The Universe in a Box:

Modeling cosmological structure formation with Blue Waters

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With:
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Special thanks to:

Manisha Gajbe, Greg Bauer, Bill Kramer (NCSA)
Ed Seidel, Gabrielle Allen, Matthew Turk (NCSA/UIUC)
Irene Qualters (NSF)
Hao Xu (UCSD; simulation wrangler)
The Enzo and yt communities:

- enzo-project.org
- yt-project.org

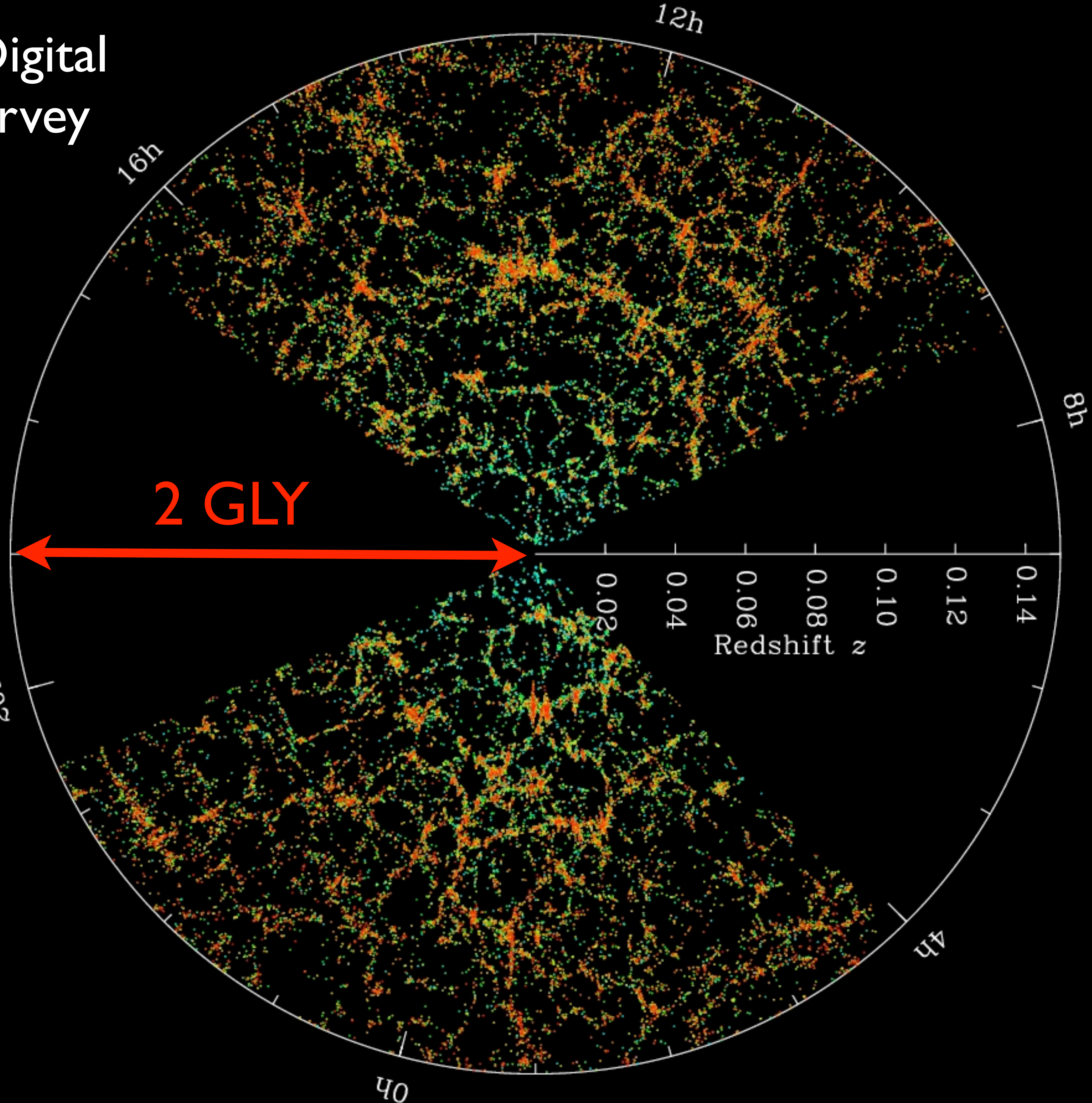
And thank you to the entire Blue Waters team!

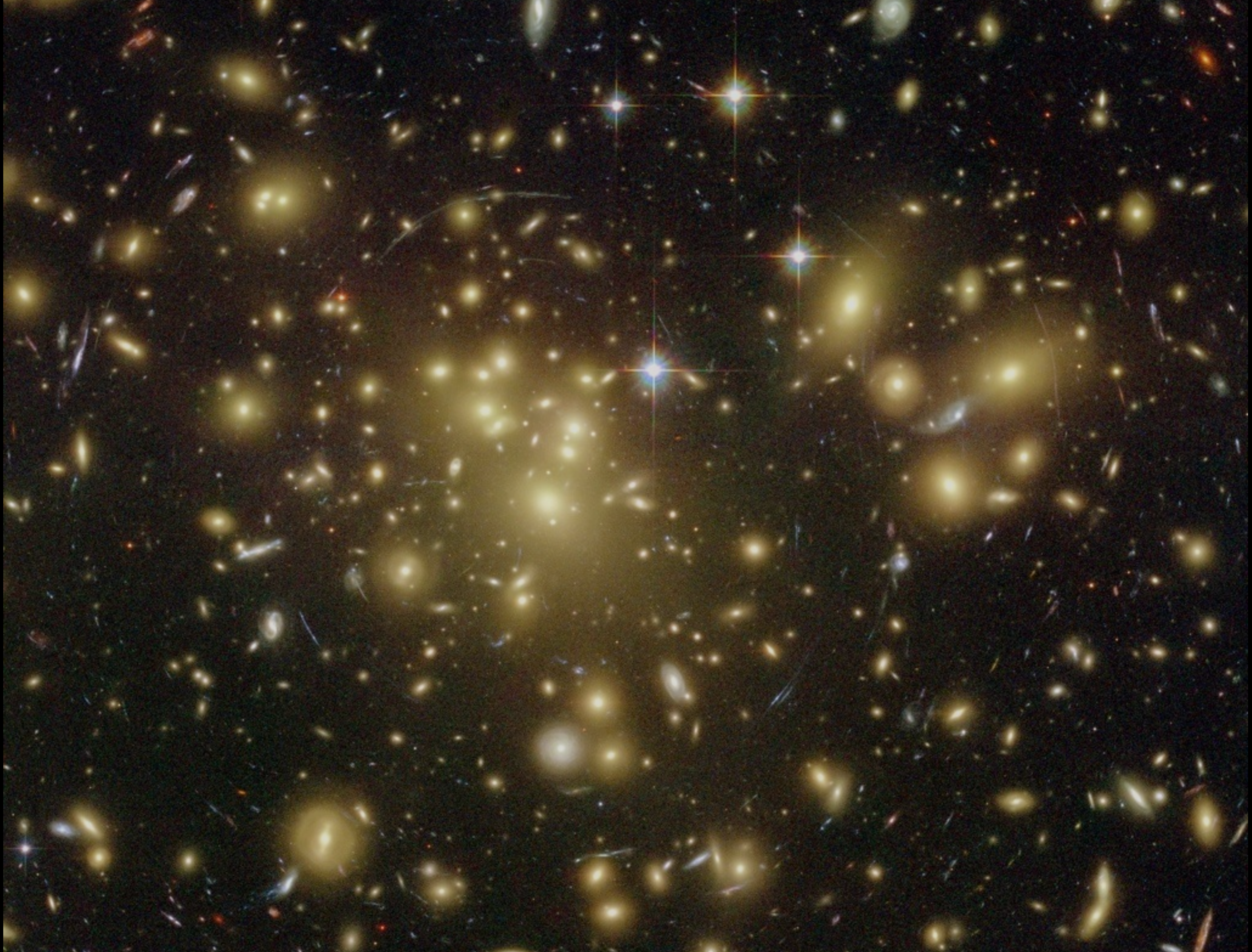
Big questions

- What do the first stars and galaxies look like?
- How do Milky Way-type galaxies form and evolve?
- How does environment affect galaxy formation (and vice versa)?

What is cosmological structure?

Sloan Digital Sky Survey



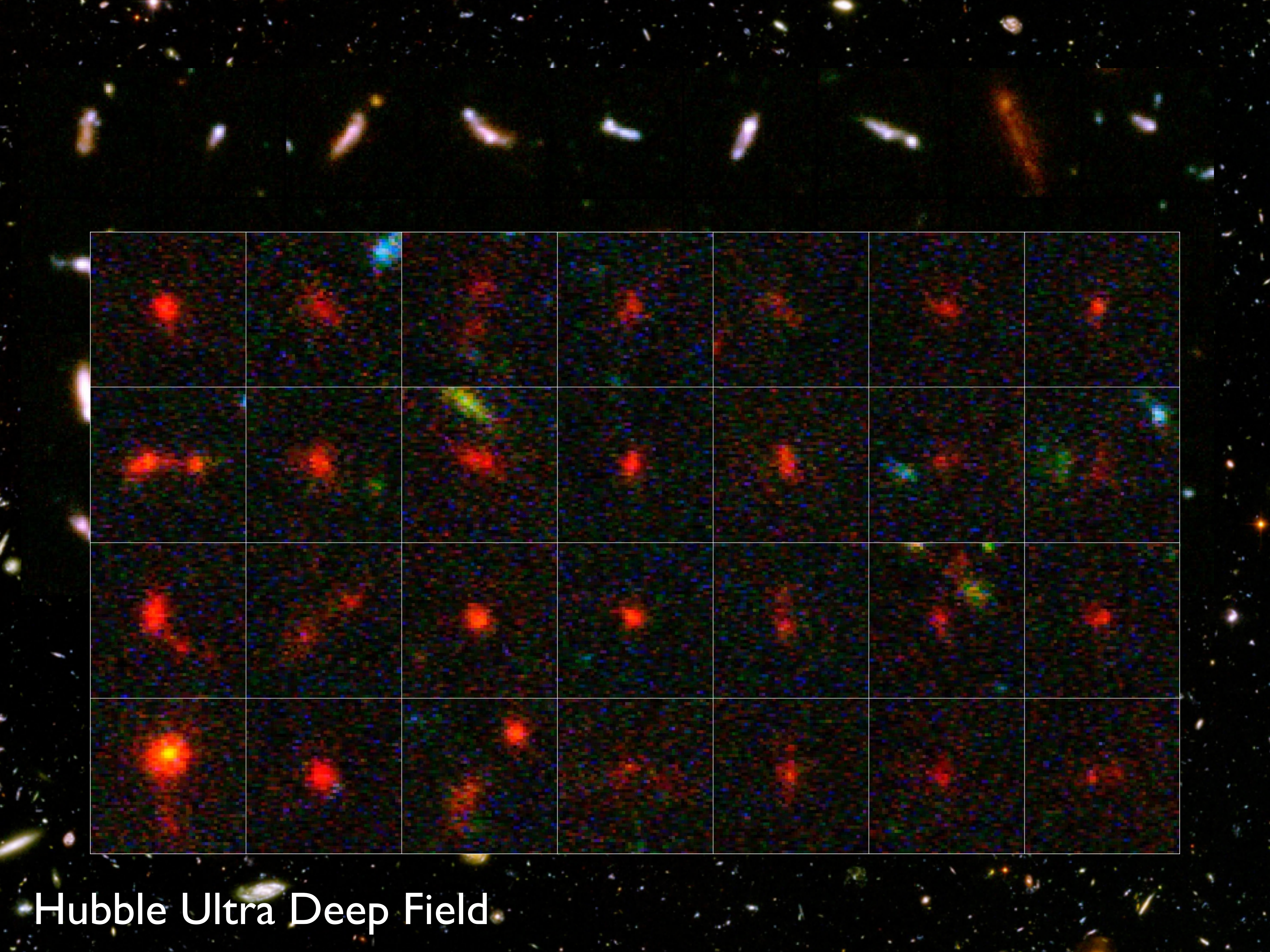


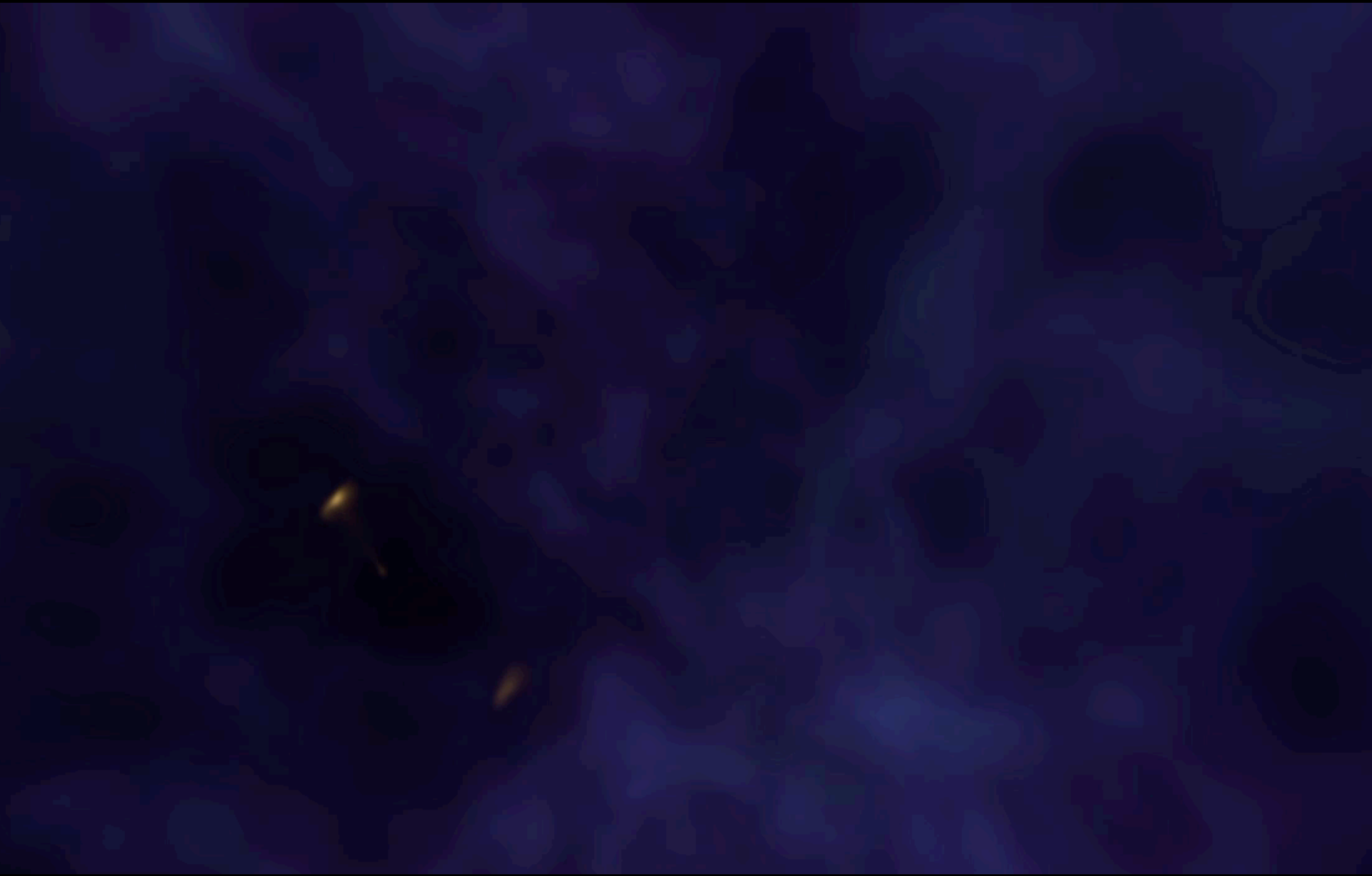

M31/Andromeda

NGC 147


Hubble Ultra Deep Field

Hubble Ultra Deep Field


Hubble Ultra Deep Field



Movie c/o NCSA Advanced Visualization Laboratory

Why is galaxy formation interesting?

