Radiation-coupled Primordial Chemistry in Simulations of the First Galaxies

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Talk Contents

- The importance of chemistry and radiation in the early universe
- Doesn’t RAMSES-RT do that already?
- Implementing *rich, radiation-coupled* non-equilibrium chemistry
- Testing the code
- Science Goals

Chemistry in the Early Universe

- In a universe devoid of metals, gas can only cool enough to form stars via H_2 and HD
- There are many chemical reactions involved in their formation, and they can be destroyed by radiation from nearby newly-formed stars
- Gas does not necessarily reach equilibrium as it cools (especially with radiation involved), therefore a *non-equilibrium* treatment is required

$$H^- + e^- \longrightarrow H + e^- + e^-$$
$$H^- + H \longrightarrow H_2 + e^-$$
$$H^- + H^+ \longrightarrow H_2^+ + e^-$$
$$H + H^+ \longrightarrow H_2^+$$
$$D + H_2 \longrightarrow HD + H$$
$$D^+ + H_2 \longrightarrow HD + H^+$$

$$H_2 + \gamma \longrightarrow H + H$$

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RAMSES-RT

- *Equilibrium* treatment of chemistry, except for H, He photoionisation.
- 'Semi-implicit' scheme for solving thermochemistry ODEs works in this case, but is inappropriate for solving large systems of highly-coupled equations.

$$x_{n+1} = x_n + \Delta t \cdot f(x_n, y_n, z_n)$$
$$y_{n+1} = y_n + \Delta t \cdot g(x_{n+1}, y_n, z_n)$$
$$z_{n+1} = z_n + \Delta t \cdot h(x_{n+1}, y_{n+1}, z_n)$$

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Implementation

- Replace semi-implicit thermochemistry solver with implicit, adaptive solver via KROME*

- KROME takes a list of chemical reactions and cooling/heating processes and generates code to solve the associated system of ODEs

- Include reactions for photons of each bin in RAMSES-RT. Cross-sections calculated on the fly by integrating stellar SEDs

$$\mathrm{H} + e^- \longrightarrow \mathrm{H}^+ + e^- + e^-$$
$$\mathrm{He} + e^- \longrightarrow \mathrm{He}^+ + e^- + e^-$$
$$\mathrm{He}^+ + e^- \longrightarrow \mathrm{He}^{2+} + e^- + e^-$$
$$\mathrm{H}^- + e^- \longrightarrow \mathrm{H} + e^- + e^-$$
$$\mathrm{H}^- + \mathrm{H} \longrightarrow \mathrm{H}_2 + e^-$$
$$\mathrm{H}^- + \mathrm{H} \longrightarrow \mathrm{H}_2 + e^-$$
$$\mathrm{H}^- + \mathrm{H} \longrightarrow \mathrm{H} + \mathrm{H} + e^-$$
$$\mathrm{H}^- + \mathrm{H} \longrightarrow \mathrm{H} + \mathrm{H} + e^-$$
$$\mathrm{H}^- + \mathrm{H}^+ \longrightarrow \mathrm{H}_2^+ + e^-$$
$$\mathrm{H} + \mathrm{H} + \mathrm{H} \longrightarrow \mathrm{H}_2 + \mathrm{H}$$
$$\mathrm{H}^- + \mathrm{H}^+ \longrightarrow \mathrm{H} + \mathrm{H}$$
$$\mathrm{H} + \mathrm{H}^+ \longrightarrow \mathrm{H}_2^+$$
$$\mathrm{H}_2^+ + \mathrm{H} \longrightarrow \mathrm{H}_2 + \mathrm{H}^+$$
$$\mathrm{H}_2 + \mathrm{H}^+ \longrightarrow \mathrm{H}_2^+ + \mathrm{H}$$
$$\mathrm{H}_2 + e^- \longrightarrow \mathrm{H} + \mathrm{H} + e^-$$
$$\mathrm{H}_2^+ + \mathrm{H}^- \longrightarrow \mathrm{H} + \mathrm{H}_2$$
$$\mathrm{H}_2 + \mathrm{H} \longrightarrow \mathrm{H} + \mathrm{H} + \mathrm{H}$$
$$\mathrm{H}_2^+ + e^- \longrightarrow \mathrm{H} + \mathrm{H}$$
$$\mathrm{H}^+ + e^- \longrightarrow \mathrm{H}$$
$$\mathrm{He}^+ + e^- \longrightarrow \mathrm{He}$$
$$\mathrm{He}^{2+} + e^- \longrightarrow \mathrm{He}^+$$
$$\mathrm{H} + e^- \longrightarrow \mathrm{H}^- + \gamma_1$$
$$\mathrm{H}^+ + e^- \longrightarrow \mathrm{H} + \gamma_4$$
$$\mathrm{He}^{2+} + e^- \longrightarrow \mathrm{He}^+ + \gamma_7$$
$$\mathrm{He}^+ + e^- \longrightarrow \mathrm{He} + \gamma_6$$

