

# **Self-Regulated Reionization and the Fluctuating $H_2$ Dissociating UV Background**

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**University of Texas at Austin**

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**The University of Texas at Austin**

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# Self-Regulated Reionization and the Fluctuating $H_2$ Dissociating UV Background

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Eiichiro Komatsu, Jun Koda, Elizabeth Fernandez, Yi Mao (U. Texas)

# Simulating Cosmic Reionization at Large Scales I. : The Geometry of Reionization

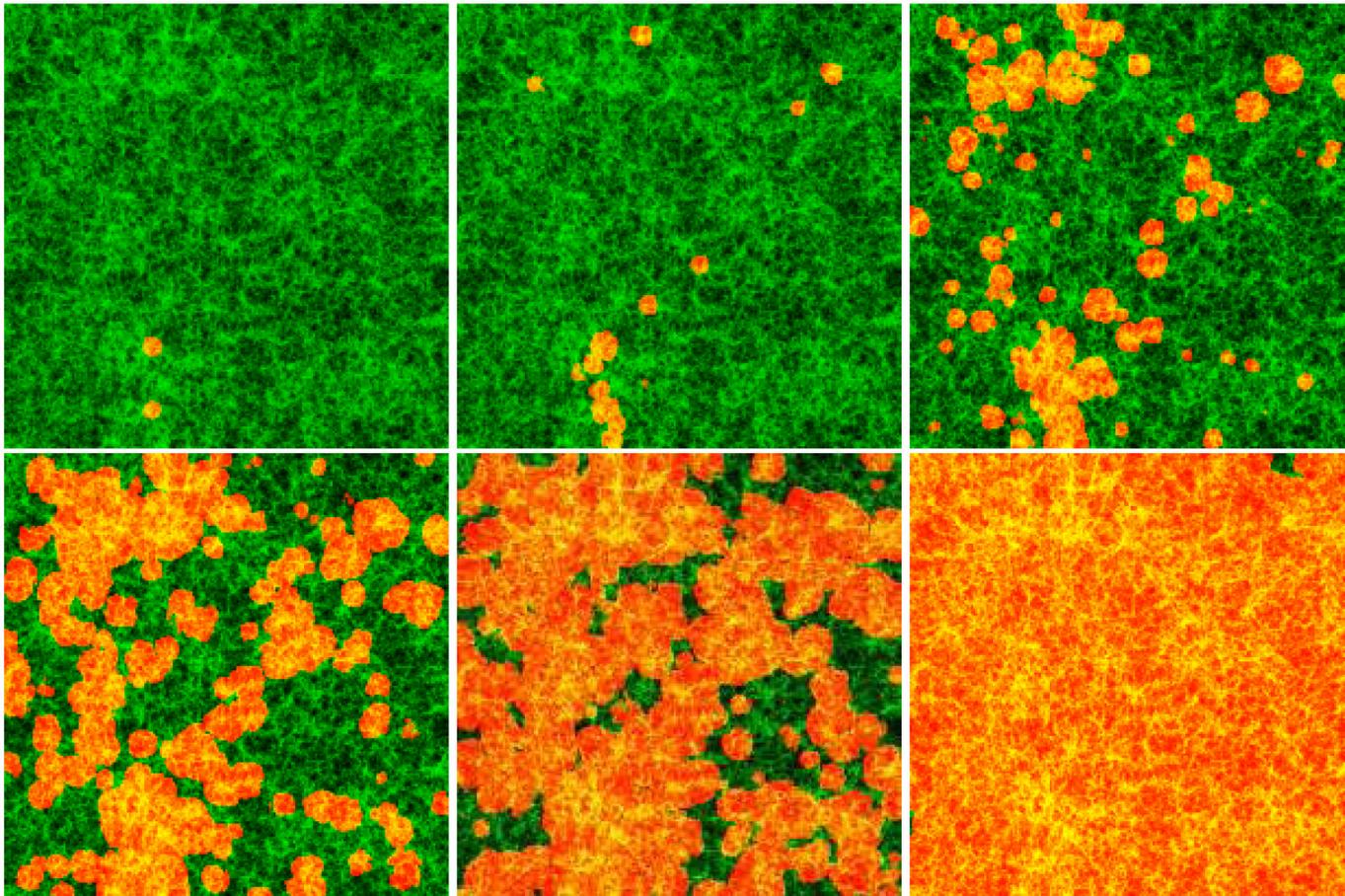
Iliev, Mellema, Pen, Merz, Shapiro & Alvarez (2006)  
MNRAS, 369, 1625 (astro-ph/0512187)

$z =$

18.5

16.1

14.5



13.6

12.6

11.3

# N-body + Radiative Transfer → Reionization simulation

- N-body simulation yields the density field and sources of ionizing radiation
  - PMFAST code (Merz, et al. 2005) with  
1624<sup>3</sup> = 4.28 billion particles, 3248<sup>3</sup> cells,  
particle mass =  $2.5 \times 10^7 M_{\text{sun}}$  (100 h<sup>-1</sup>Mpc box),  
  
- Halo finder “on-the-fly” yields location, mass, other  
properties of all galaxies,  
 $M \geq 2.5 \times 10^9 M_{\text{sun}}$  (100 h<sup>-1</sup>Mpc box),  
e.g.  $N_{\text{halo}} \sim 4 \times 10^5$  by  $z \sim 8$  (WMAP1)  
 $\sim 3 \times 10^5$  by  $z \sim 6$  (WMAP3)

# N-body + Radiative Transfer → Reionization simulation

- Radiative transfer simulations evolve the radiation field and nonequilibrium ionization state of the gas
  - New, fast, efficient C<sup>2</sup>-Ray code (Conservative, Causal Ray-Tracing) (Mellema, Ilev, Alvarez, & Shapiro 2006, *New Astronomy*, 11, 374) uses short-characteristics to propagate radiation throughout the evolving gas density field provided by the N-body results, re-gridded to  $(203)^3$  and  $(406)^3$  cells, for different resolution runs, from each and every galaxy halo source in the box.

e.g.  $N_{\text{halo}} \sim 4 \times 10^5$  by  $z \sim 8$  (WMAP1)  
 $\sim 3 \times 10^5$  by  $z \sim 6$  (WMAP3)

# Every galaxy in the simulation volume emits ionizing radiation

- We assume a constant mass-to-light ratio for simplicity:

$$f_{\gamma} = \# \text{ ionizing photons released} \\ \text{by each galaxy per halo baryon} \\ = f_{*} f_{\text{esc}} N_i,$$

where

$f_{*}$  = star-forming fraction of halo baryons,

$f_{\text{esc}}$  = ionizing photon escape fraction,

$N_i$  = # ionizing photons emitted per stellar baryon over stellar lifetime

e.g.  $N_i = 50,000$  (top-heavy IMF),  $f_{*} = 0.2$ ,  $f_{\text{esc}} = 0.2 \rightarrow$   
 $f_{\gamma} = 2000$

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 $f_{\gamma} = 2000$

- This yields source luminosity:  $dN_{\gamma}/dt = f_{\gamma} M_{\text{bary}} / (\mu m_{\text{H}} t_{*})$ ,  
 $t_{*}$  = source lifetime (e.g.  $2 \times 10^7$  yrs),  
 $M_{\text{bary}}$  = halo baryonic mass

# Self-Regulated Reionization

Iliev, Mellema, Shapiro, & Pen (2007), MNRAS, 376, 534; (astro-ph/0607517)