Why is studying galaxy formation challenging?

Complex physics

- Cosmology
- Gravity
- Hydrodynamics
- Heating and cooling of gas
- Formation and feedback of stars & black holes
- Radiation transport
- Magnetic fields
- Etc...

Dynamic range

“Fair sample” of the universe: 10^8 ly

Milky Way and satellites: 10^6 ly

Star-forming cloud: 10^2 ly

Factor of 10^6!

Age of universe: $\sim 10^{10}$ years

Dynamical time of star-forming regions: $\sim 10^4$ years

Factor of 10^6!

Statistics/sampling

Outcome: a Blue Waters-worthy problem!

Our goal:

Understanding the first generations of galaxy formation

Our simulation tool:
The Enzo AMR code

http://enzo-project.org

[Intimidating equations slide]

$$\frac{\partial \rho}{\partial t} + \frac{1}{a}\nabla \cdot (\rho \mathbf{v}) = 0$$

$$\frac{\partial \rho \mathbf{v}}{\partial t} + \frac{1}{a}\nabla \cdot \left(\rho \mathbf{v}\mathbf{v} + \mathbf{I}p^{*} - \frac{\mathbf{B}\mathbf{B}}{a}\right) = -\frac{\dot{a}}{a}\rho \mathbf{v} - \frac{1}{a}\rho \nabla \phi$$

$$\frac{\partial E}{\partial t} + \frac{1}{a}\nabla \cdot \left[(E + p^{*})\mathbf{v} - \frac{1}{a}\mathbf{B}(\mathbf{B}\cdot\mathbf{v})\right] = -\frac{\dot{a}}{a}\left(2E - \frac{B^2}{2a}\right) - \frac{1}{a}\mathbf{v}\cdot\nabla\phi - \Lambda + \Gamma + \frac{1}{a^2}\nabla\cdot\mathbf{F}_{\rm cond}$$

$$\frac{\partial \mathbf{B}}{\partial t} - \frac{1}{a}\nabla \times (\mathbf{v} \times \mathbf{B}) = 0$$

$$\frac{d\mathbf{x}}{dt} = \frac{1}{a}\mathbf{v},$$

$$\frac{d\mathbf{v}}{dt} = -\frac{\dot{a}}{a}\mathbf{v} - \frac{1}{a}\nabla\phi$$

$$\frac{\partial E_r}{\partial t} + \frac{1}{a}\nabla \cdot (E_r \mathbf{v}) = \nabla \cdot (D \nabla E_r) - \frac{\dot{a}}{a}E_r - c\kappa E_r + \eta$$

$$\frac{\ddot{a}}{a} = -\frac{4\pi G}{3a^3}(\rho_0 + 3p_0/c^2) + \Lambda_c/3 \qquad p^{*} = p + \frac{B^2}{2a}$$

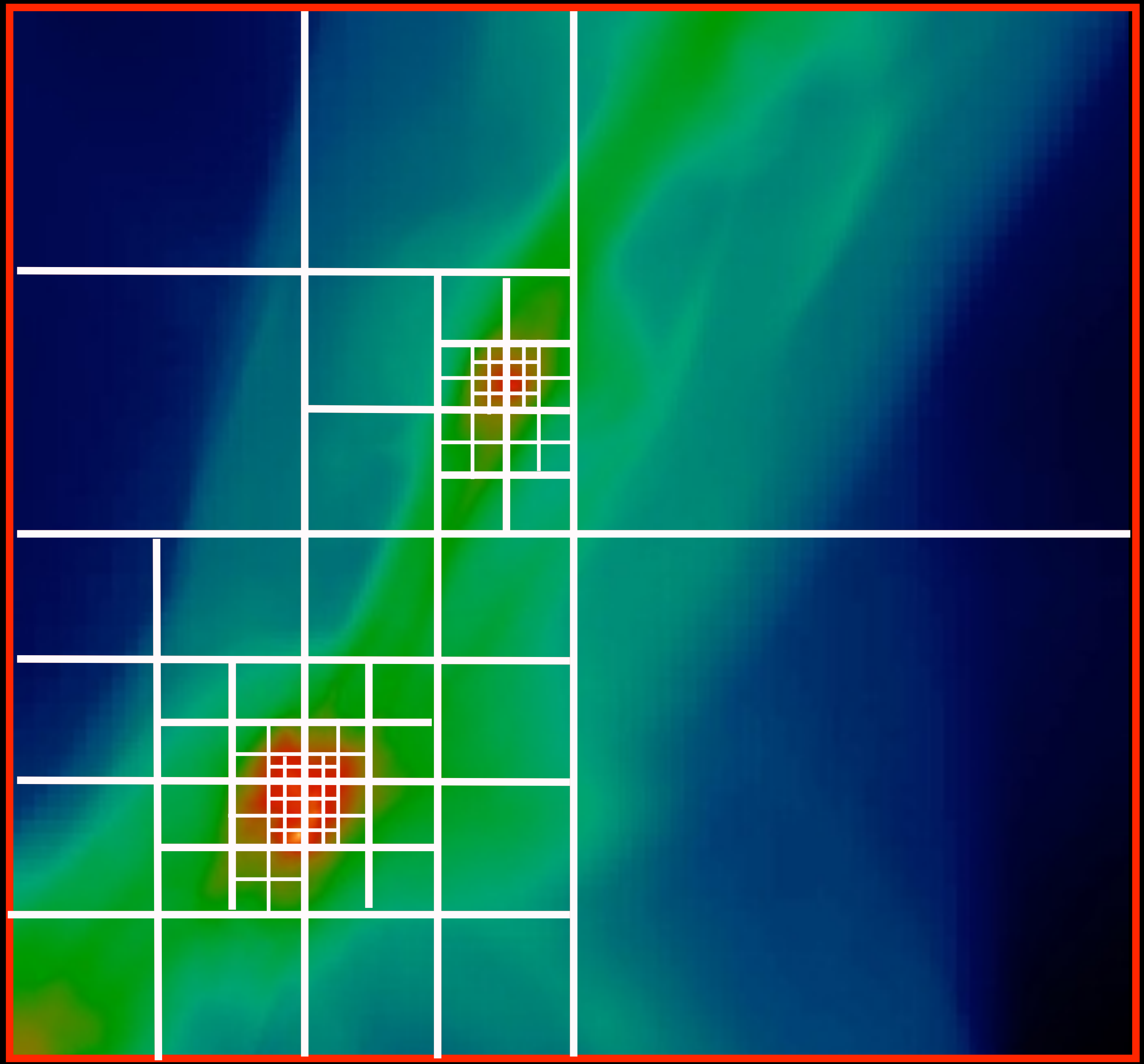
$$e = p/[(\gamma - 1)\rho]$$

$$\nabla^2 \phi = 4\pi G \rho_{\rm total}$$

$$E = e + \frac{\rho v^2}{2} + \frac{B^2}{2a}$$

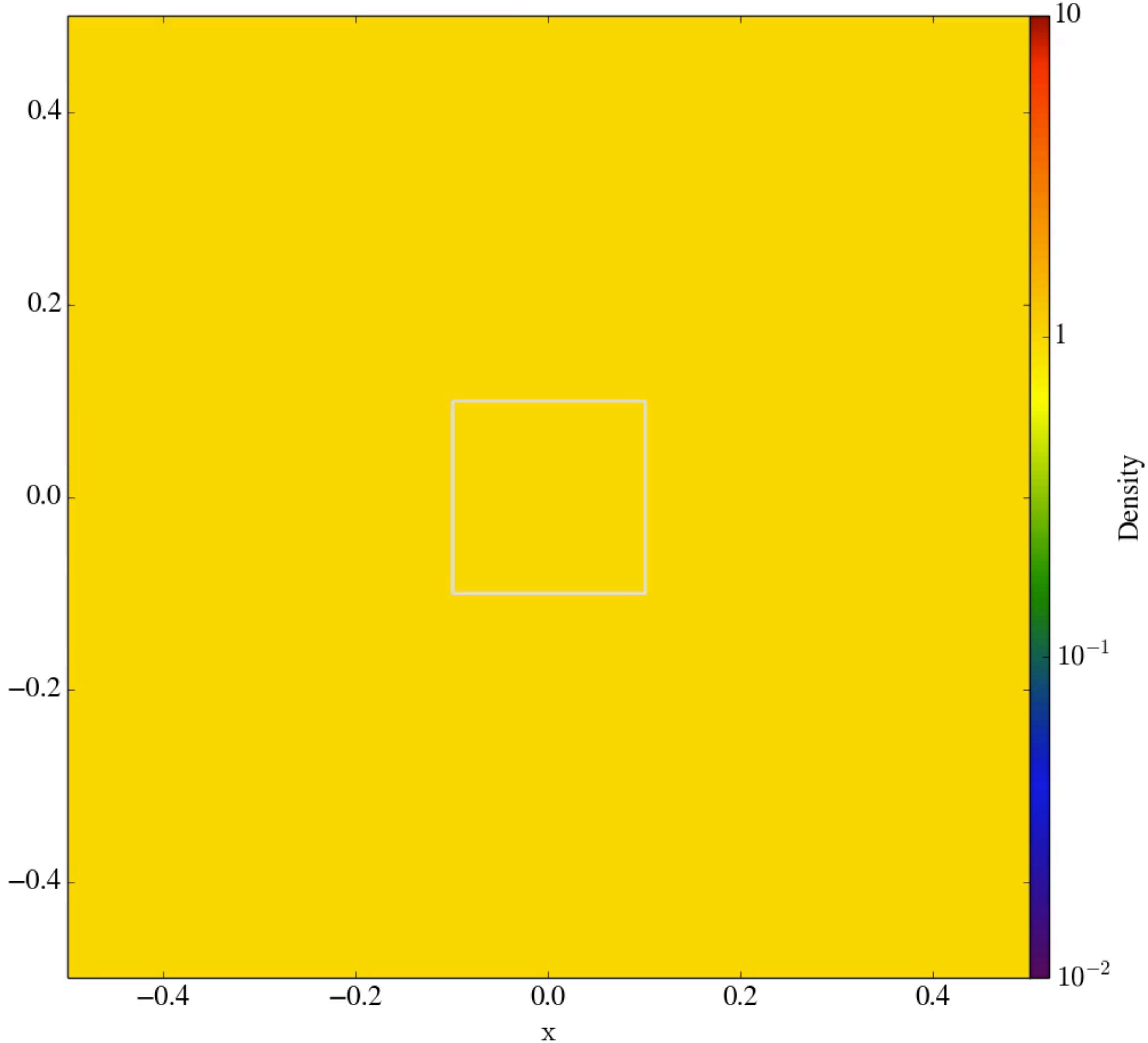
$$\frac{\partial n_i}{\partial t} + \frac{1}{a}\nabla \cdot (n_i \mathbf{v}) = k_{ij}(T) n_i n_j + \Gamma_j^{ph} n_j$$

