properties, and impact”. Preprint. 2023. arXiv: 2303.12500.

References IV

[9] Muhammad A. Latif and Andrea Ferrara. "Formation of Supermassive Black Hole Seeds". In: *Publications of the Astronomical Society of Australia* 33 (2016). ISSN: 1448-6083. DOI: 10.1017/pasa.2016.41. arXiv: 1605.07391. URL: http://dx.doi.org/10.1017/pasa.2016.41.

[10] Fulvio Melia. "The cosmic timeline implied by the highest redshift quasars". Preprint. 2024. arXiv: 2412.02706.

[11] George Stein, Marcelo A Alvarez, and J Richard Bond. "The mass-Peak Patch algorithm for fast generation of deep all-sky dark matter halo catalogues and itsN-body validation". In: *Monthly Notices of the Royal Astronomical Society* 483.2 (2018), pp. 2236–2250. ISSN: 1365-2966. DOI: 10.1093/mnras/sty3226. arXiv: 1810.07727. URL: http://dx.doi.org/10.1093/mnras/sty3226.

References V

[12] Kazuyuki Sugimura et al. "Formation of Massive and Wide First-star Binaries in Radiation Hydrodynamic Simulations". In: *The Astrophysical Journal* 959.1 (2023), p. 17. ISSN: 1538-4357. DOI: 10.3847/1538-4357/ad02fc. arXiv: 2307.15108. URL: http://dx.doi.org/10.3847/1538-4357/ad02fc.

[13] Tao Wang et al. "MAssive galaxies aCRoss cOSmic time revealed by JWST/MIRI (MACROSS): The true number density of massive galaxies in the early Universe". Preprint. 2024. arXiv: 2403.02399.