- Jeans-mass filtering →

low-mass source halos

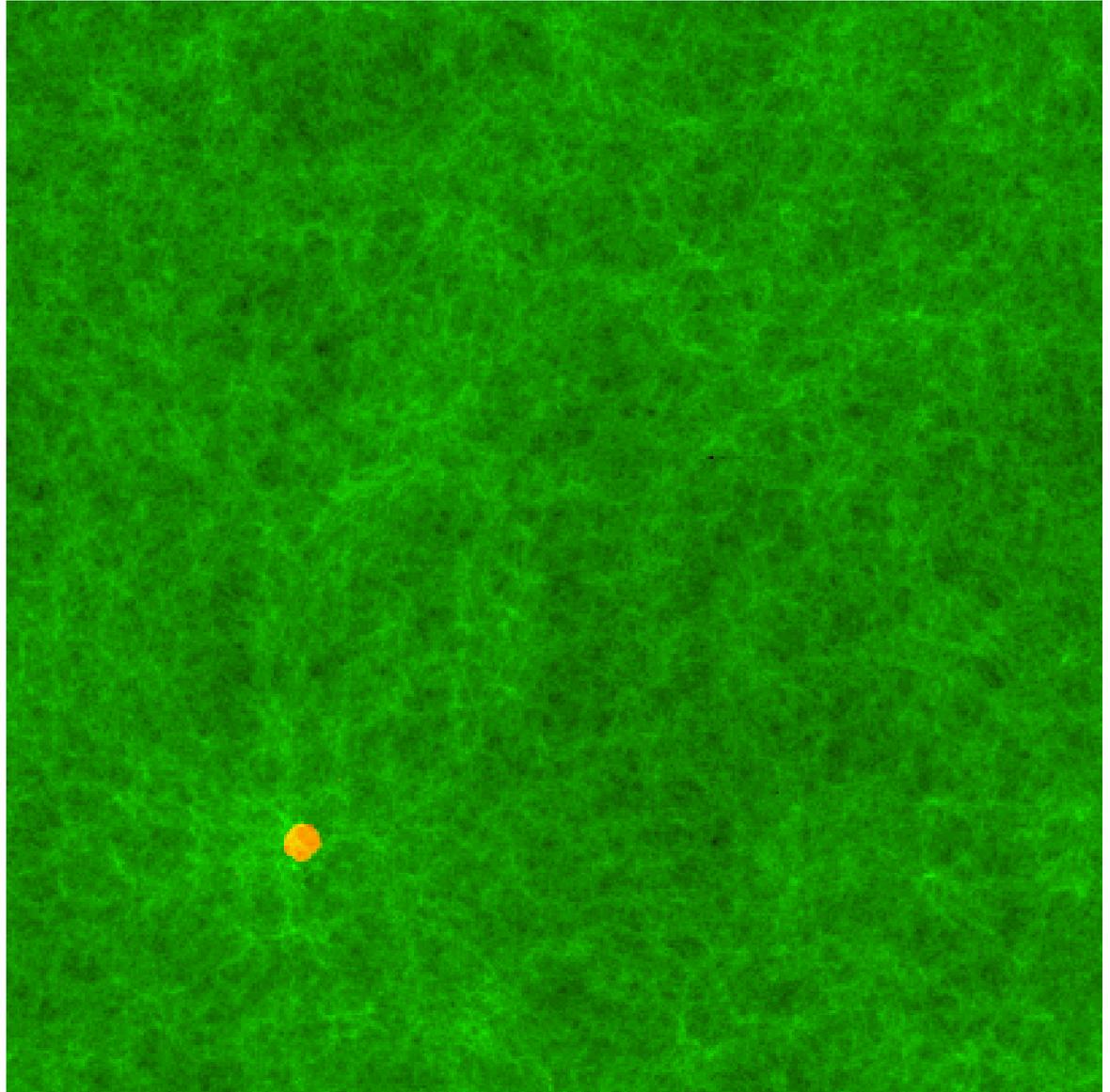
( $M < 10^9 M_{\text{solar}}$ ) cannot form  
inside H II regions ;

- 35/h Mpc box,  $406^3$  radiative  
transfer simulation, WMAP3,  
 $f_{\gamma} = 250$ ;

- resolved all halos with

$M > 10^8 M_{\text{solar}}$  (i.e. all  
atomically-cooling halos),  
(blue dots = source cells);

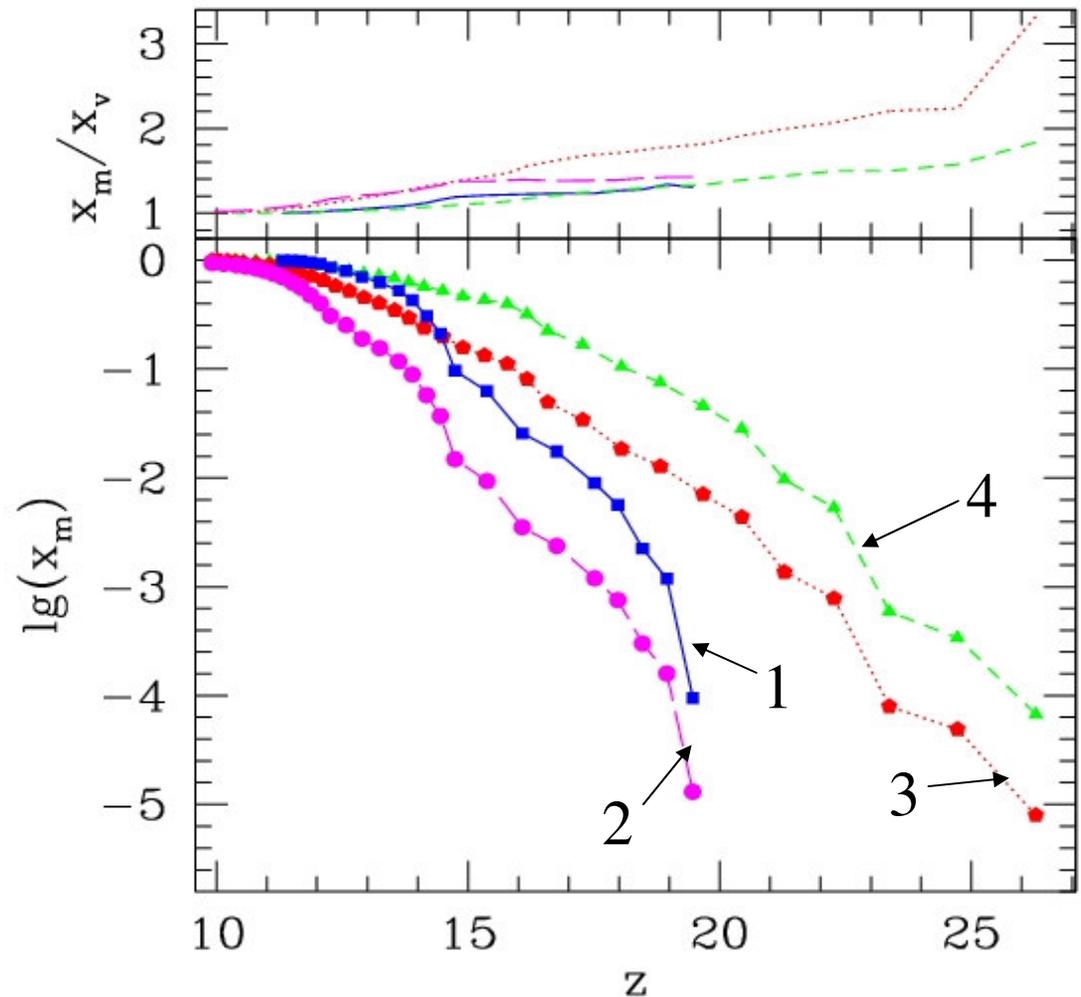
- Evolution:  $z=21$  to  $z_{\text{ov}} = 7.5$ .



# Extended reionization: Jeans-mass filtering, halo-mass-dependent emissivity

## Cases

1. Halo masses  $M_{\text{solar}} > 10^9$   
 $f_{\gamma} = 2000$  (e.g. Pop III);
2. Halo masses  $M_{\text{solar}} > 10^9$   
 $f_{\gamma} = 250$  (e.g. Pop II);
3. Halo masses  $M_{\text{solar}} > 10^8$   
 $f_{\gamma} = 250$  (e.g. Pop II),  
lower-mass halos  
suppressed inside H II regions  
(Jeans-mass filtering) ;
4. Same as 3., but  
 $f_{\gamma} = 2000$  ( $M_{\text{solar}} < 10^9$ )  
 $f_{\gamma} = 250$  ( $M_{\text{solar}} > 10^9$ )