Schematic example of AMR

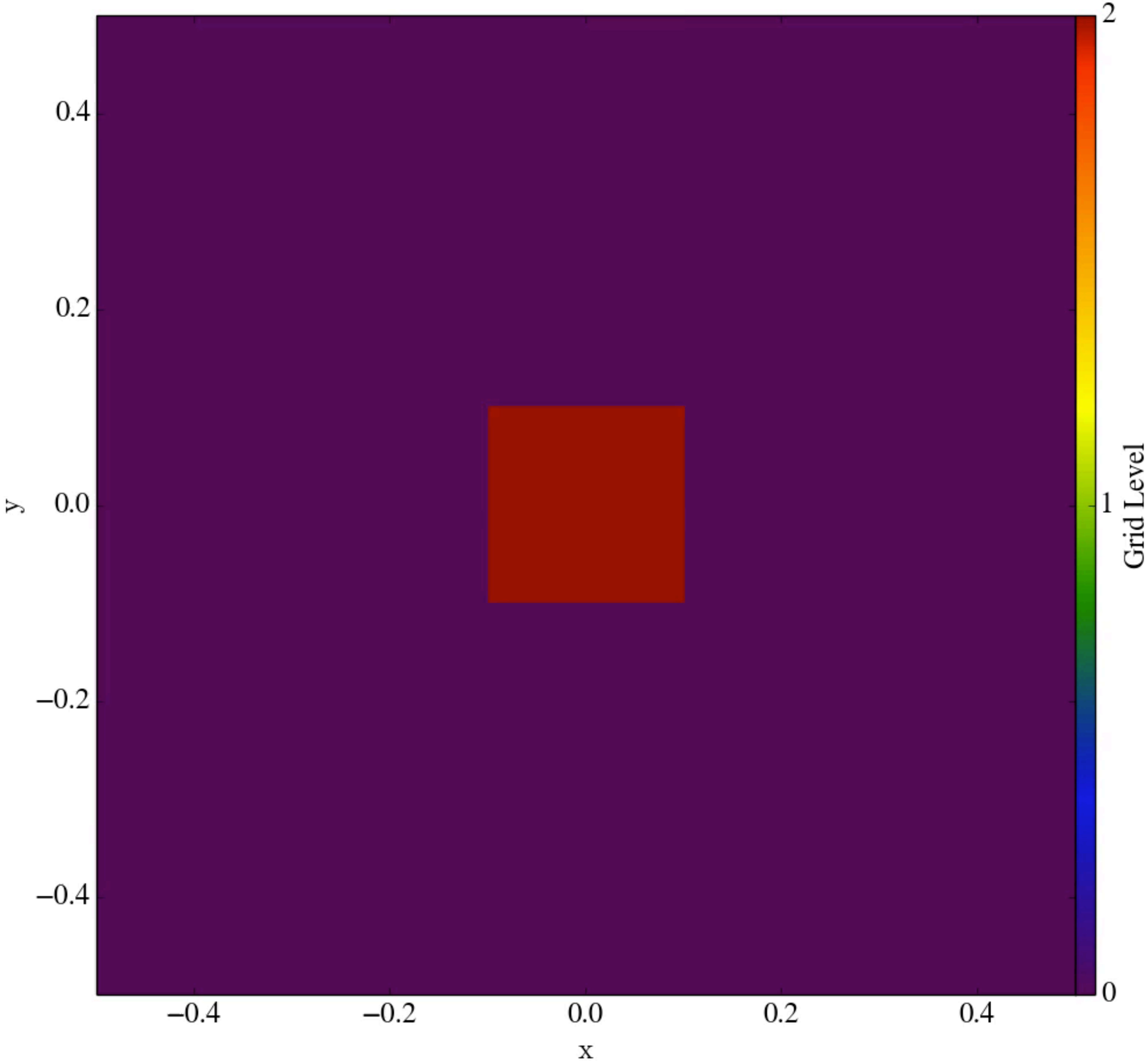


Dynamic example of AMR

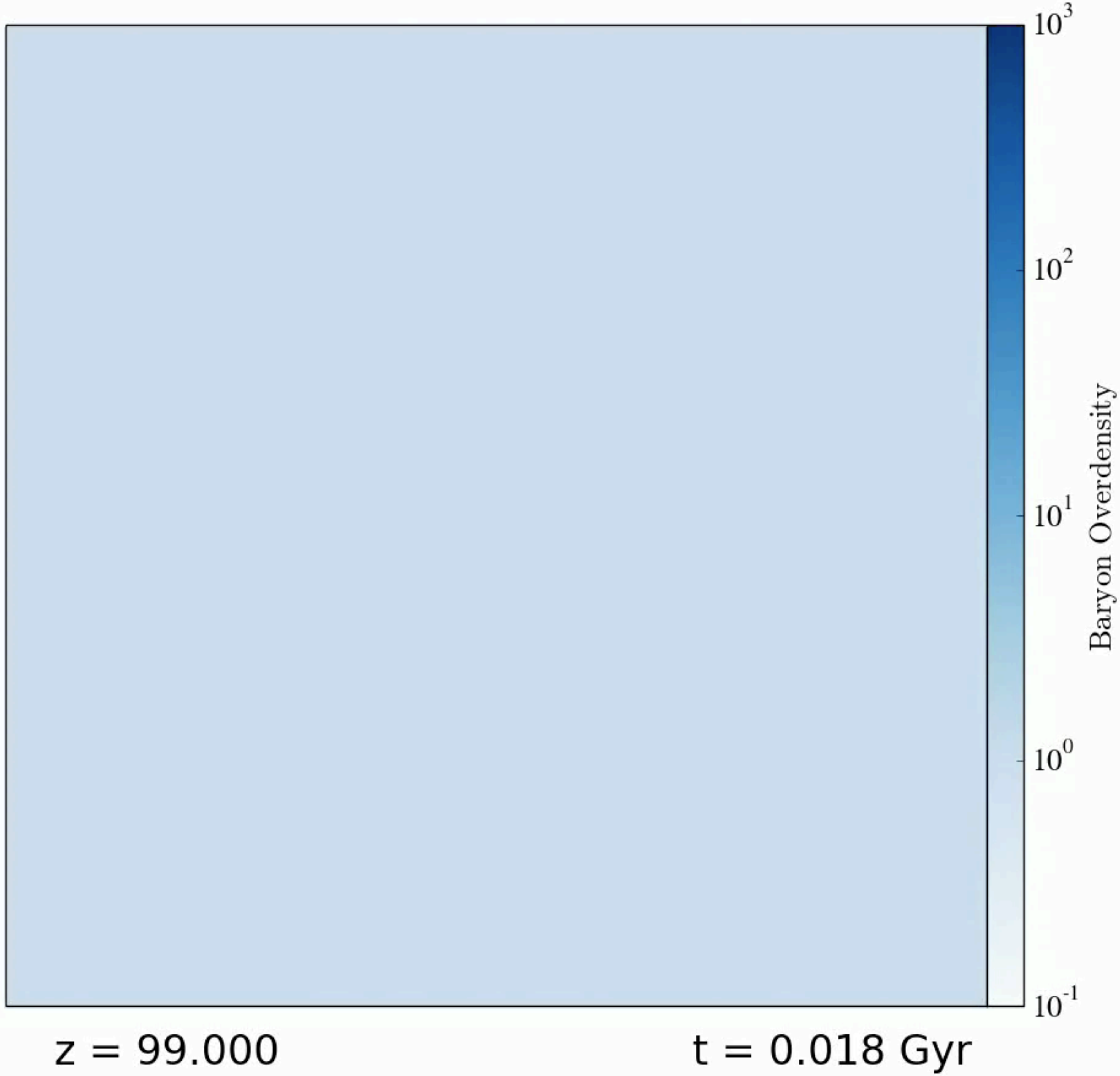
Note: movies available at
http://www.pa.msu.edu/~oshea/



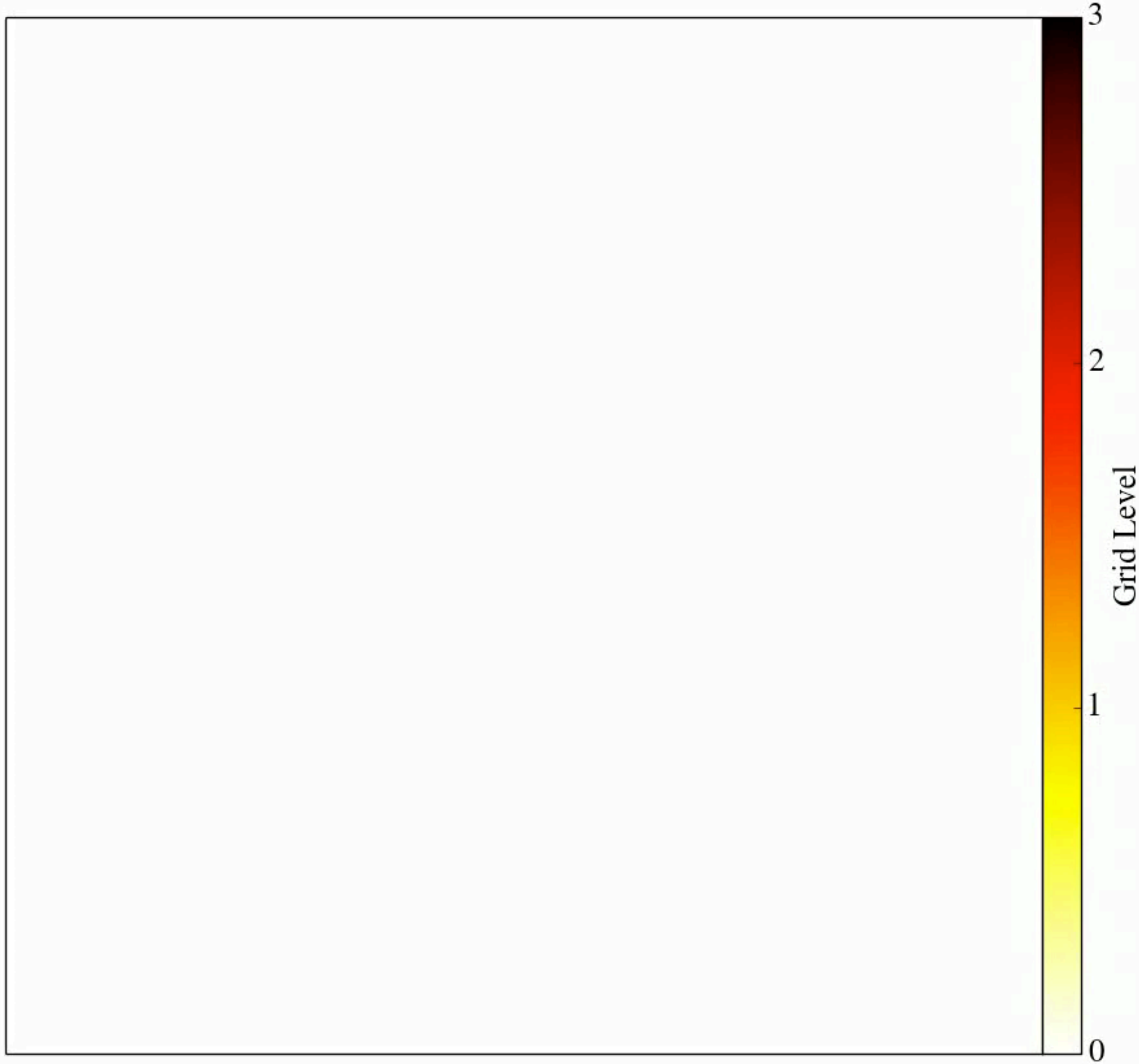
0.4
0.2
0.0
−0.2
−0.4
y
−0.4
−0.2
0.0
0.2
0.4
x
10
1
10^{-1}
10^{-2}
Density



0.4
0.2
0.0
−0.2
−0.4
y
−0.4
−0.2
0.0
0.2
0.4
x
2
1
0
Grid Level



10^{3}
10^{2}
10^{1}
10^{0}
10^{-1}
Baryon Overdensity
z = 99.000
t = 0.018 Gyr



z = 99.000

t = 0.018 Gyr

Our analysis and visualization tool:

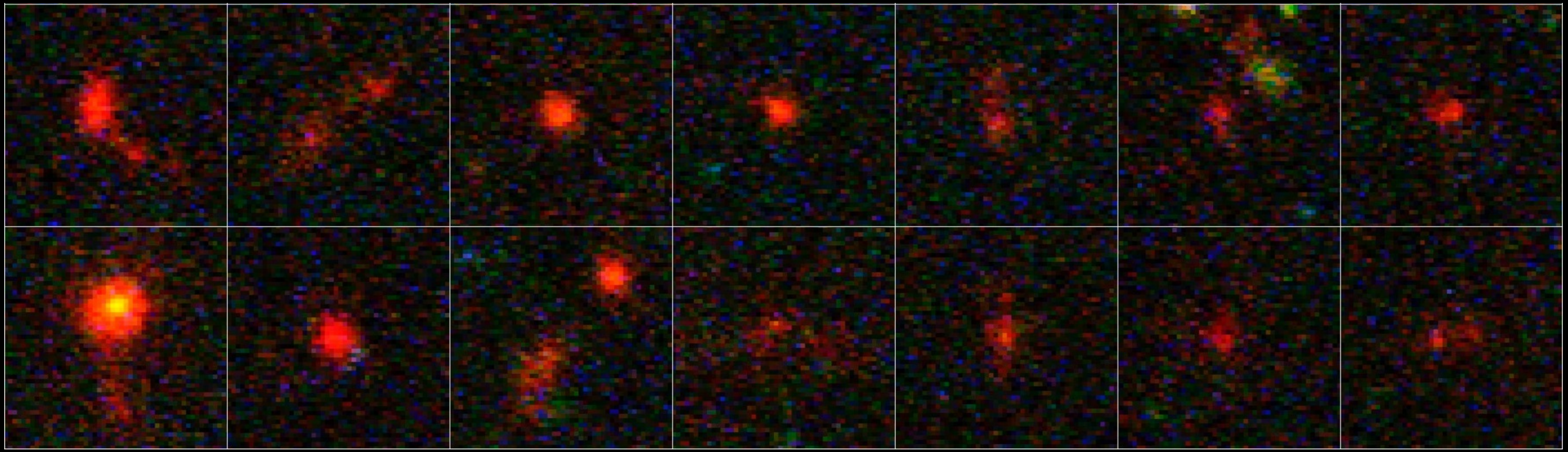
Turk et al. 2011, ApJS, 192, 9

http://yt-project.org

Why Blue Waters?

- Excellent interconnect + lots of memory per node: great scaling! (Esp. for radiation transport)
- Excellent file system: easy to create and manipulate simulation data
- Rapid turnaround for simulations and analysis
- Result: we can perform simulations on Blue Waters that are **10-100x larger** than is possible on XSEDE systems!

The big question: How do the first galaxies form?



Critical and unique simulation characteristics:

Radiation transport, unprecedented spatial, mass resolution, star-by-star HII regions and supernovae

Lots of results!

- Xu et al., "Heating the Intergalactic Medium by X-Rays from Population III Binaries in High-redshift Galaxies," 2014, ApJ, 791, 110
- Chen et al., "Scaling Relations for Galaxies Prior to Reionization," 2014, ApJ, 795, 144
- Ahn et al., "Spatially Extended 21 cm Signal from Strongly Clustered UV and X-Ray Sources in the Early Universe", 2015, ApJ, submitted
- O'Shea et al., "The ultraviolet luminosity function of the first galaxies," 2015, ApJ submitted
- Smith et al., "The First Population II Stars Formed in Externally Enriched Mini-halos," 2015, ApJ submitted
- Xu et al., "Ionising Photons From Faint Galaxies During the Epoch of Reionization," 2015, ApJ, in prep (submitting ~end of March)
- Shi et al., "The Dynamics of Seed Black Holes in the First Galaxies," 2015, ApJ, in prep. (submitting ~April)

And much more to come!