$$\mathrm{H}^- + \gamma_1 \longrightarrow \mathrm{H} + e^-$$
$$\mathrm{H}^- + \gamma_2 \longrightarrow \mathrm{H} + e^-$$
$$\mathrm{H}^- + \gamma_3 \longrightarrow \mathrm{H} + e^-$$
$$\mathrm{H}^- + \gamma_4 \longrightarrow \mathrm{H} + e^-$$
$$\mathrm{H} + \gamma_4 \longrightarrow \mathrm{H}^+ + e^-$$
$$\mathrm{H} + \gamma_5 \longrightarrow \mathrm{H}^+ + e^-$$
$$\mathrm{H} + \gamma_6 \longrightarrow \mathrm{H}^+ + e^-$$
$$\mathrm{H} + \gamma_7 \longrightarrow \mathrm{H}^+ + e^-$$
$$\mathrm{H}_2 + \gamma_3 \longrightarrow \mathrm{H} + \mathrm{H}$$
$$\mathrm{H}_2 + \gamma_4 \longrightarrow \mathrm{H} + \mathrm{H}$$
$$\mathrm{H}_2 + \gamma_5 \longrightarrow \mathrm{H} + \mathrm{H}$$
$$\mathrm{H}_2 + \gamma_5 \longrightarrow \mathrm{H}_2^+ + e^-$$
$$\mathrm{H}_2 + \gamma_6 \longrightarrow \mathrm{H}_2^+ + e^-$$
$$\mathrm{H}_2 + \gamma_7 \longrightarrow \mathrm{H}_2^+ + e^-$$
$$\mathrm{H}_2^+ + \gamma_2 \longrightarrow \mathrm{H}^+ + \mathrm{H}$$
$$\mathrm{H}_2^+ + \gamma_3 \longrightarrow \mathrm{H}^+ + \mathrm{H}$$
$$\mathrm{H}_2^+ + \gamma_4 \longrightarrow \mathrm{H}^+ + \mathrm{H}$$
$$\mathrm{He} + \gamma_6 \longrightarrow \mathrm{He}^+ + e^-$$
$$\mathrm{He} + \gamma_7 \longrightarrow \mathrm{He}^+ + e^-$$
$$\mathrm{He}^+ + \gamma_7 \longrightarrow \mathrm{He}^{2+} + e^-$$

*Grassi et al. 2014 (https://arxiv.org/abs/1311.1070)

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Drawbacks

- **Slow**
- High memory cost
- Adaptive solver tries very hard to resolve short-timescale phenomena, e.g. photoheating and ionisation in cells containing newly-formed stars (good for accuracy, potentially bad for stability and performance)