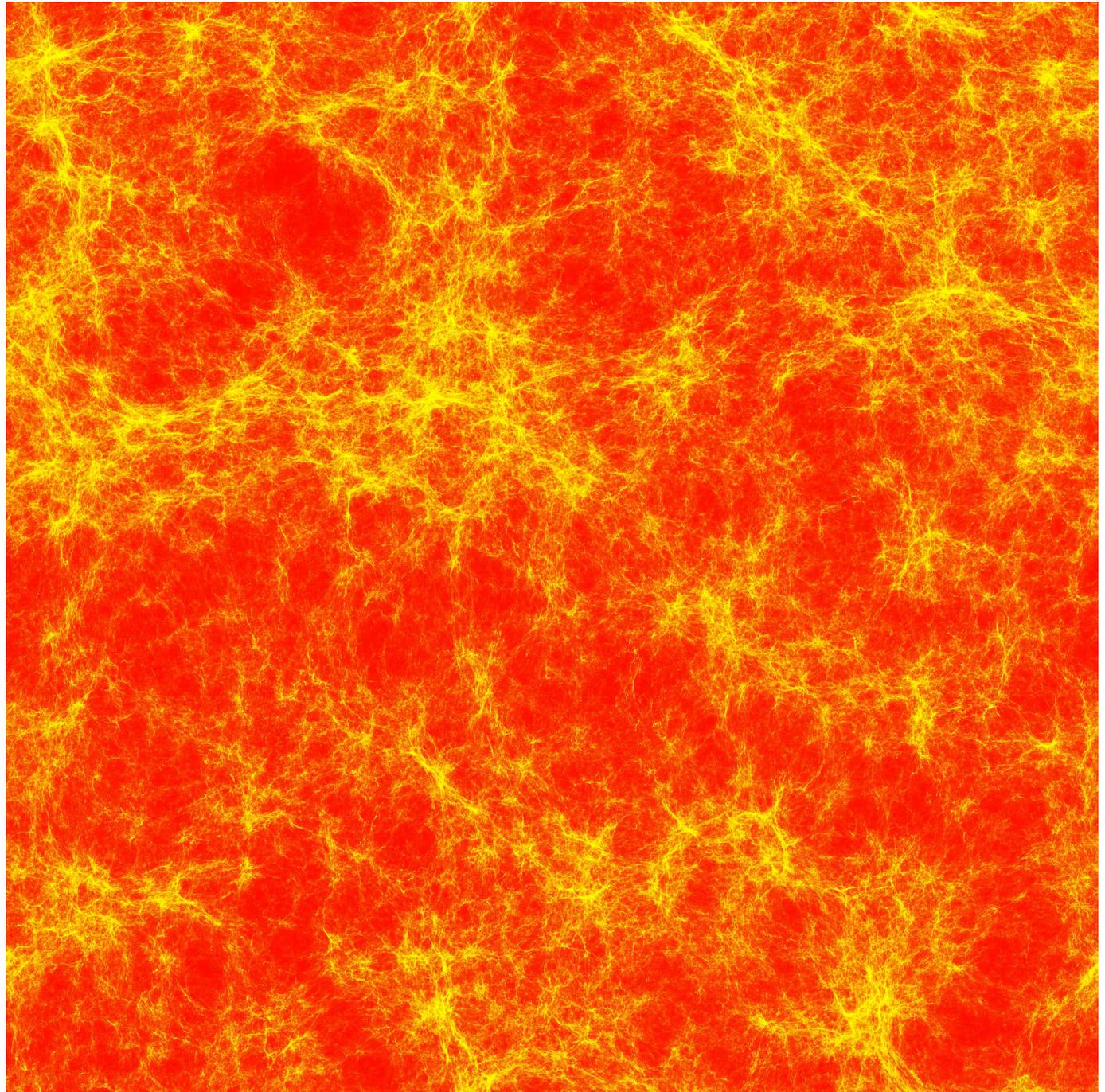


# New, Large-Scale Simulations of Self-Regulated Reionization

Iliev, Mellema, Pen,  
Shapiro, and Merz  
(2008), in press (astro-  
ph/0806.2887);

Shapiro, Iliev, Mellema,  
Pen, & Merz (2008),  
AIPC, 1035, 68  
(astro-ph/0806.3091)

**CubeP<sup>3</sup>M** N-body  
 $\Lambda$ CDM sim with  
 $3072^3$  (29 billion)  
particles,  
 $6144^3$  cells,  
box size = 160 Mpc;  
particle mass =  
5 million solar  
masses

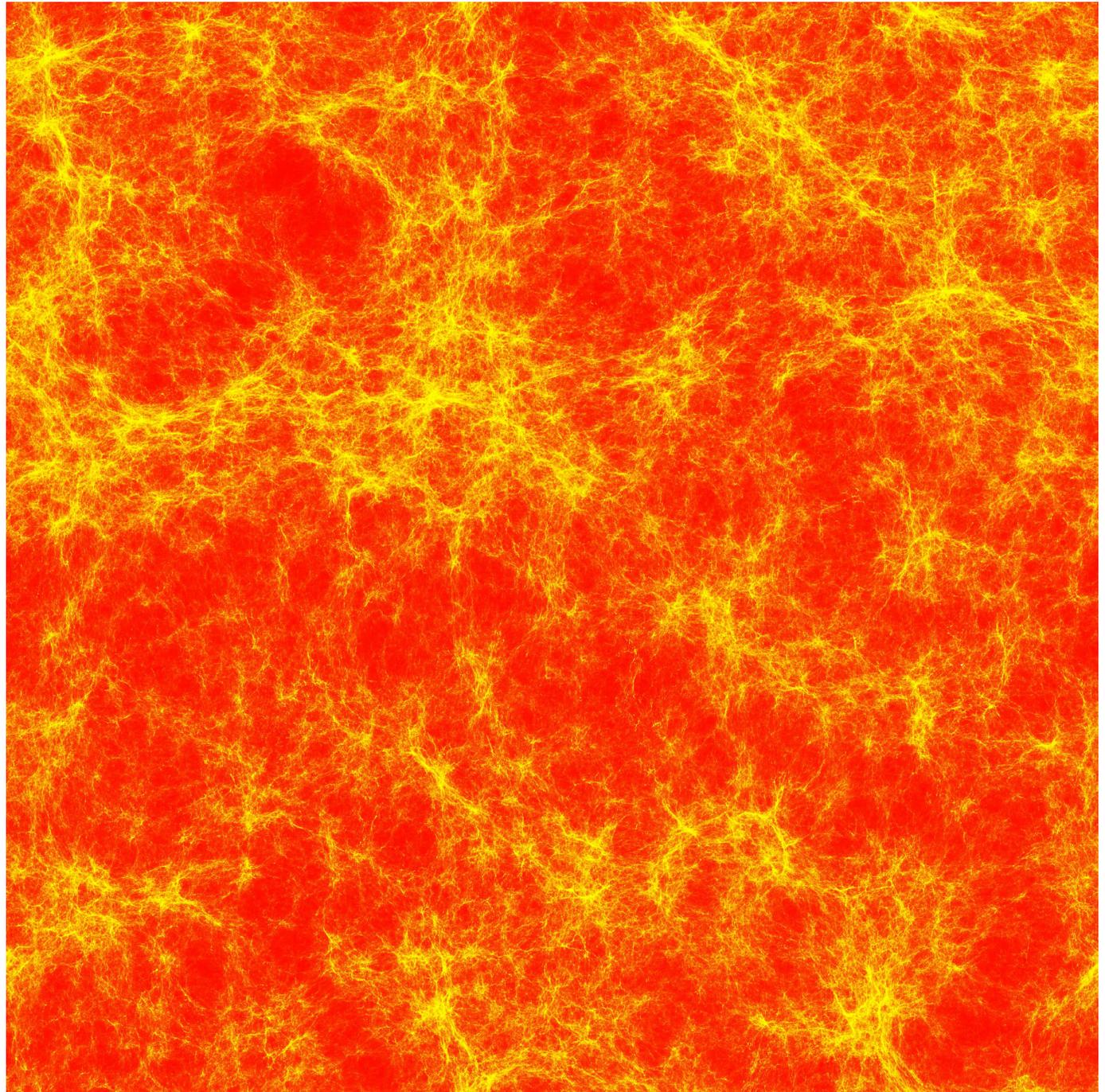


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**CubeP<sup>3</sup>M** N-body  
 $\Lambda$ CDM sim with  
 $3072^3$  (29 billion)  
particles,  
resolves halos above  
 $10^8$  solar masses