Two sets of simulations

The transition to metal-enriched star formation: Britton Smith*, John Wise*, BWO

Evolution of early galaxy populations: Hao Xu*, Pengfei Chen, Mike Norman, BWO

* Ran the simulations

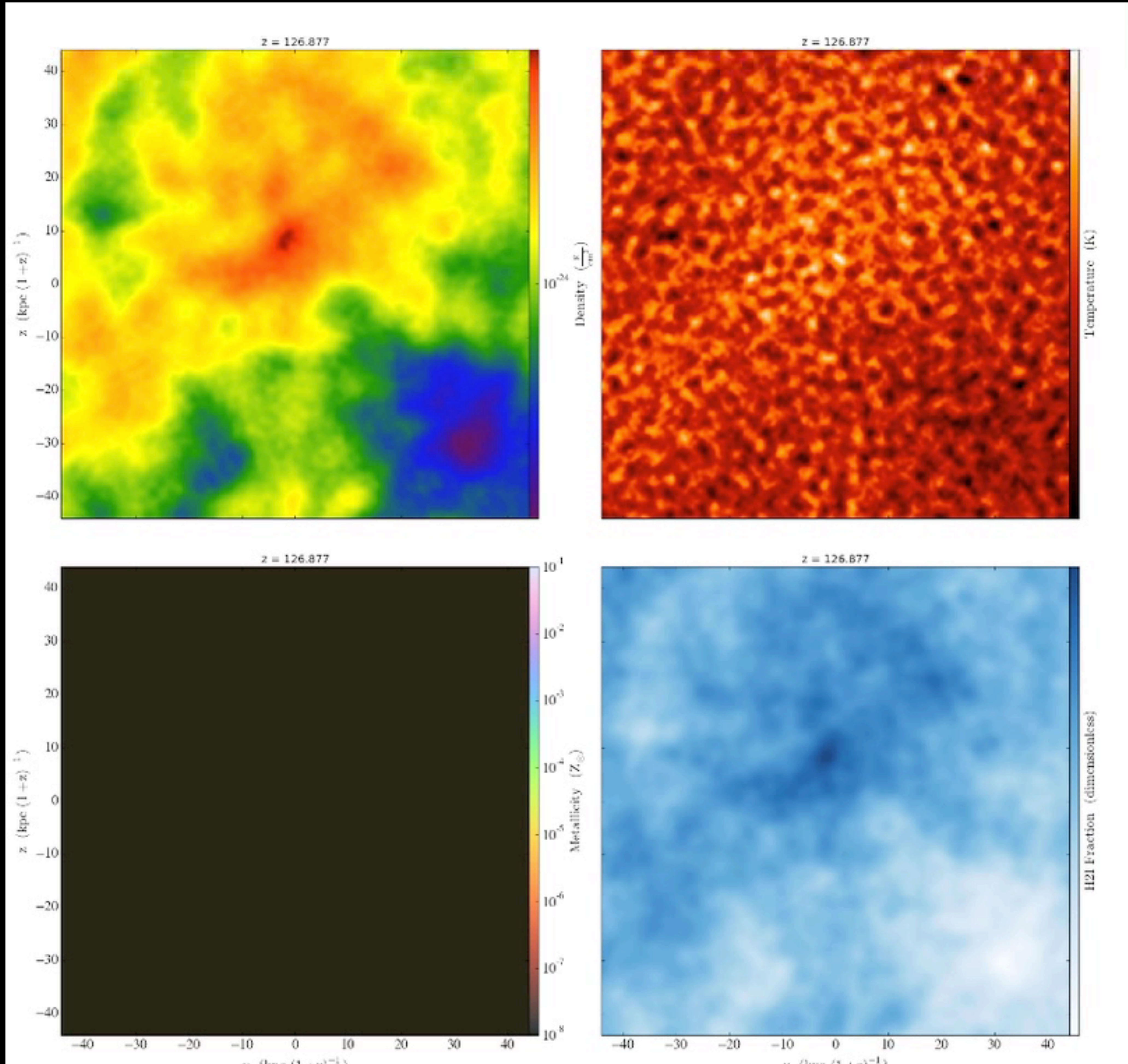
The transition to metal-enriched star formation

- 0.5 Mpc/h box
- 13 levels of AMR prior to explosion (0.119 pc comoving max); 30 after (~1 au comoving)
- ~0.19 $M_\odot$ gas, 0.92 $M_\odot$ dm mass resolution
- Primordial gas + metal + dust chemistry & cooling
- Radiation transport for Pop III stars; core-collapse supernovae w/11.2 $M_\odot$ of metals

Smith, Wise, O'Shea & Norman 2015

Density

Temp.

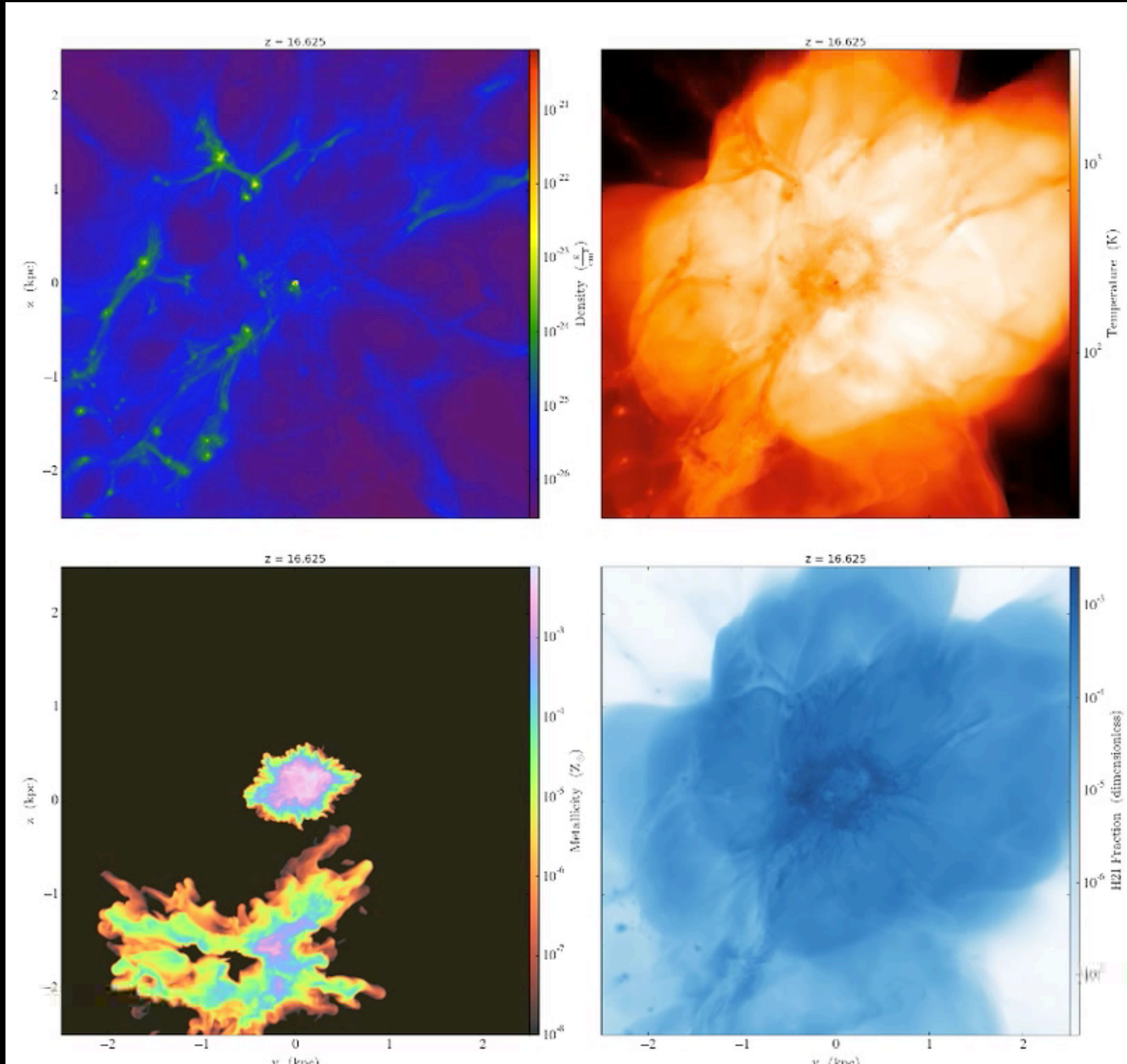


Metallicity

H_2

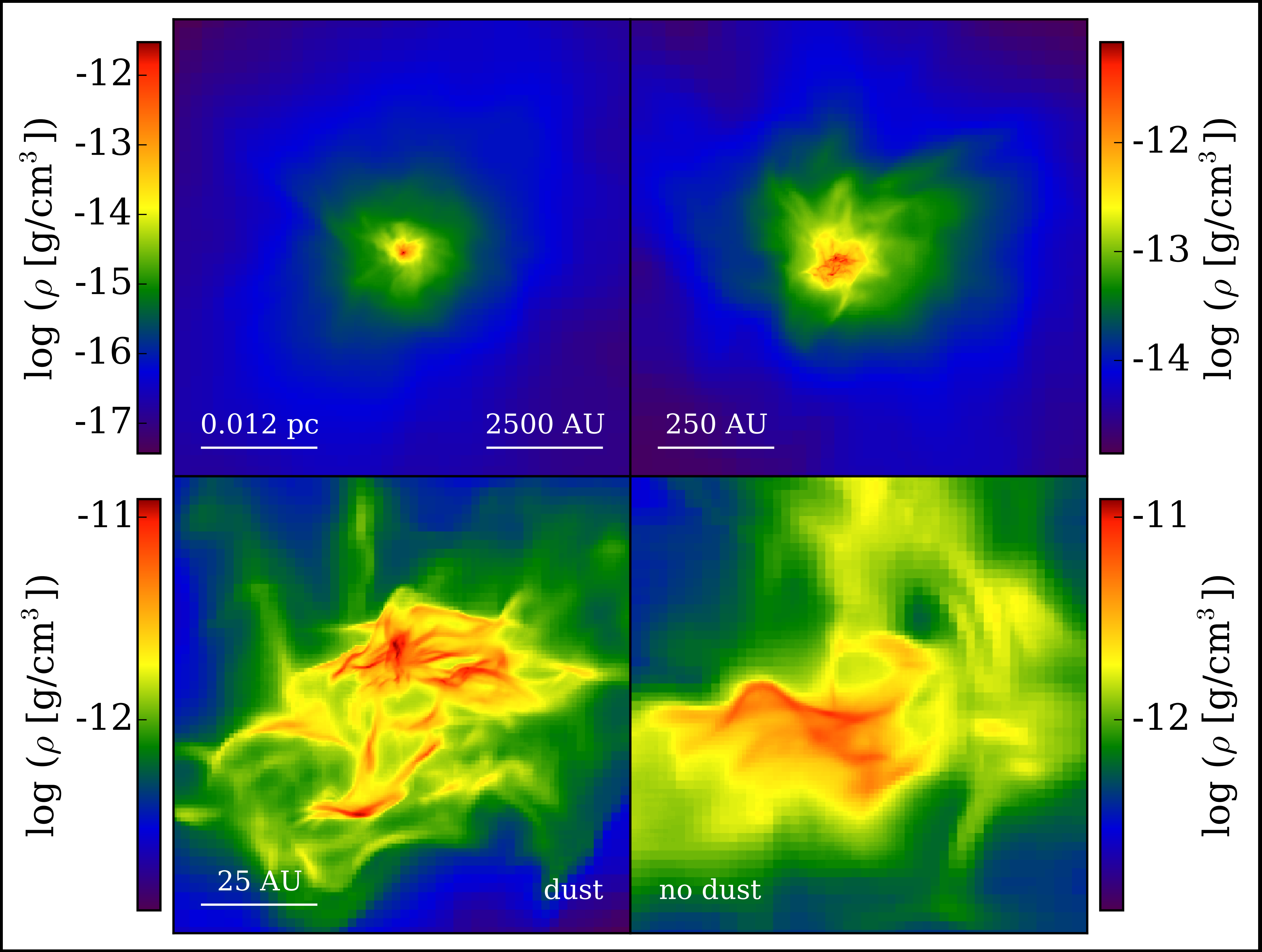
Density

Temp.