$$\begin{aligned}
&H + e^- \longrightarrow H^+ + e^- + e^- \\
&He + e^- \longrightarrow He^+ + e^- + e^- \\
&He^+ + e^- \longrightarrow He^{2+} + e^- + e^- \\
&H^- + e^- \longrightarrow H + e^- + e^- \\
&H^- + H \longrightarrow H_2 + e^- \\
&H^- + H \longrightarrow H_2 + e^- \\
&H^- + H \longrightarrow H + H + e^- \\
&H^- + H \longrightarrow H + H + e^- \\
&H^- + H^+ \longrightarrow H_2^+ + e^- \\
&H + H + H \longrightarrow H_2 + H \\
&H^- + H^+ \longrightarrow H + H \\
&H + H^+ \longrightarrow H_2^+ \\
&H_2^+ + H \longrightarrow H_2 + H^+ \\
&H_2 + H^+ \longrightarrow H_2^+ + H \\
&H_2 + e^- \longrightarrow H + H + e^- \\
&H_2^+ + H^- \longrightarrow H + H_2 \\
&H_2 + H \longrightarrow H + H + H \\
&H_2^+ + e^- \longrightarrow H + H \\
&H^+ + e^- \longrightarrow H \\
&He^+ + e^- \longrightarrow He \\
&He^{2+} + e^- \longrightarrow He^+ \\
&H + e^- \longrightarrow H^- + \gamma_1 \\
&H^+ + e^- \longrightarrow H + \gamma_4 \\
&He^{2+} + e^- \longrightarrow He^+ + \gamma_7 \\
&He^+ + e^- \longrightarrow He + \gamma_6
\end{aligned}$$

$$\begin{aligned}
&H^- + \gamma_1 \longrightarrow H + e^- \\
&H^- + \gamma_2 \longrightarrow H + e^- \\
&H^- + \gamma_3 \longrightarrow H + e^- \\
&H^- + \gamma_4 \longrightarrow H + e^- \\
&H + \gamma_4 \longrightarrow H^+ + e^- \\
&H + \gamma_5 \longrightarrow H^+ + e^- \\
&H + \gamma_6 \longrightarrow H^+ + e^- \\
&H + \gamma_7 \longrightarrow H^+ + e^- \\
&H_2 + \gamma_3 \longrightarrow H + H \\
&H_2 + \gamma_4 \longrightarrow H + H \\
&H_2 + \gamma_5 \longrightarrow H + H \\
&H_2 + \gamma_5 \longrightarrow H_2^+ + e^- \\
&H_2 + \gamma_6 \longrightarrow H_2^+ + e^- \\
&H_2 + \gamma_7 \longrightarrow H_2^+ + e^- \\
&H_2^+ + \gamma_2 \longrightarrow H^+ + H \\
&H_2^+ + \gamma_3 \longrightarrow H^+ + H \\
&H_2^+ + \gamma_4 \longrightarrow H^+ + H \\
&He + \gamma_6 \longrightarrow He^+ + e^- \\
&He + \gamma_7 \longrightarrow He^+ + e^- \\
&He^+ + \gamma_7 \longrightarrow He^{2+} + e^-
\end{aligned}$$