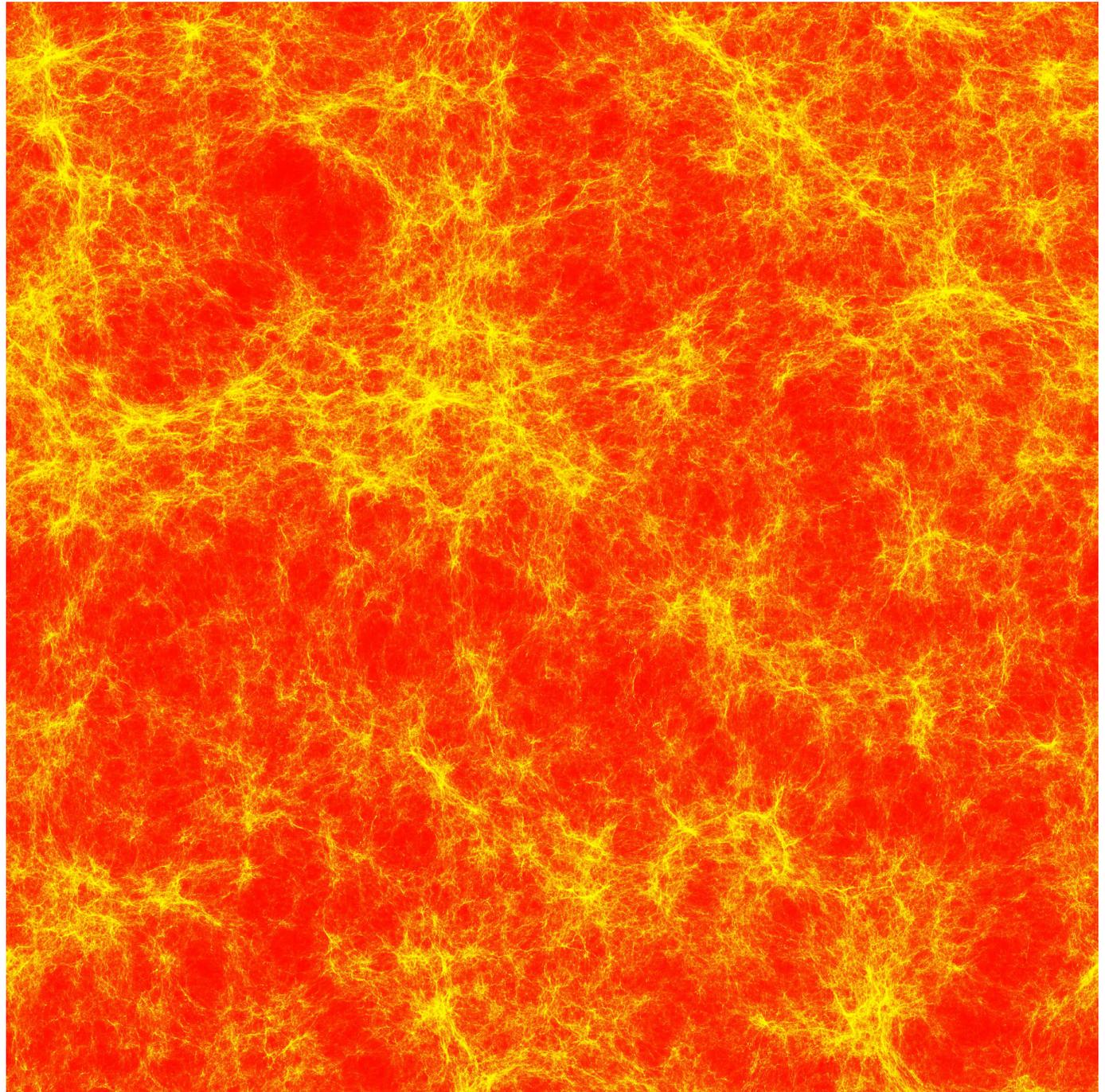
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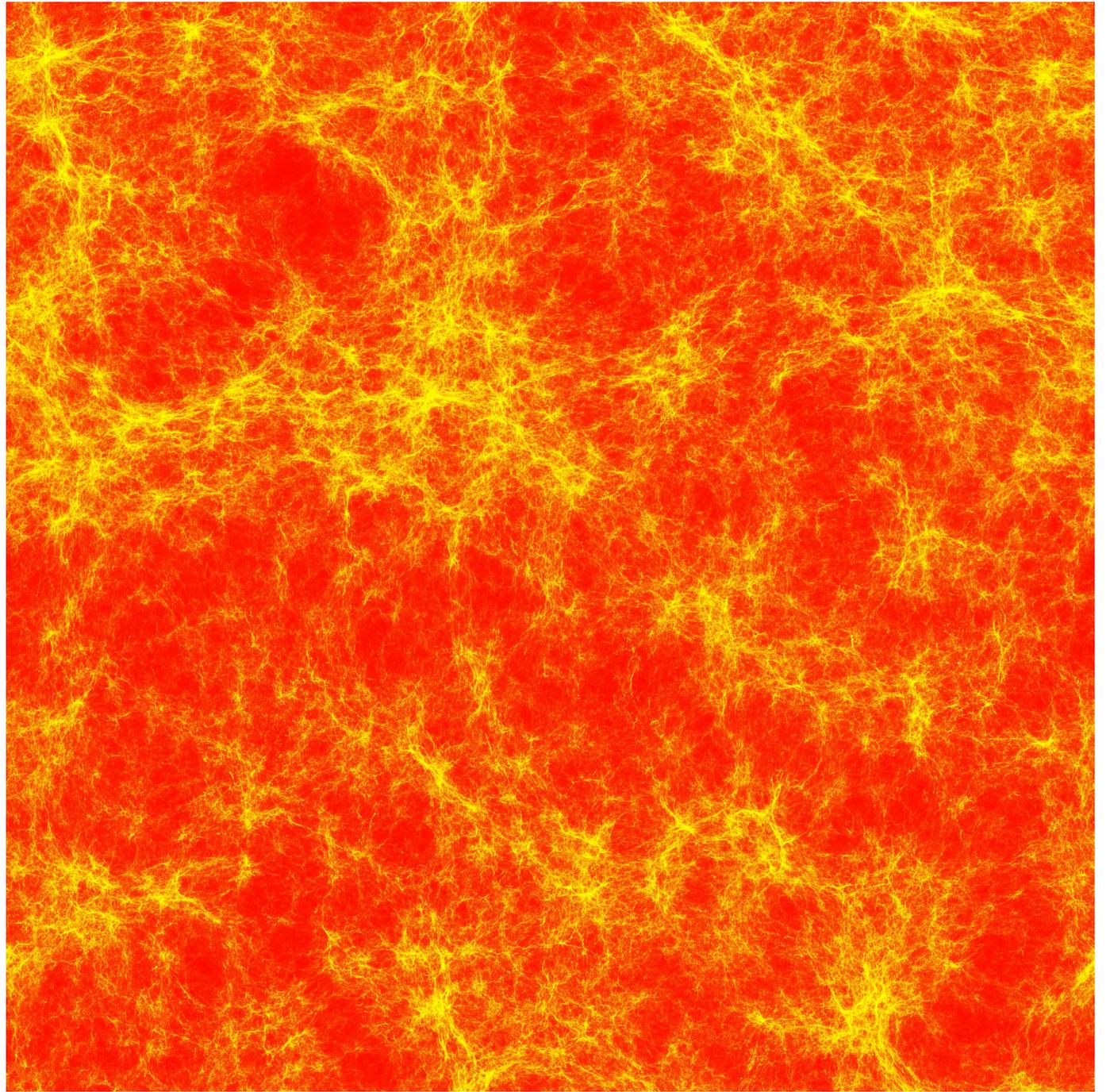
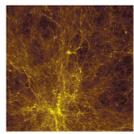