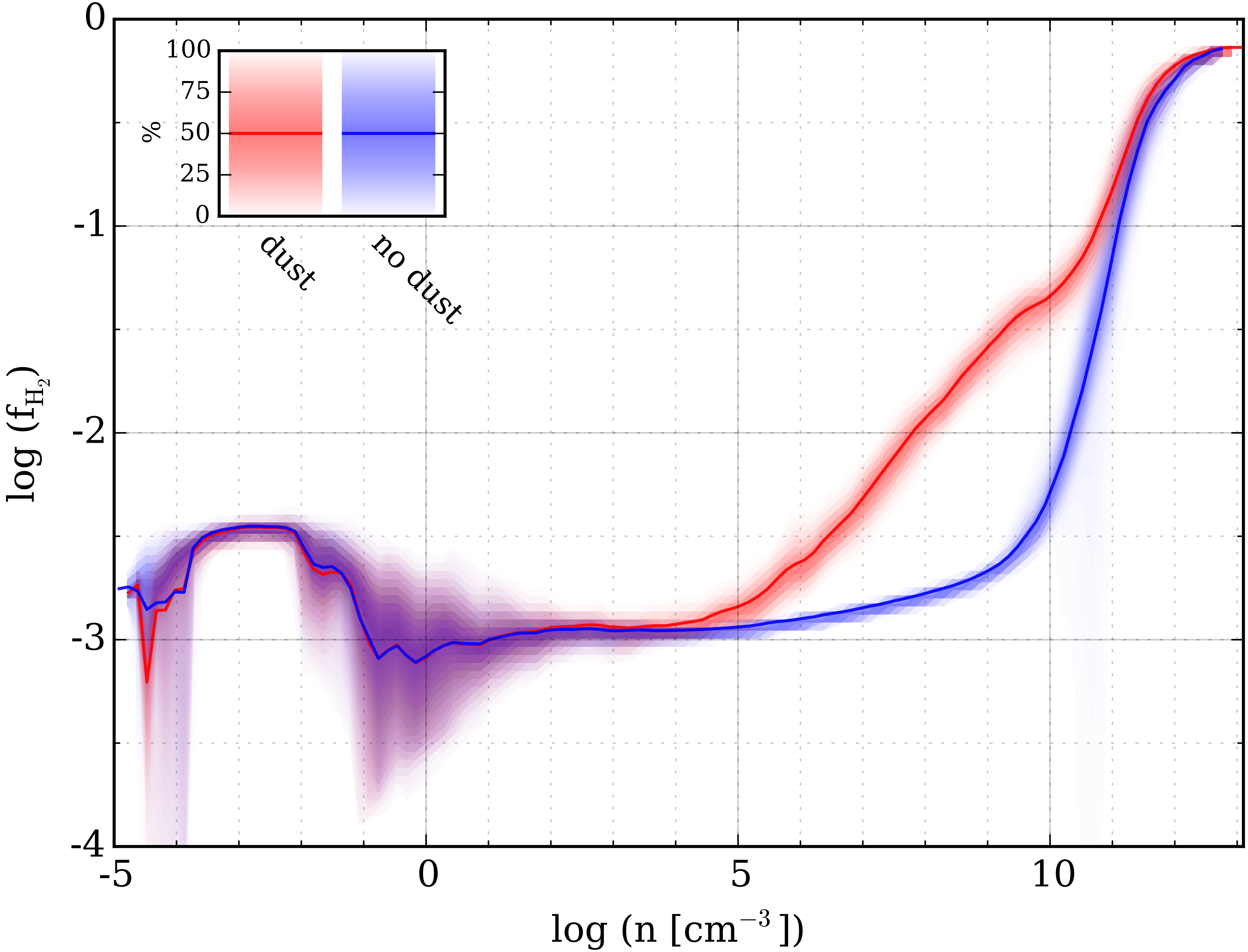


Metallicity

H_2



-12
-13
-14
-15
-16
-17
log (ρ [g/cm^3])
0.012 pc
2500 AU
250 AU
-12
-13
-14
log (ρ [g/cm^3])
-11
-12
log (ρ [g/cm^3])
25 AU
dust
no dust
-11
-12
log (ρ [g/cm^3])



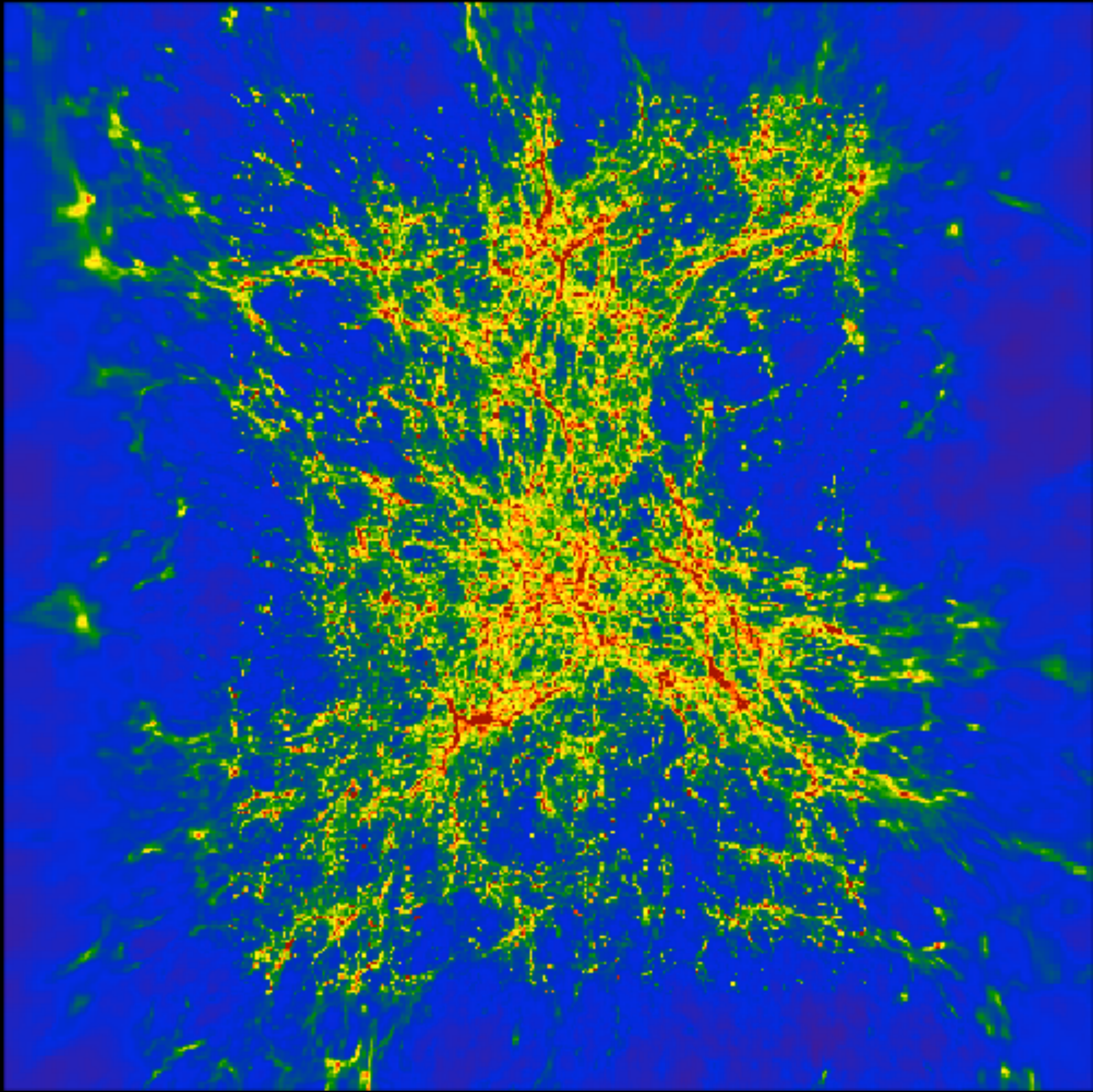
0
-1
-2
-3
-4
-5
0
5
10
log (n [cm^{-3}])
log (f_{H_2})
100
75
50
25
0
%
dust
no dust

Evolution of early galaxy populations

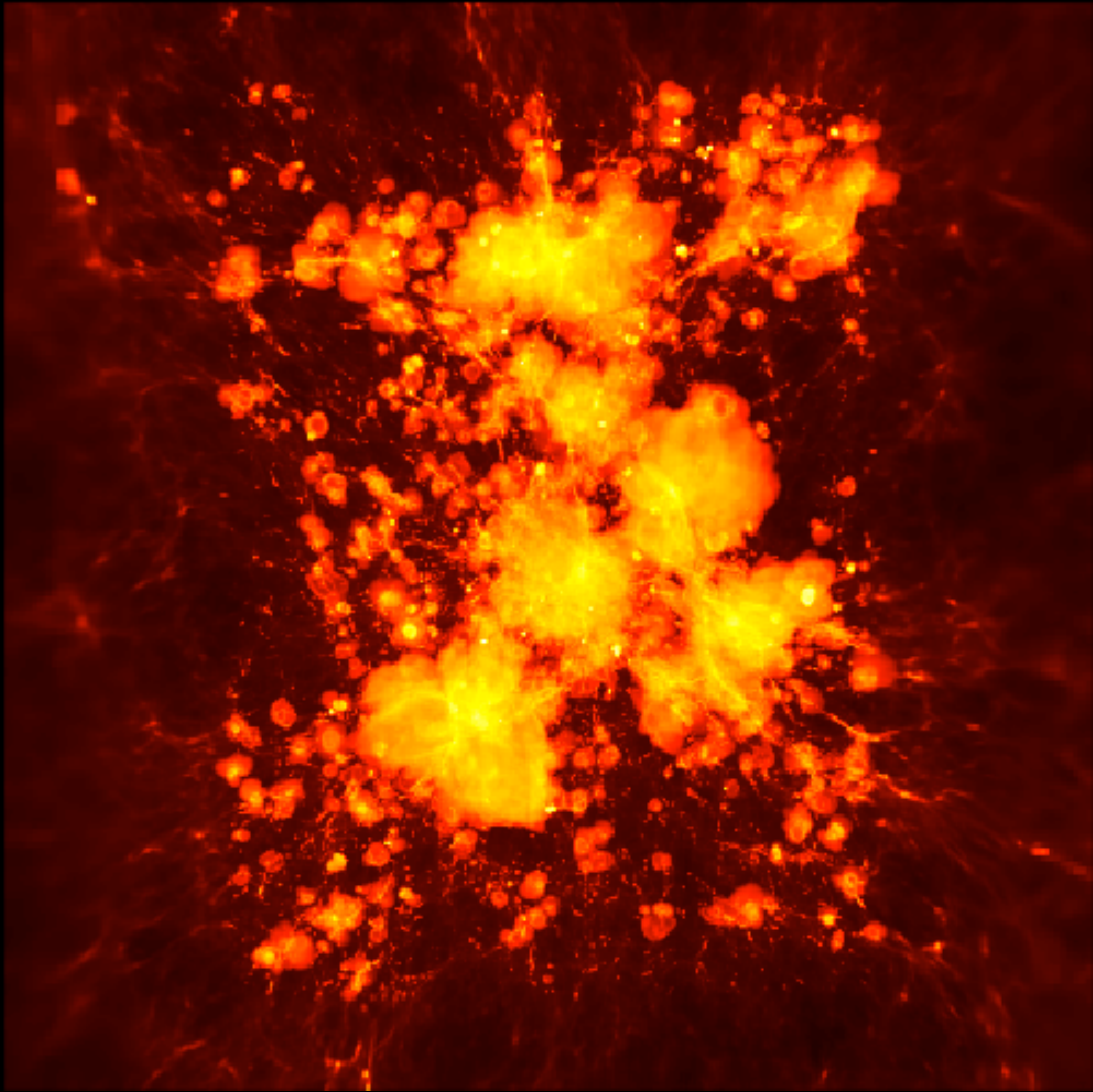
- 40 Mpc box, refine on three separate ~300 Mpc^3 regions (overdense, average, low density)
- Simulation at 12 levels of AMR (19 comoving pc), primordial + metal-enriched chemistry, Pop III and metal-enriched SF
- 13,000 Pop III stars formed, ~3,000 halos > 10^7 $M_\odot$ (with star formation) by end of simulations
- Multiple Pop III stars per halo at later times!