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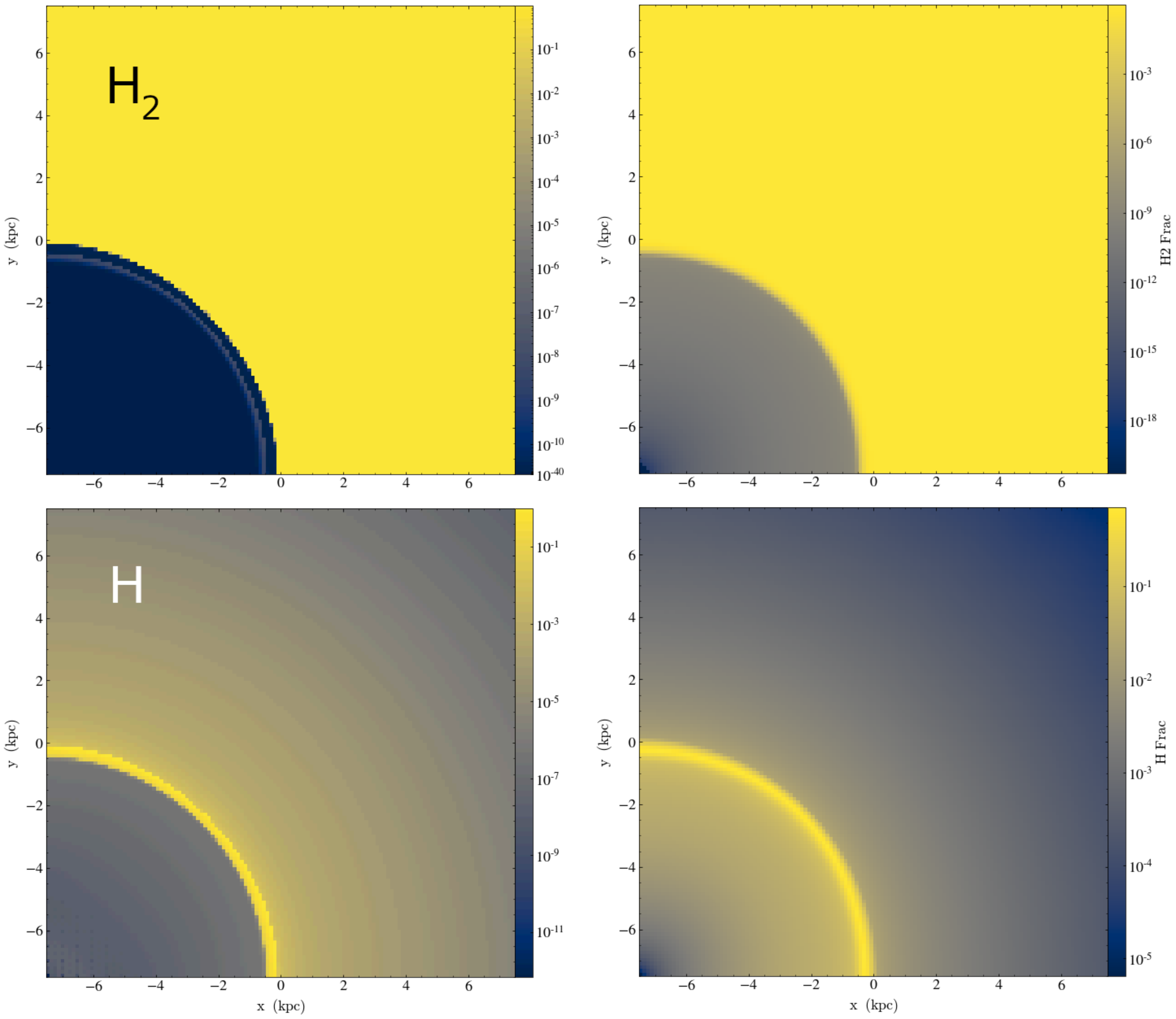
Testing

- Seek to test two main problems:
  - Photoionisation/dissociation
  - Gas collapse