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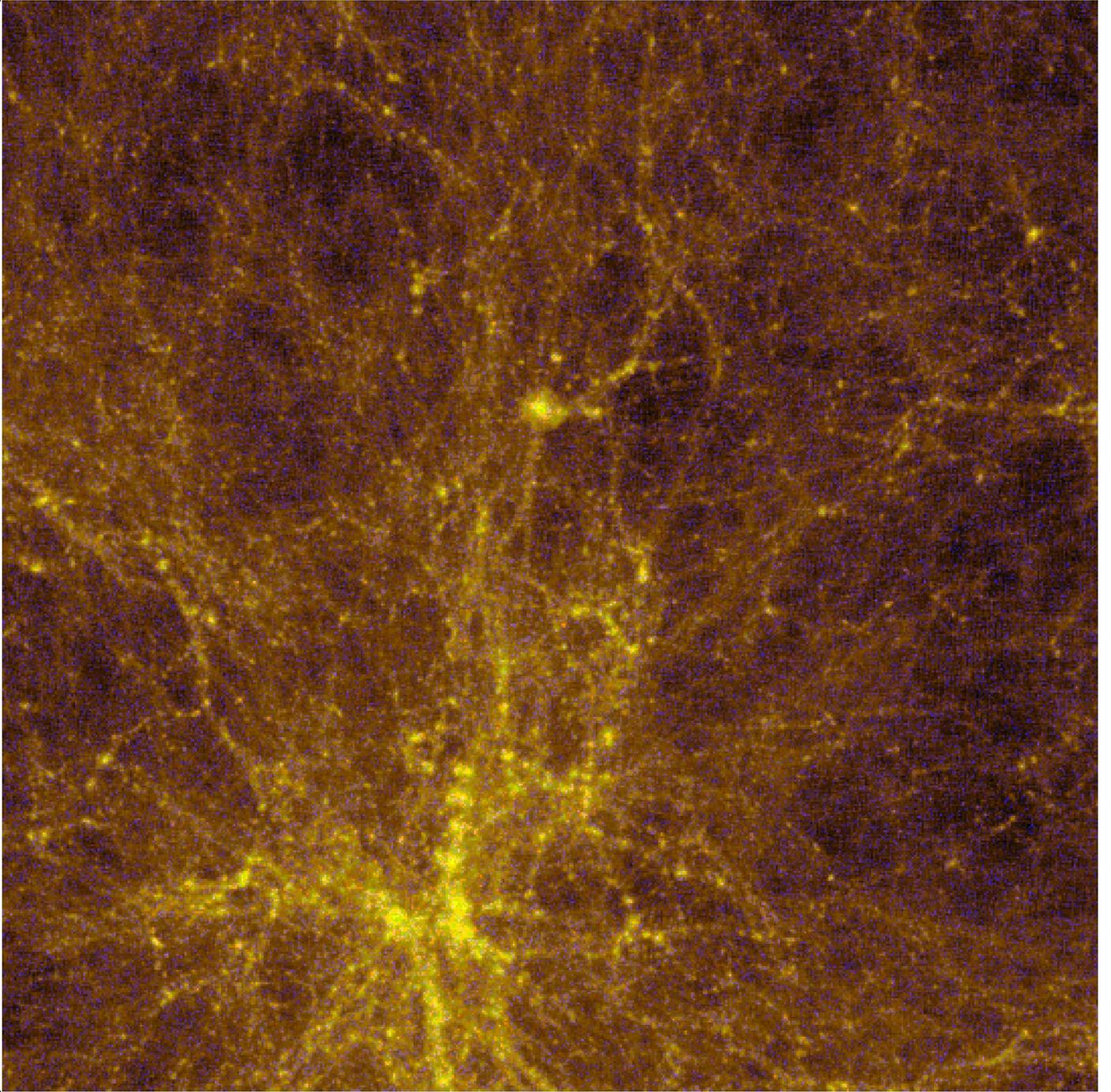
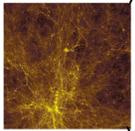
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## **CubeP<sup>3</sup>M** N-body