Hao Xu et al. 2014, 15; Chen et al. 2014; O'Shea et al. 2015

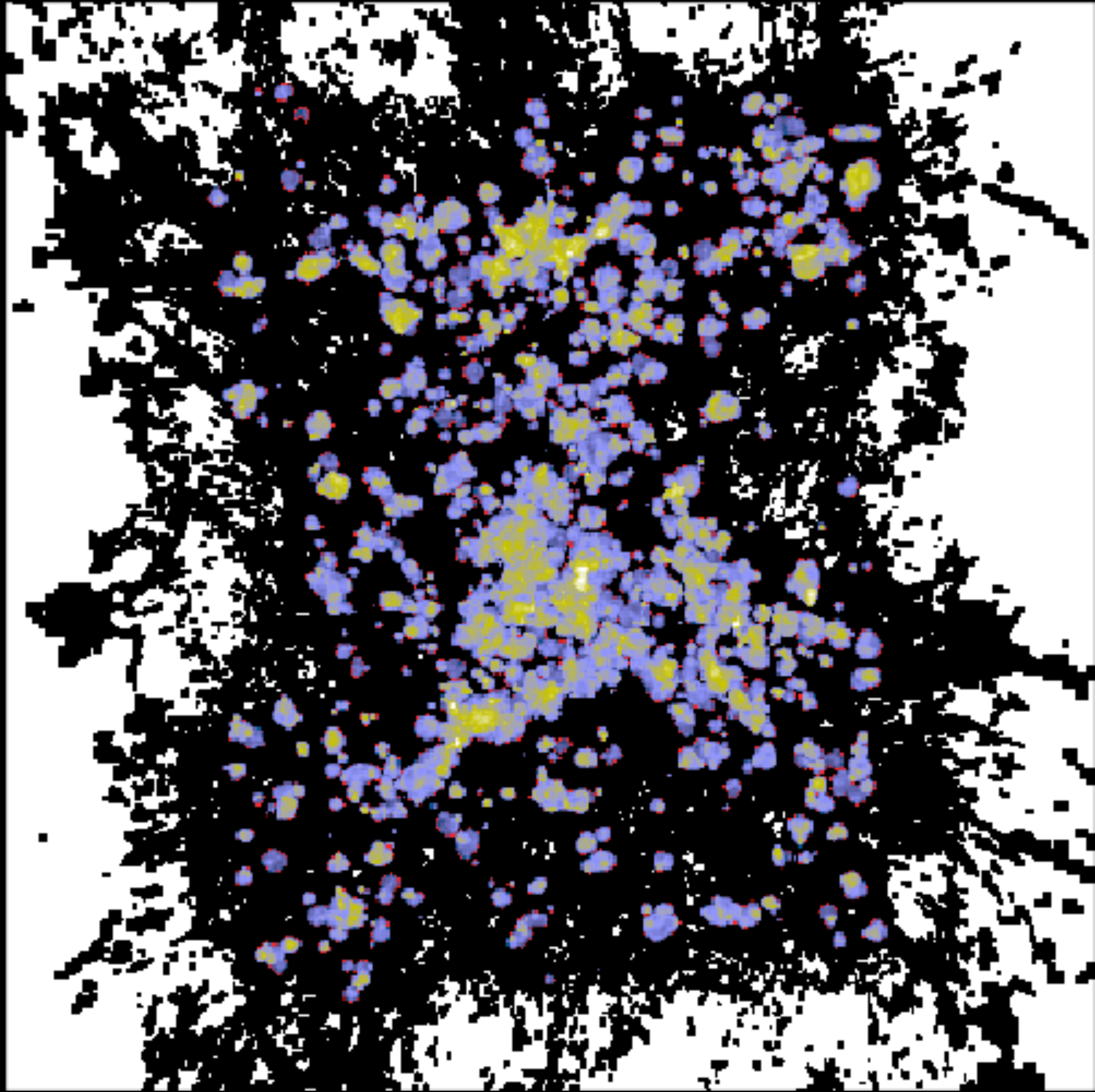
Density



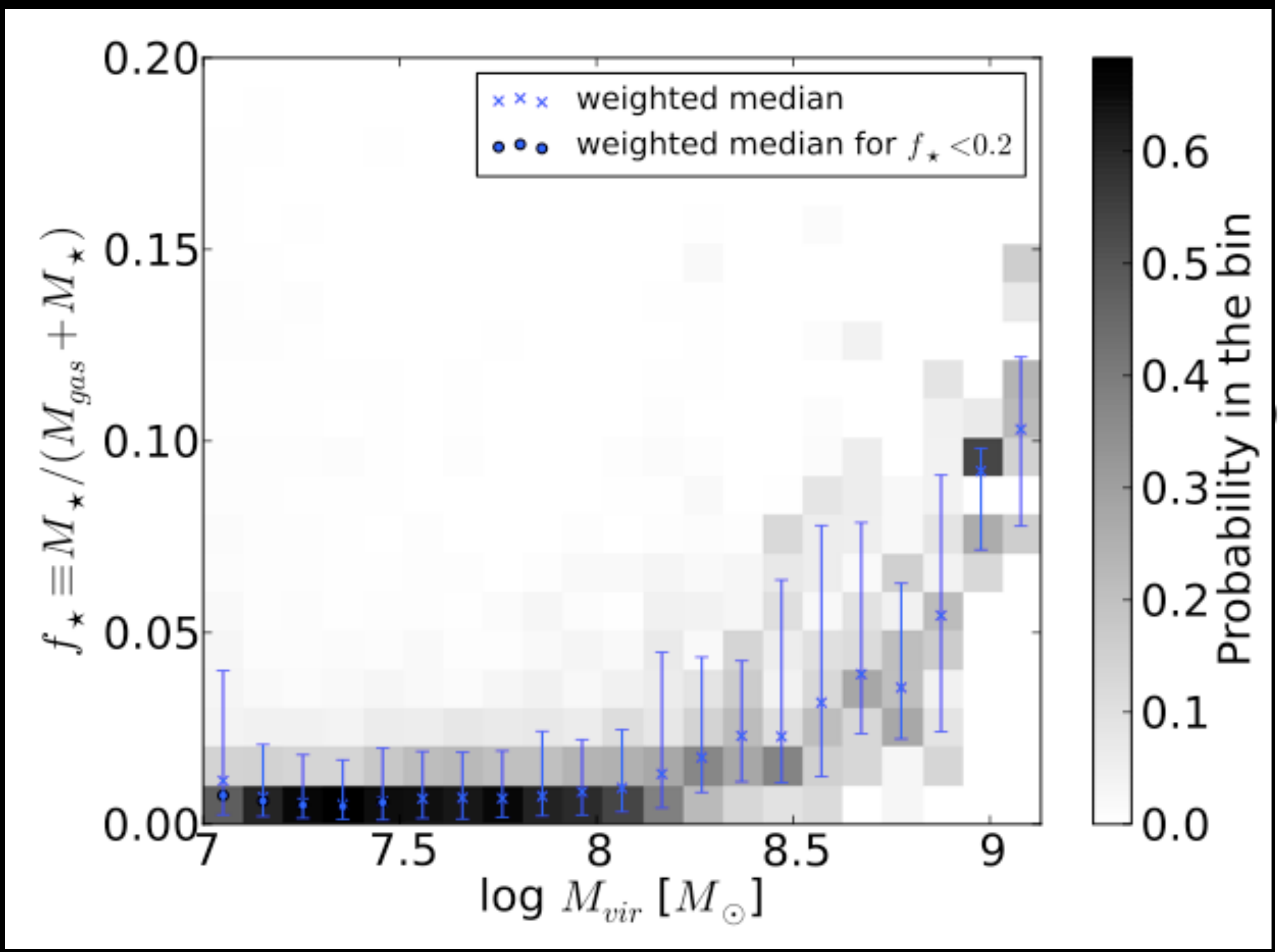
Temperature

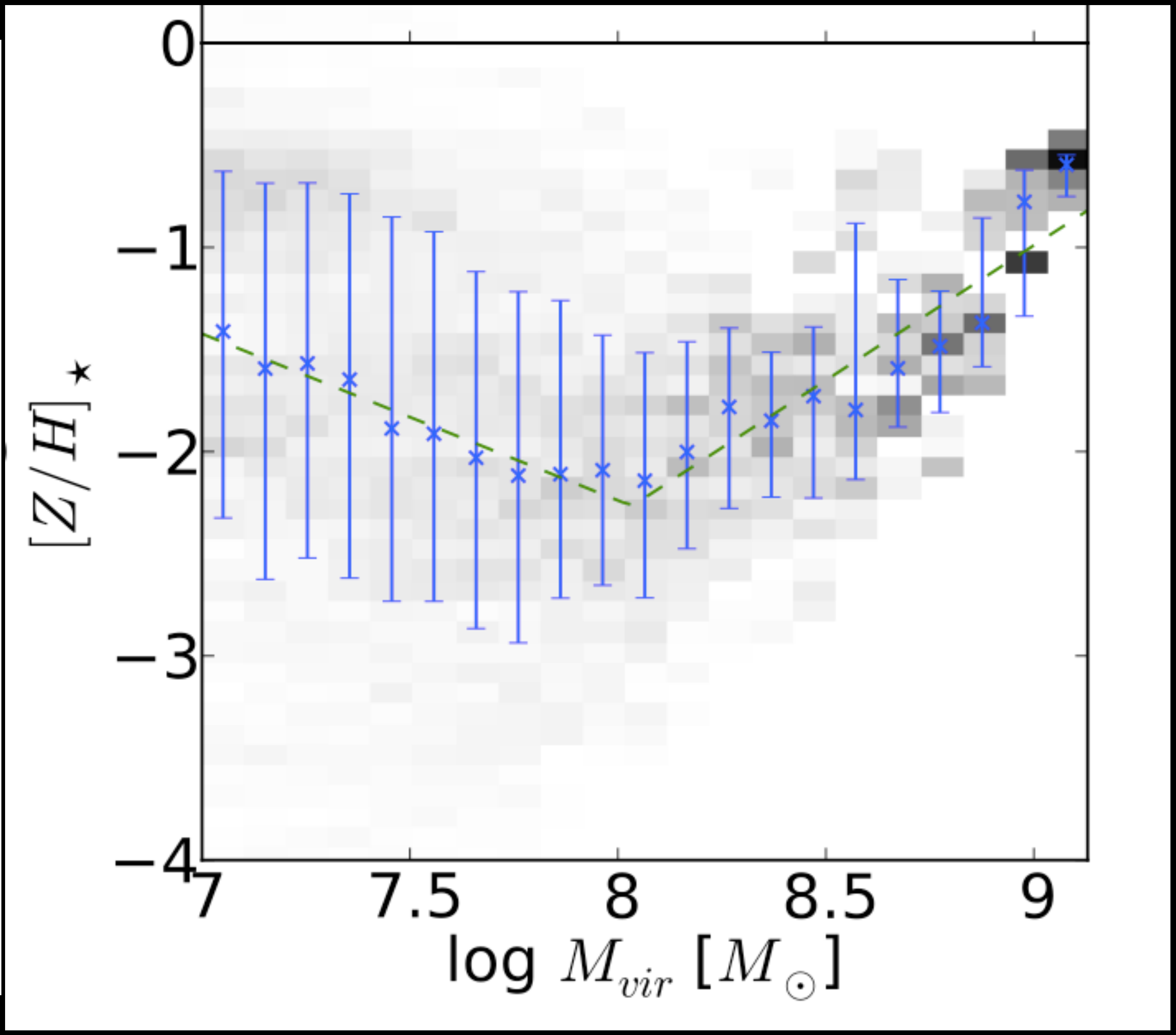


Metals



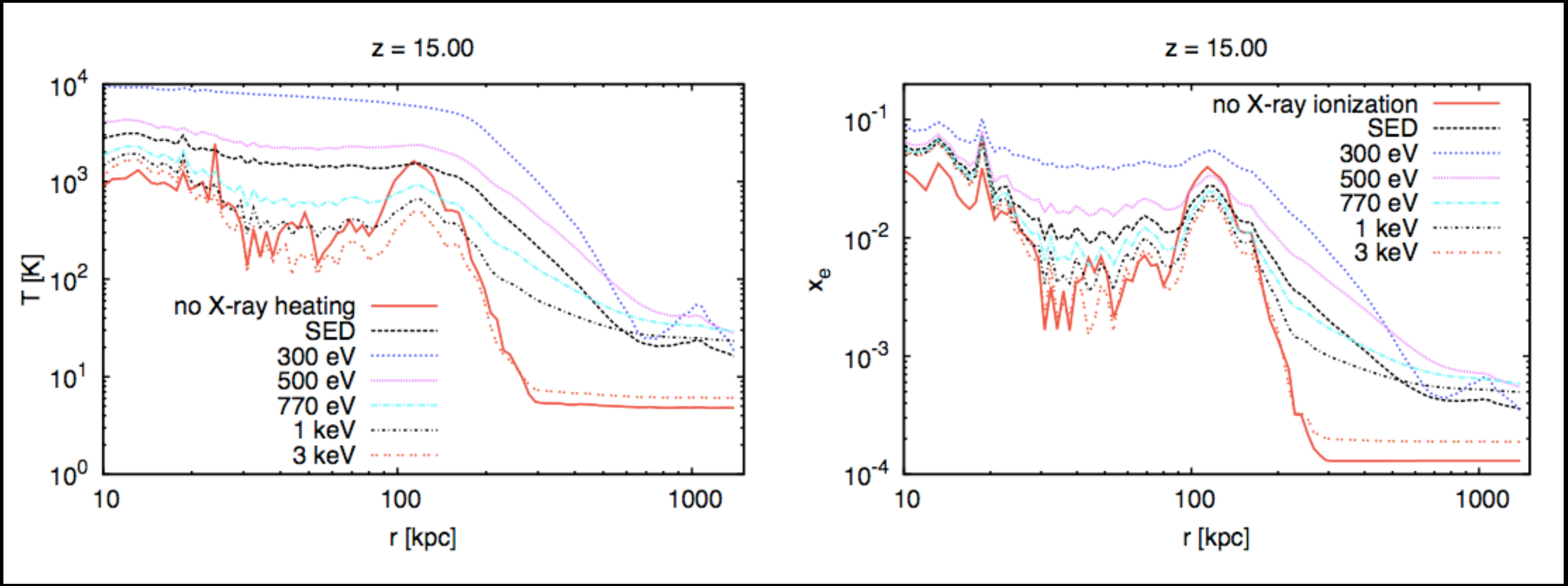
Formation of high-redshift dwarf galaxies