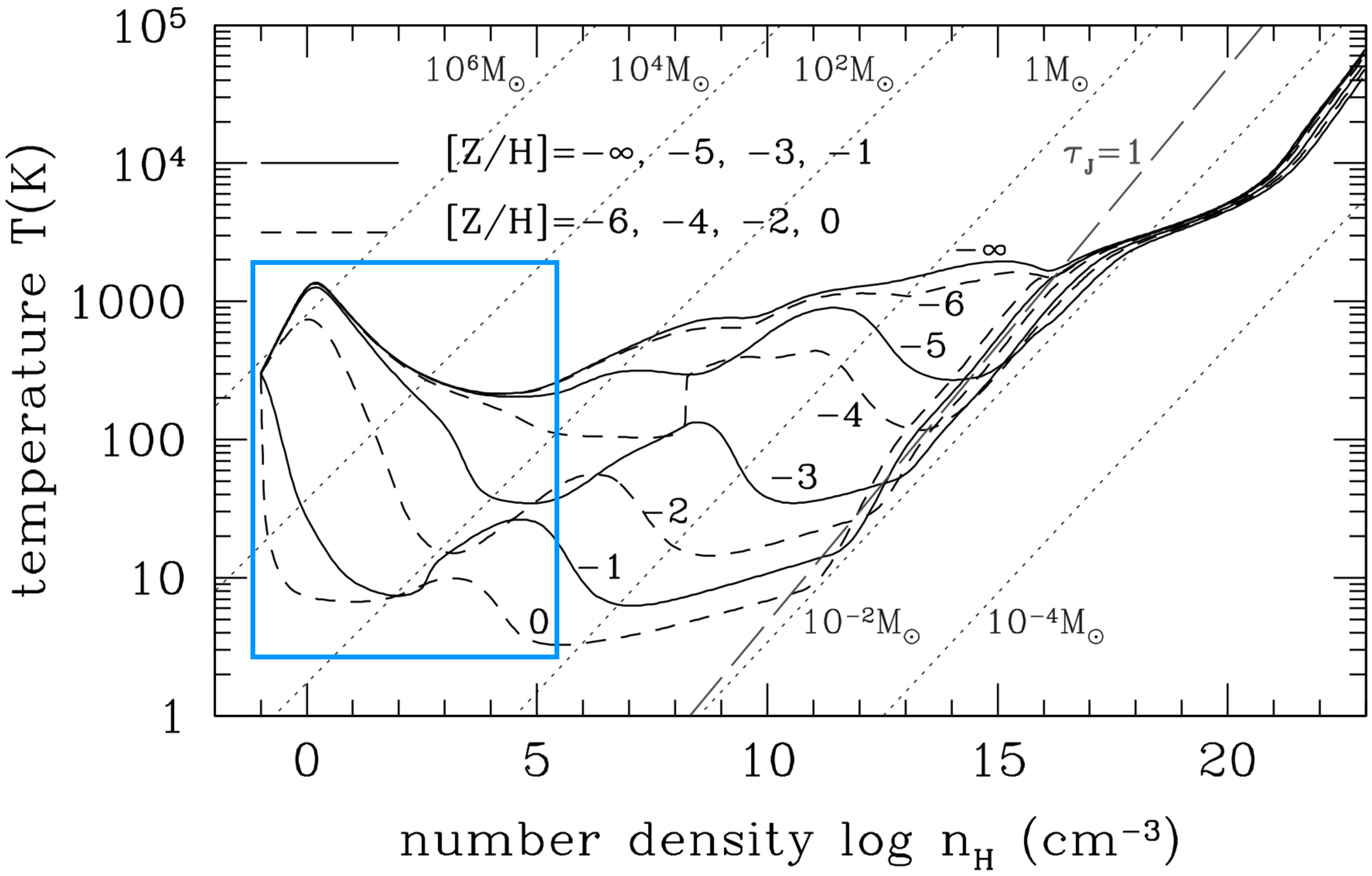
H_2 Strömgren Sphere

- Left Column: H_2 and H gas fractions with ‘semi-implicit’ temperature update, decoupled from chemistry solver
- Right Column: with fully coupled temperature update
- Without full treatment, gas in photoionisation regions is heated, dissociated and ionised too much



Gas Collapse

- Simulate collapse of spherically symmetric cloud of atomic gas
- Seek to reproduce the T vs. n curve of Omukai et al. 2005 (zero-D protostellar collapse simulation) at least up to n = 10^5 cm^{-3}