- new Texas Sun  
Constellation Linux  
Cluster, *Ranger*,  
2048 cores, 159,000  
SUs (cores x hours)

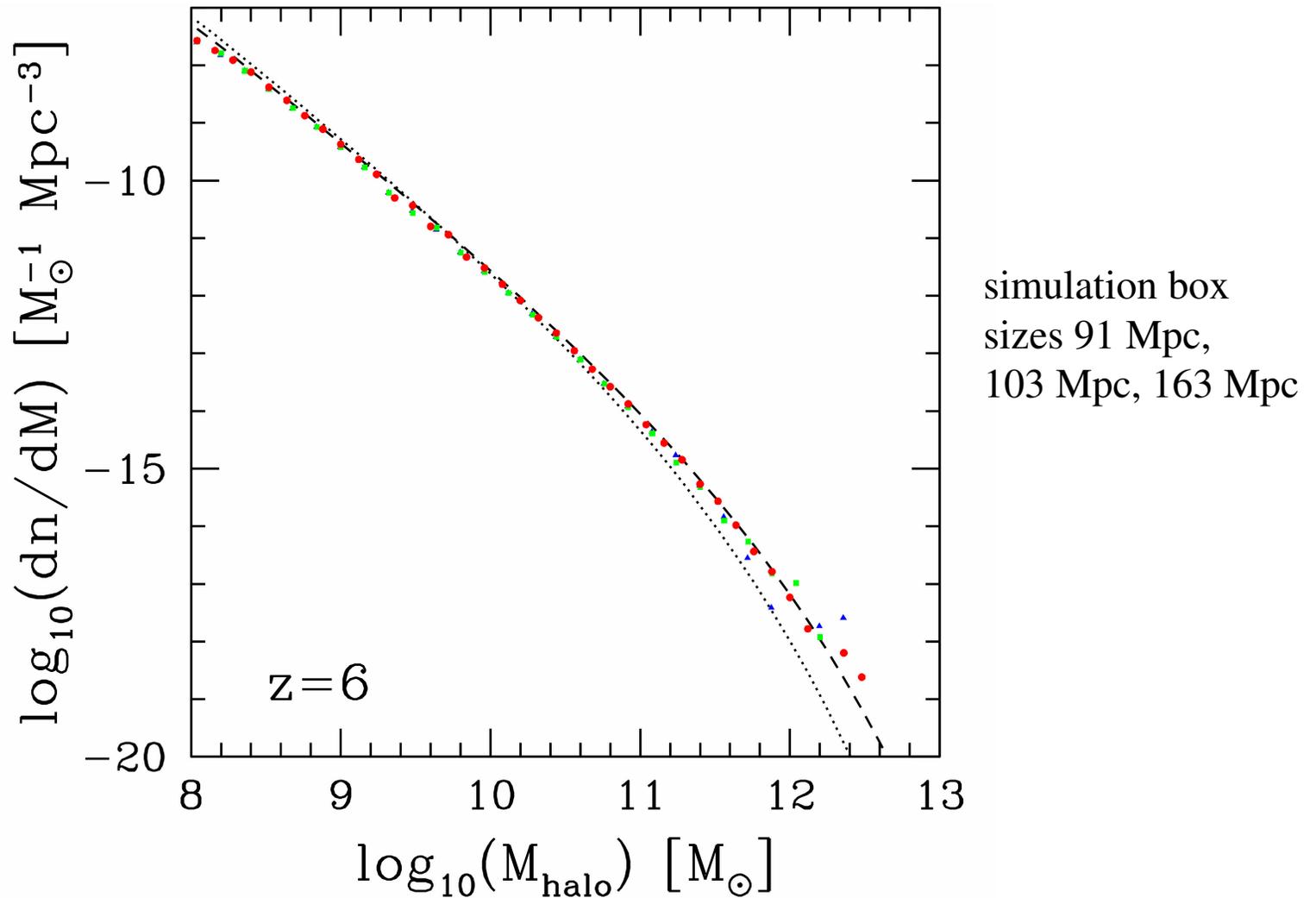






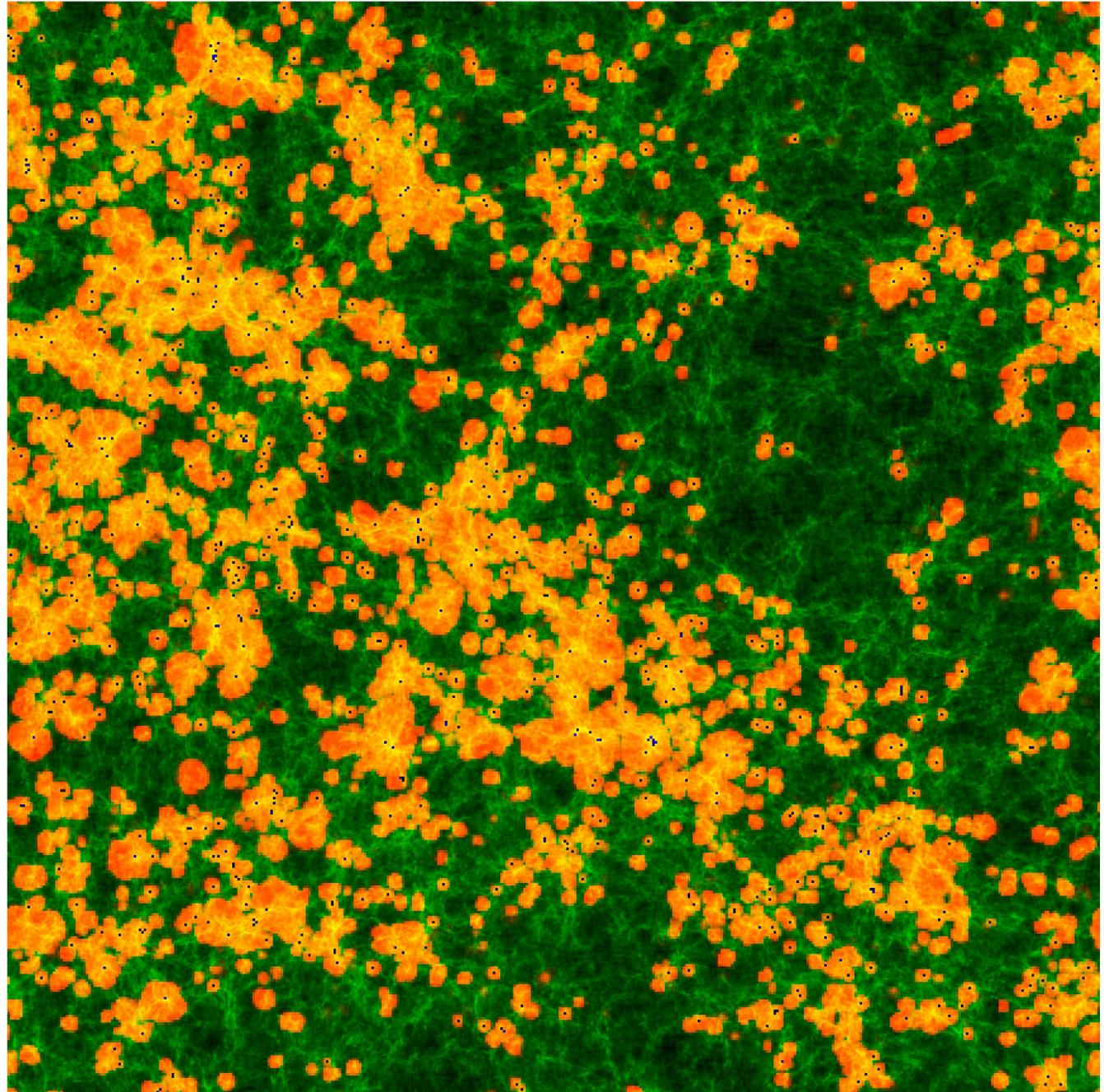
# $\Lambda$ CDM Halo Mass Function ( $M > 10^8$ Solar Masses)