Chen et al. 2014

Heating the intergalactic medium with X-ray binaries



Xu et al. 2014

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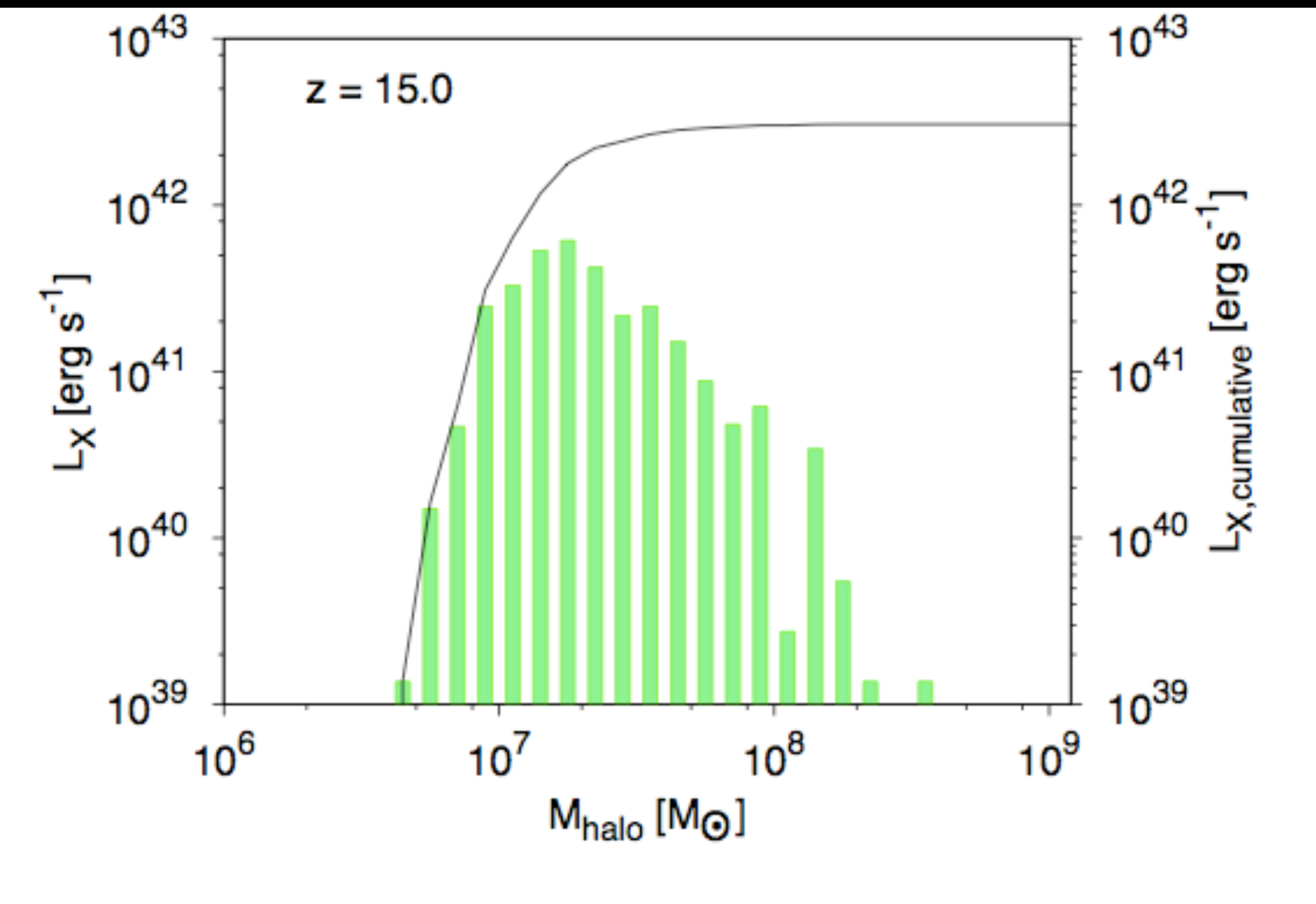
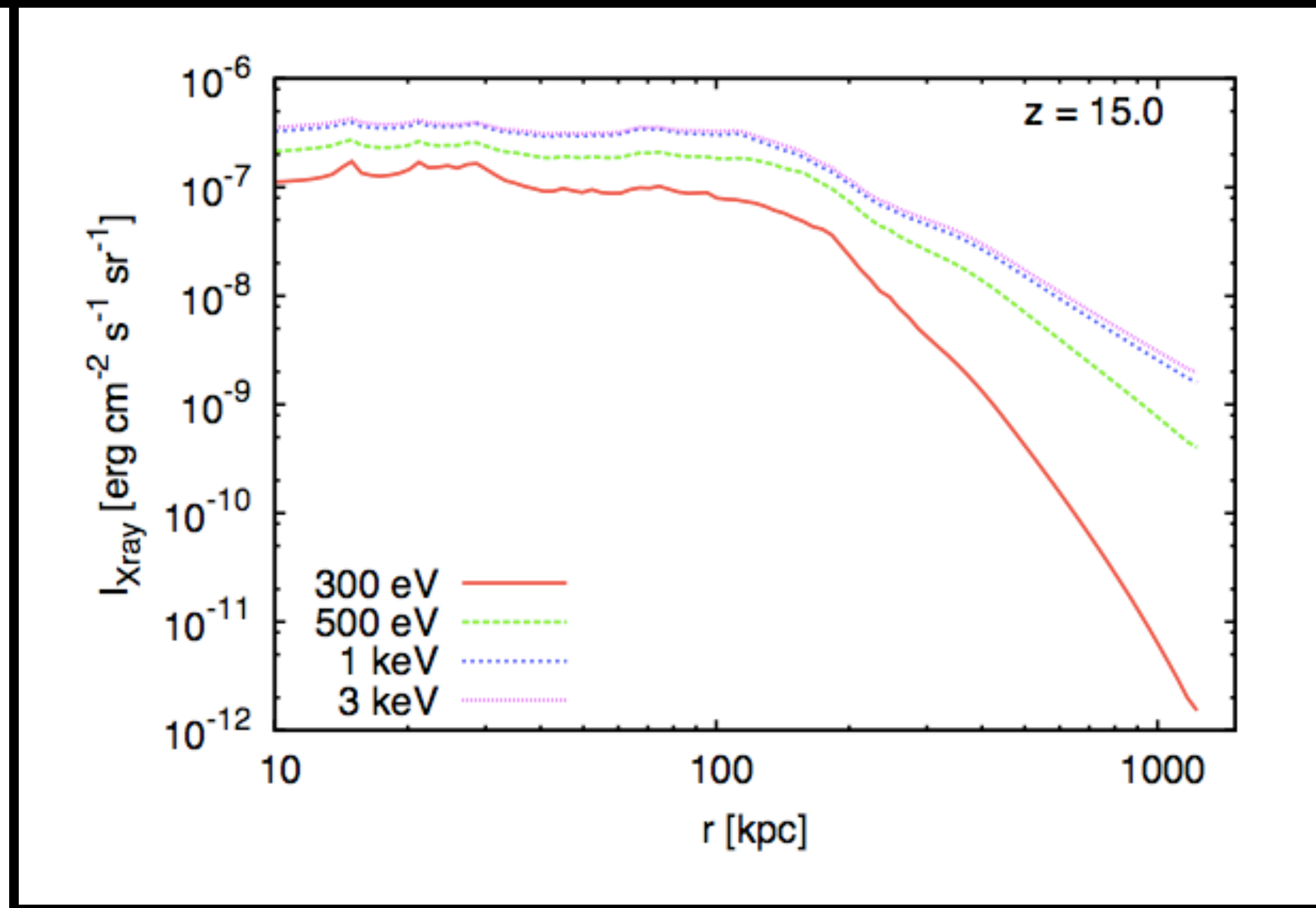
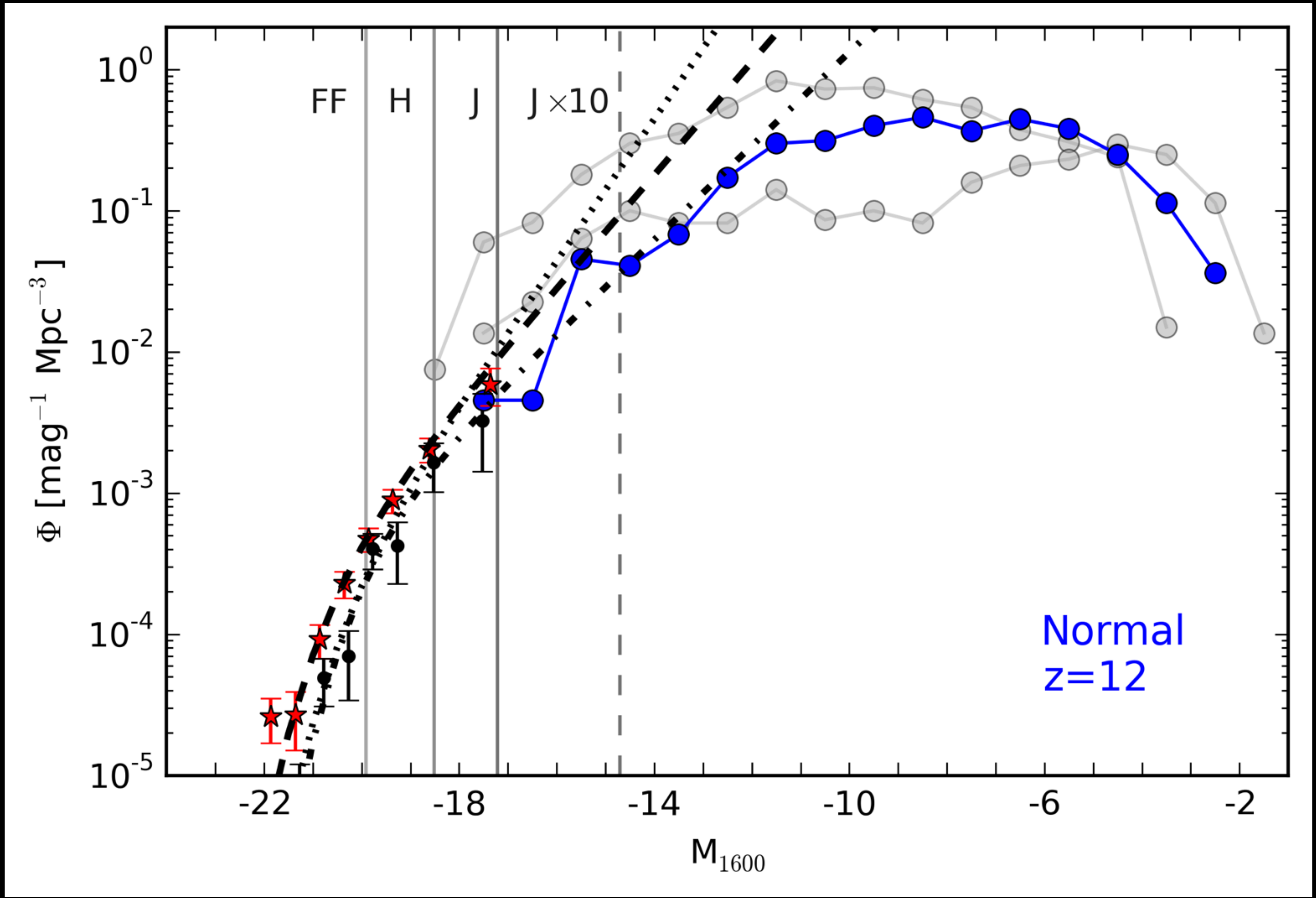