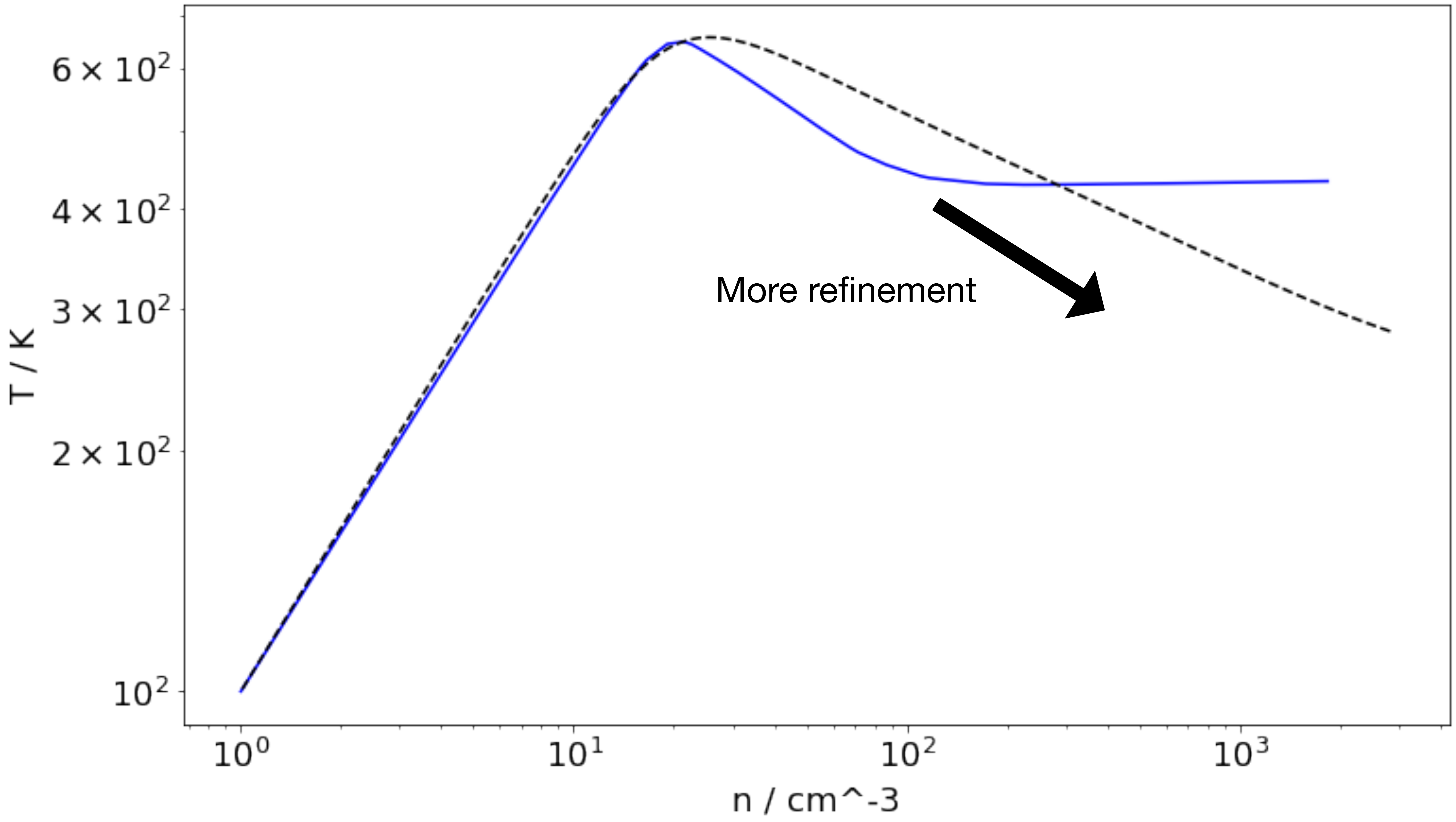


Omukai et al. 2005 (https://arxiv.org/abs/astro-ph/0503010)

Gas Collapse

- Dashed black line is the reference zero-D simulation with my network (no hydro), blue line is my simulation

- Discrepancy due to hydrodynamics, and insufficient refinement at higher densities