from CubeP<sup>3</sup>M N-body Simulations



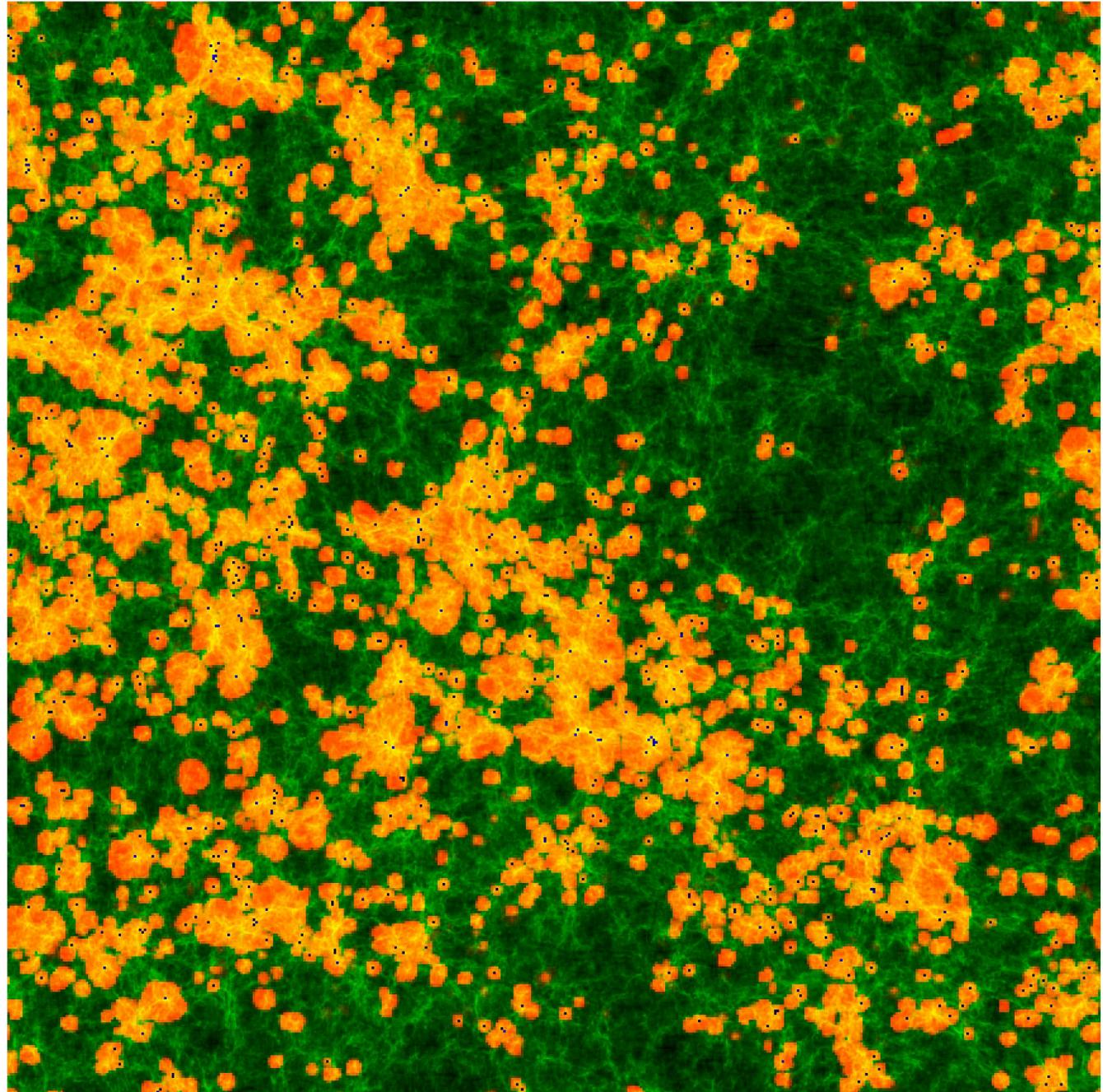
# C<sup>2</sup>Ray radiative transfer

- RT grid  $432^3$   
cells
- box size = 90  
Mpc



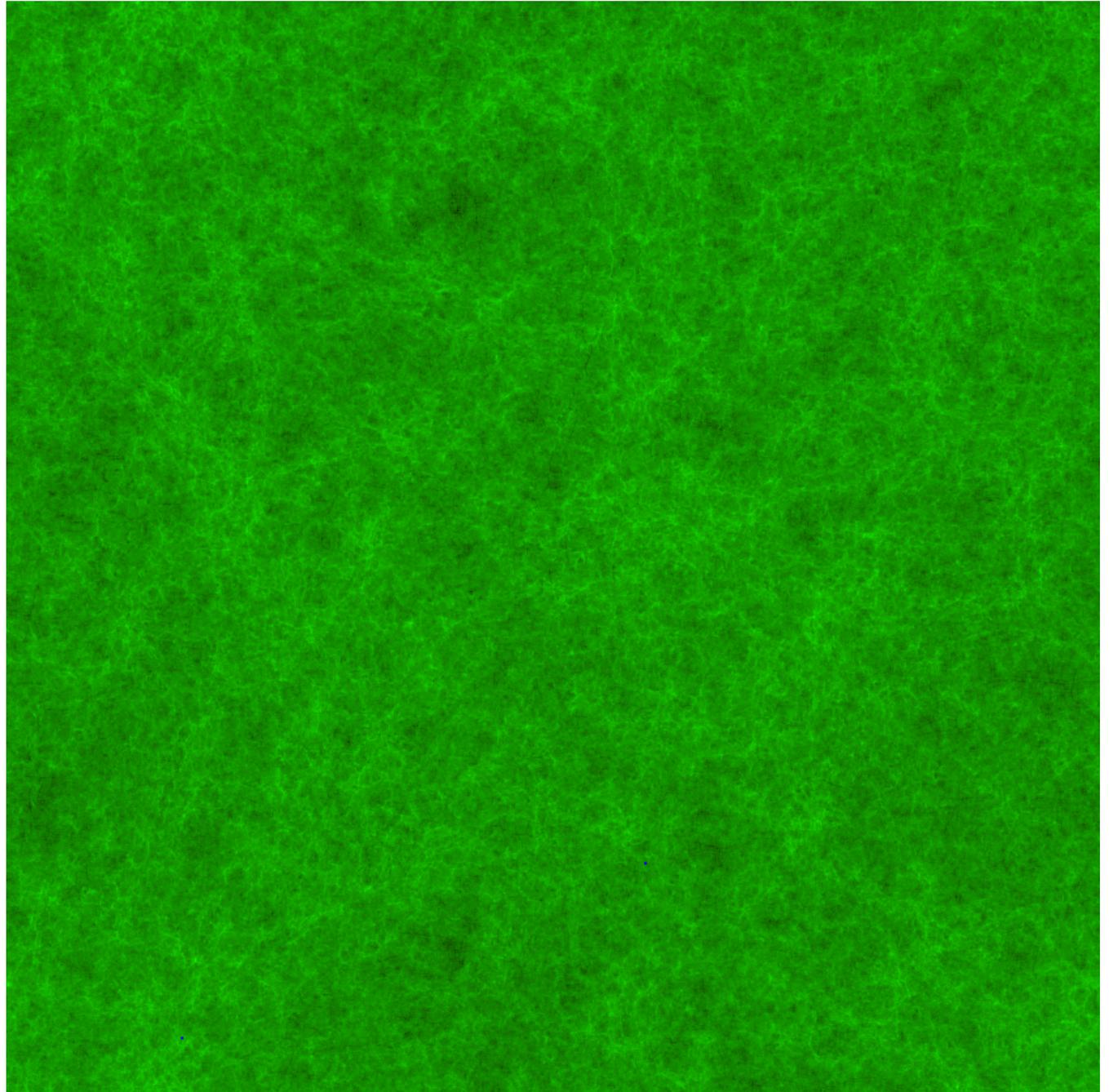
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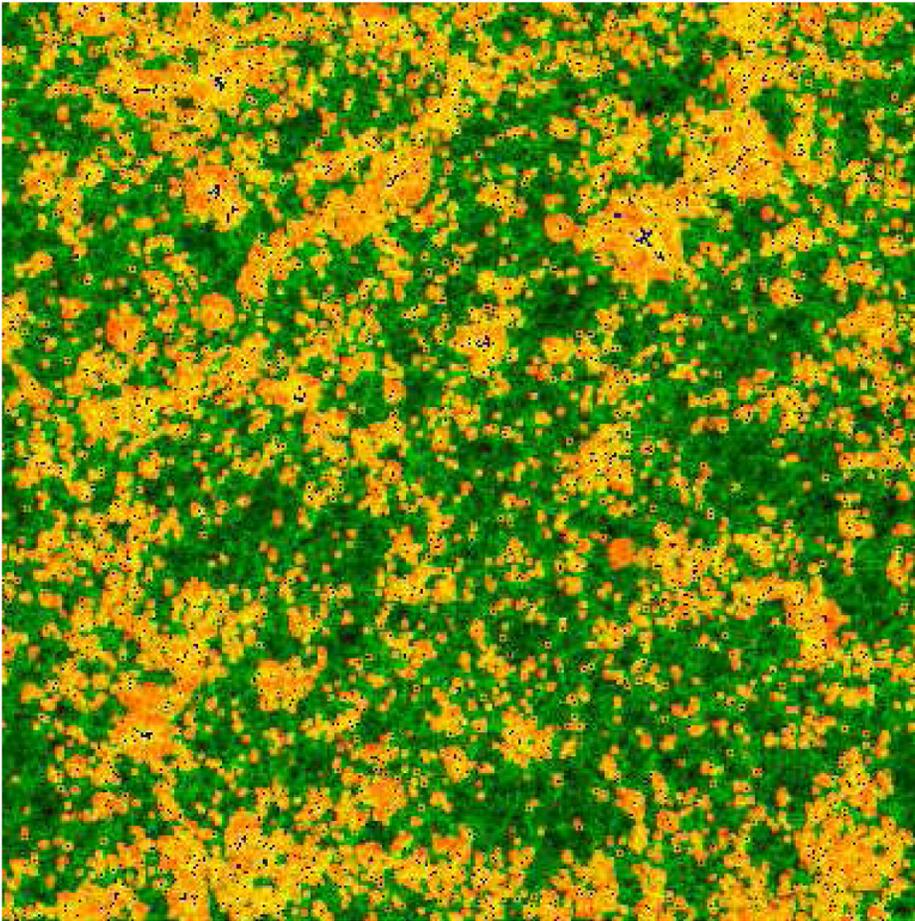
- RT grid  $432^3$   
cells
- box size = 90  
Mpc
- *Ranger*,  
Texas Sun  
Constellation  
Linux Cluster,  
700,000 SUs  
(cores x hours),  
up to 10,000  
cores