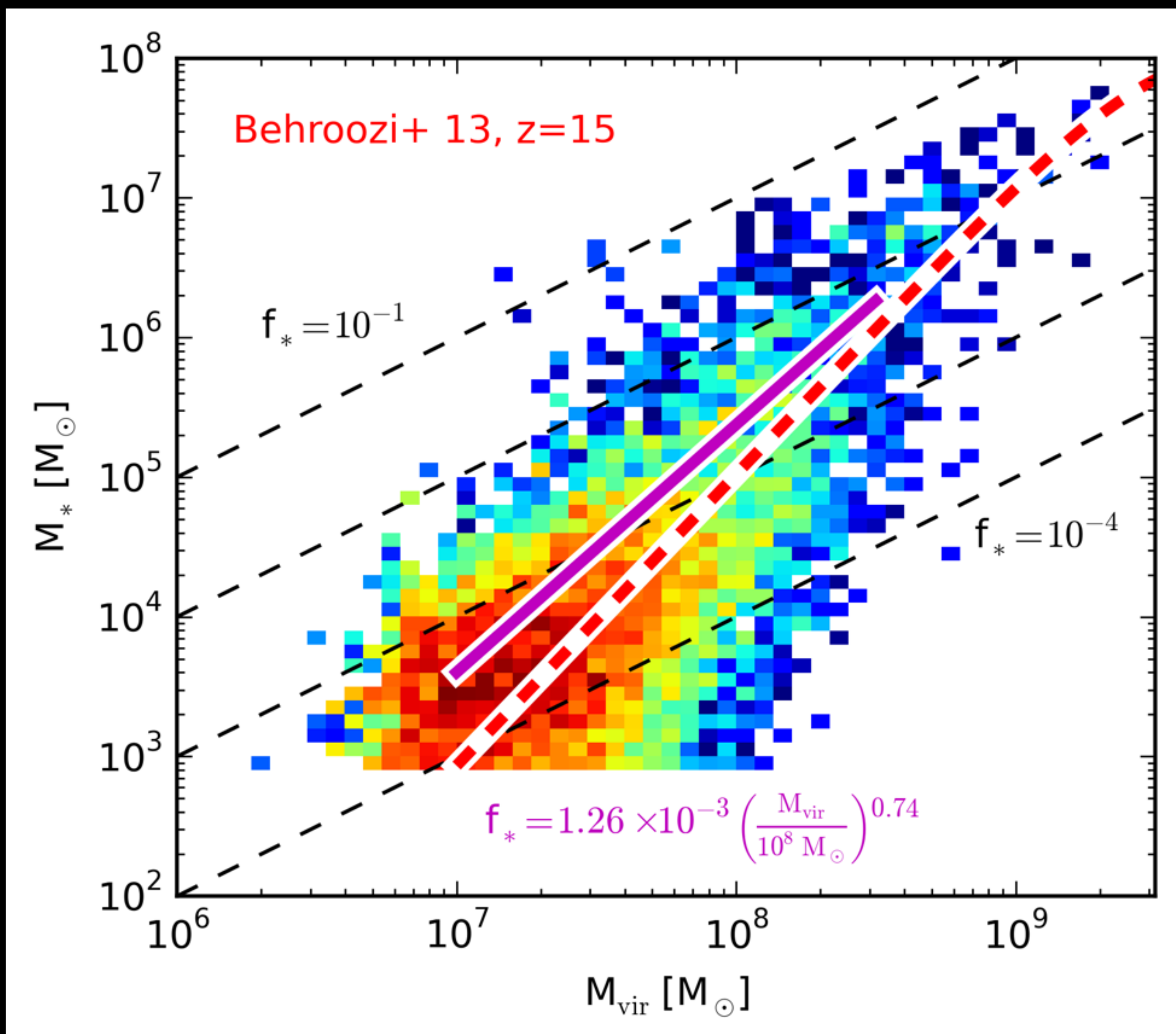
Xu et al. 2014

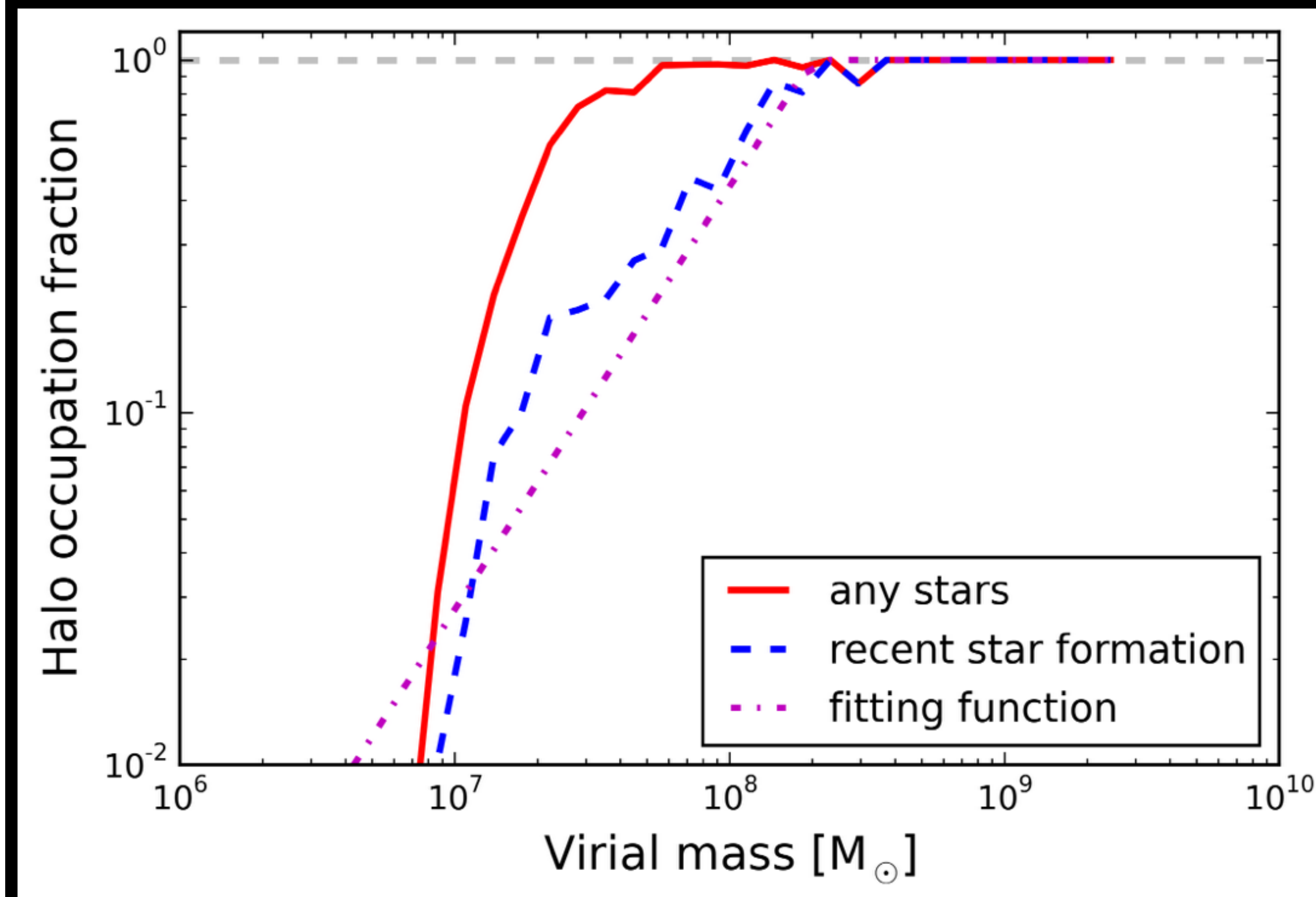
Luminosity function of early galaxies



O’Shea et al. 2015

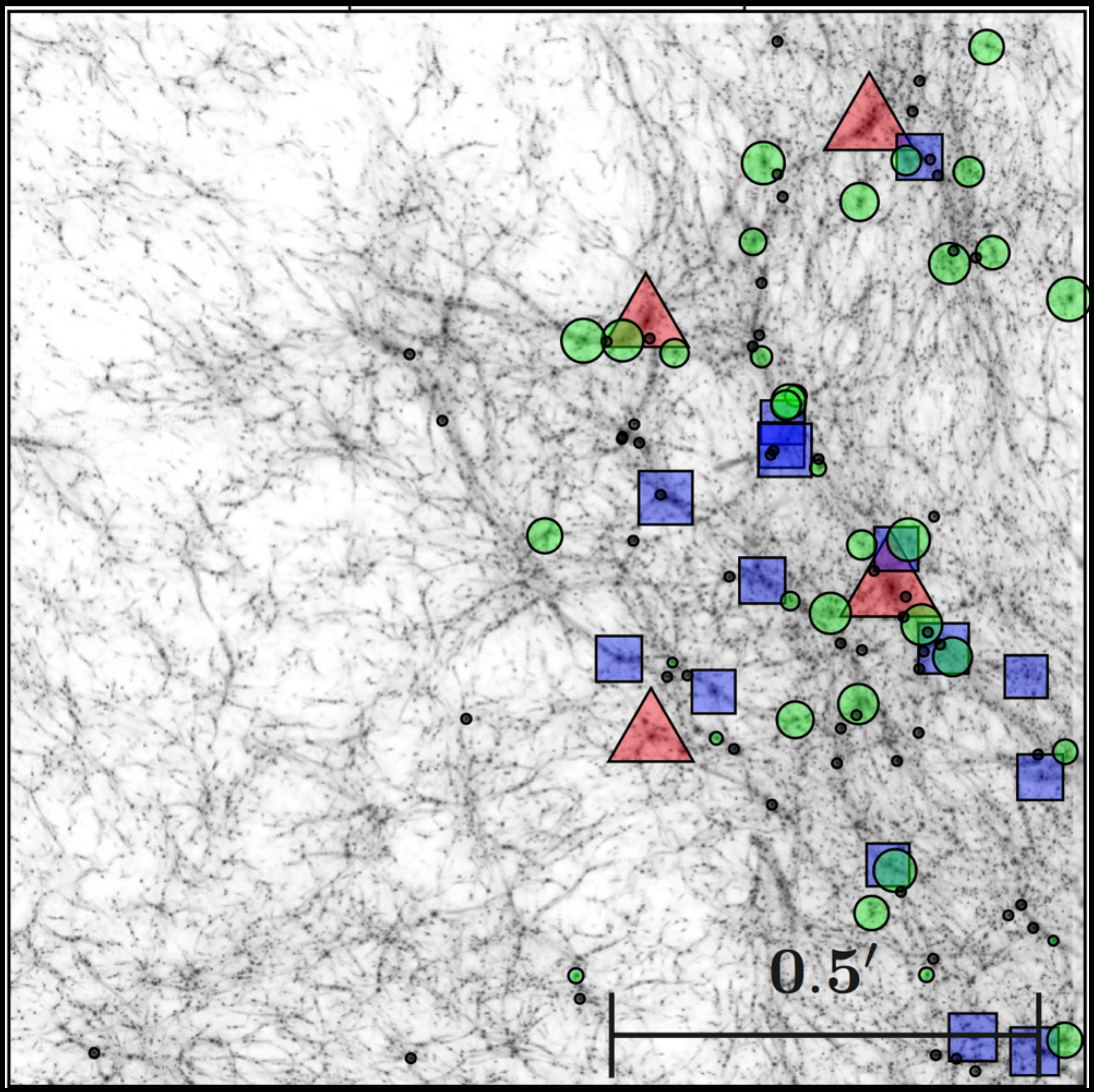
Luminosity function of early galaxies



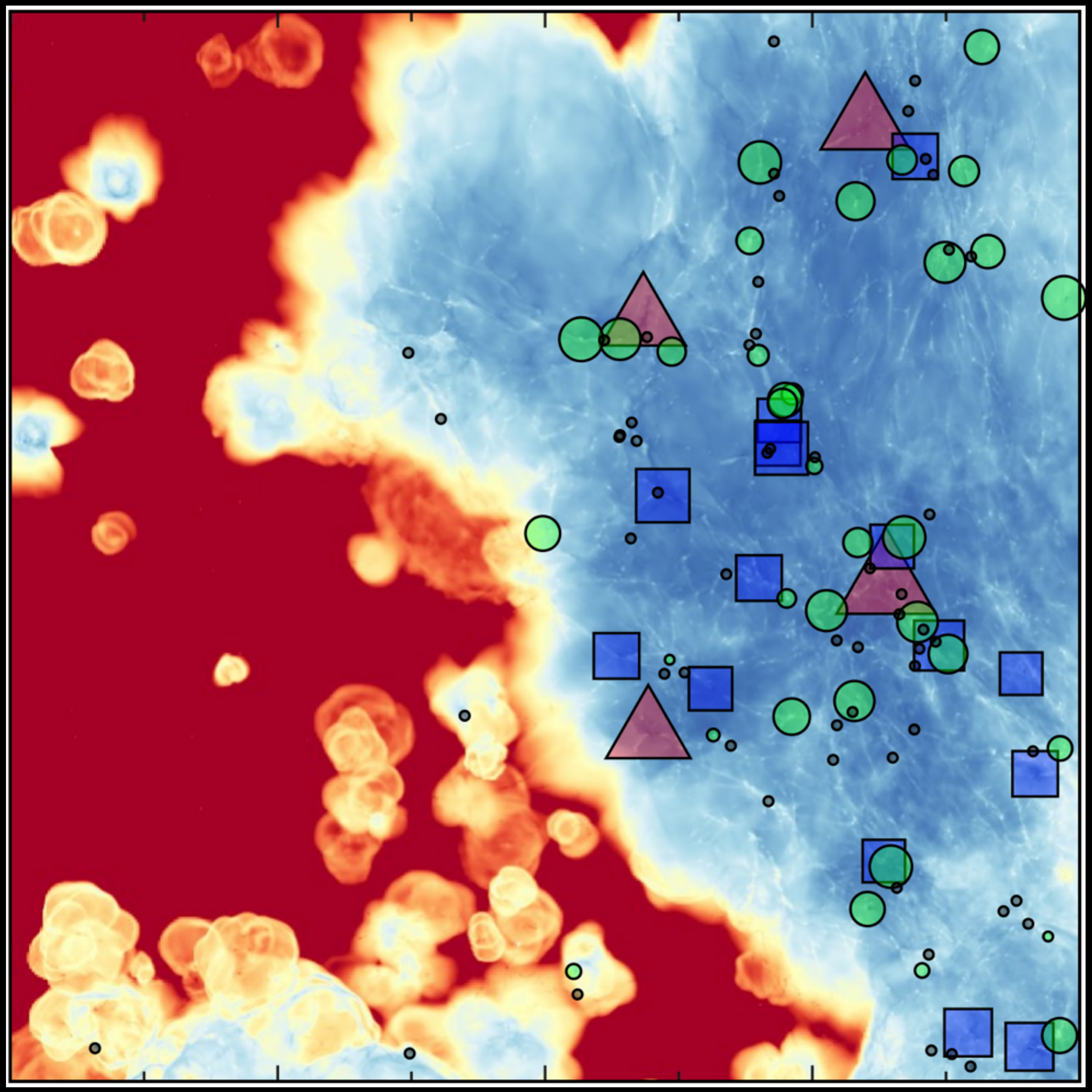


O'Shea et al. 2015

Luminosity function of early galaxies



Density



Electron fraction
(ionizing radiation)

Blue Waters data as a community resource

- Simulation tool (Enzo) and analysis/viz tool (yt) are open-source community codes.
- We plan to make all of our datasets available to the astronomical community and the public via the National Data Service very soon.
- These simulations were expensive and will be a community resource for years to come.

Cutting-edge simulations have a long tail of utility!

Takeaways

- Modeling galaxy formation is physically complex and requires both high dynamic range and a large sample size: computationally challenging!
- We are using Blue Waters to perform cutting-edge simulations of the first generations of stars and galaxies - simulations that cannot be done on other NSF or NASA resources.
- The transition between metal-free and metal-enriched star formation is locally complex and globally extended over time
- We that star formation is inefficient (and sometimes suppressed entirely) in small galaxies - this is observable!

Special thanks to:

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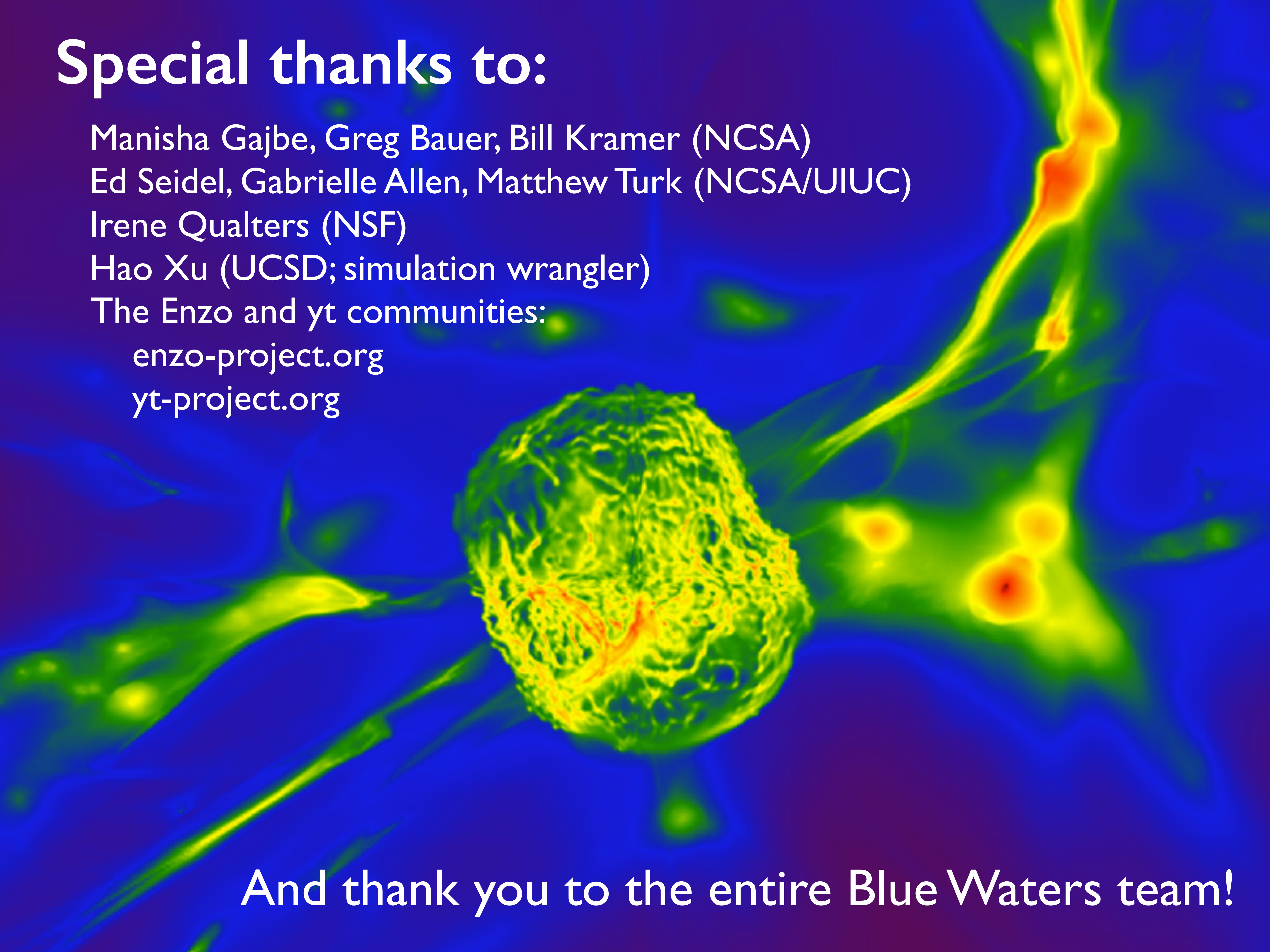

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