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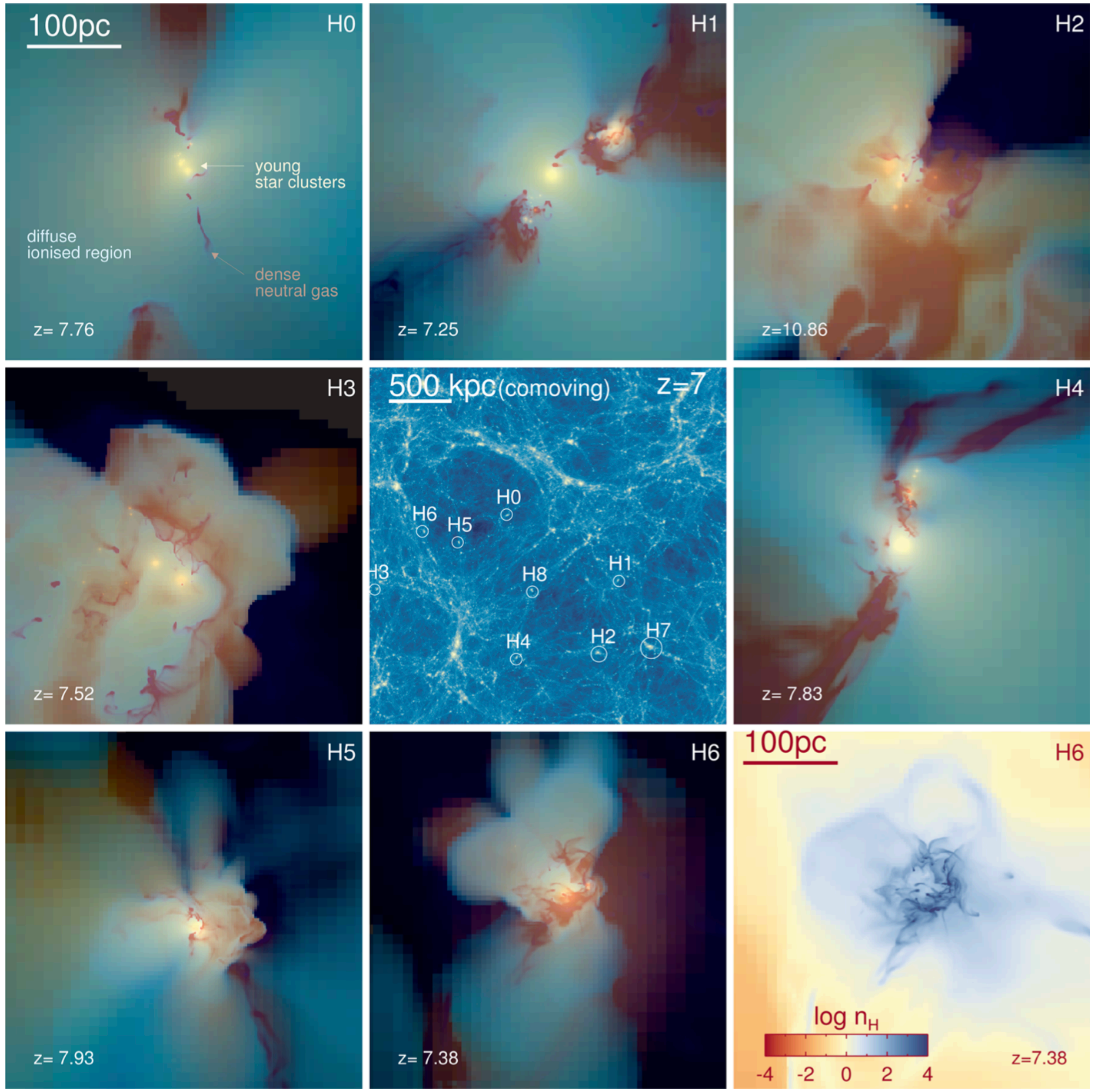
Science Goals

- Resimulate the mini-haloes of Kimm et al. 2017*, including their physics suite but adding my chemistry

- Investigate the effects of baryon-DM streaming and the primordial magnetic field on mini-halo evolution (via initial conditions with different power spectra)



*Feedback-regulated star formation and escape of LyC photons from mini-haloes during reionization — Taysun Kimm, Harley Katz, Martin Haehnelt, Joakim Rosdahl, Julien Devriendt and Adrianne Slyz (https://arxiv.org/abs/1608.04762)