# Self-Regulated Reionization in $\Lambda$ CDM

- 90 Mpc box

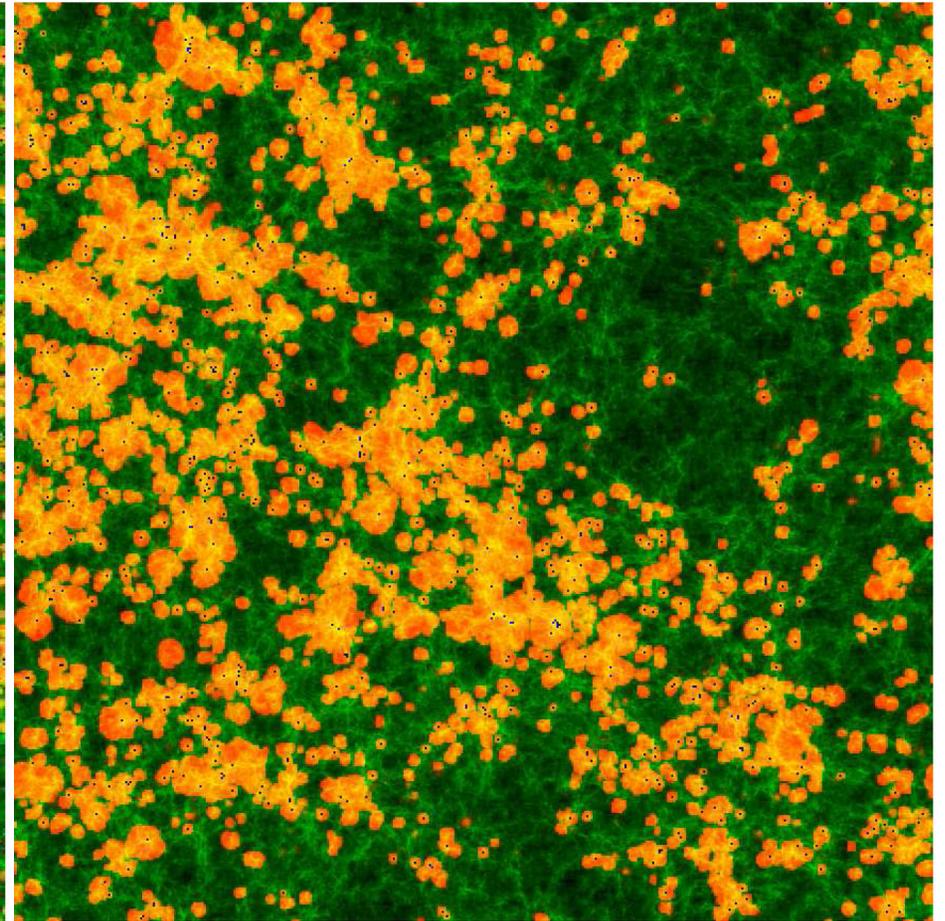




160 Mpc box

$z = 11.6$

when mass-weighted mean ionized fraction of universe  $x_m = 0.3$

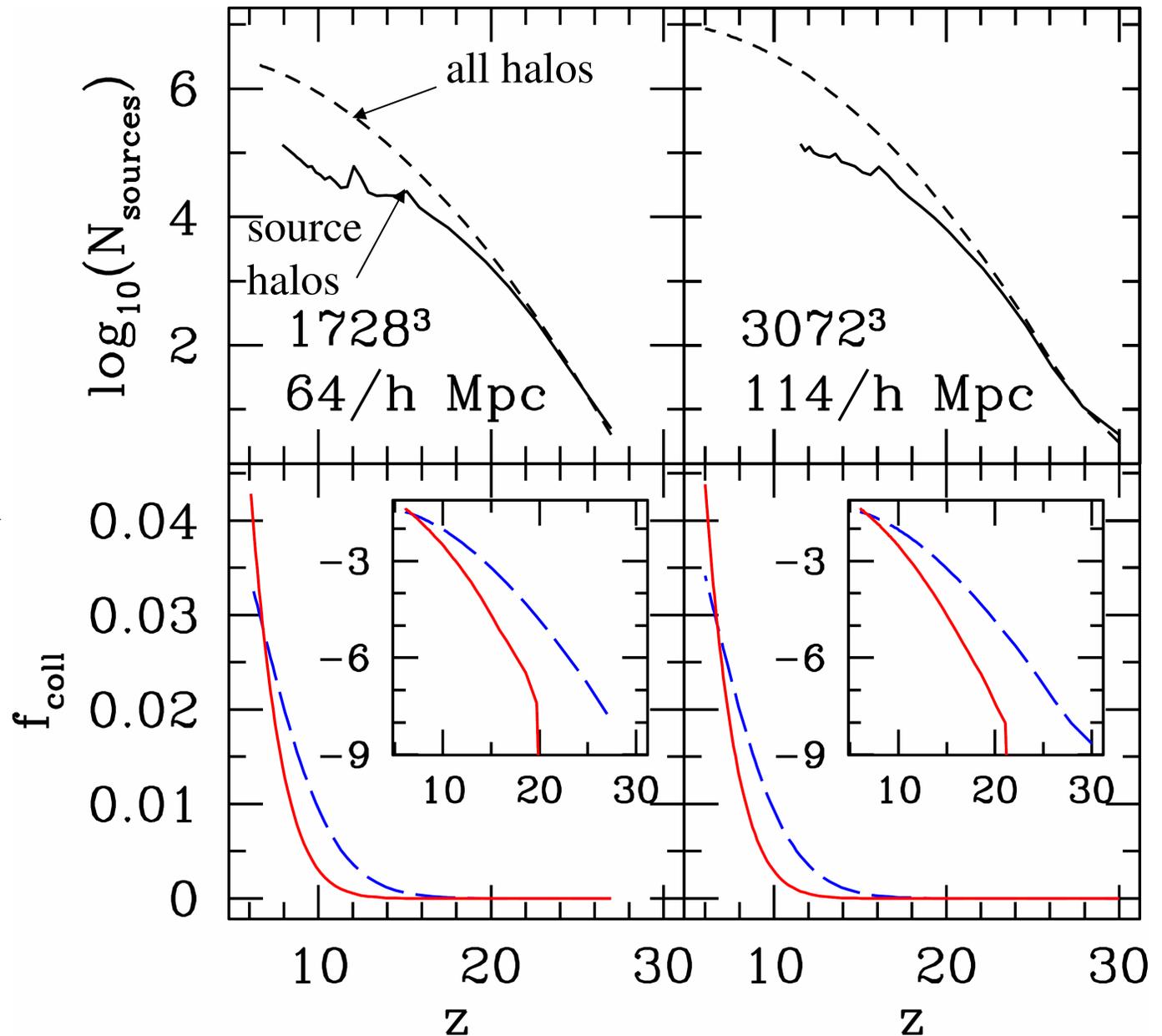


90 Mpc box

$z = 11.9$

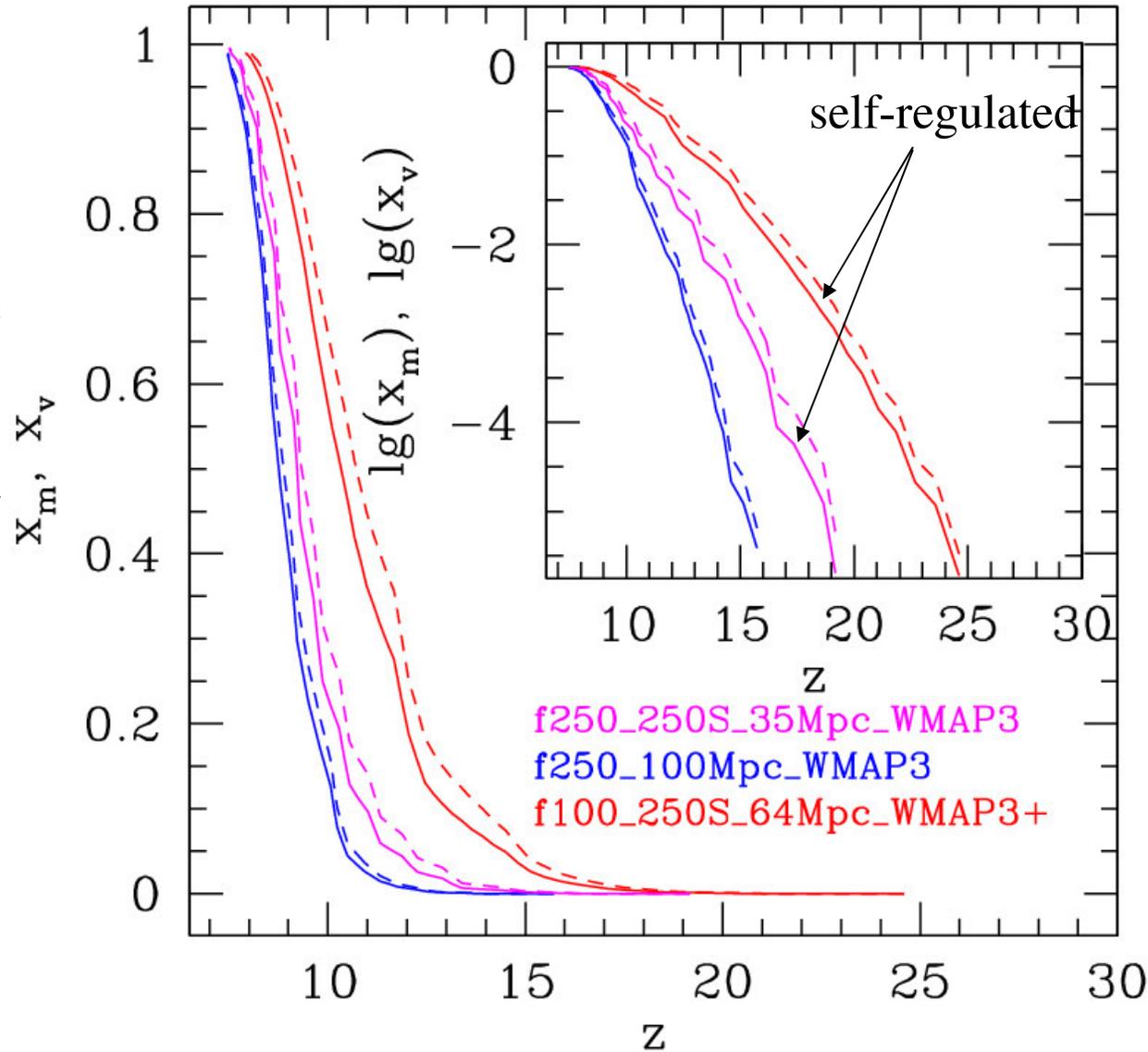
## Self-regulated halo mass function

- Jeans-mass filtering suppresses formation of sources in small-mass halos which form inside H II regions
- clustering of small-mass halos around density peaks enhances this effect → suppression is strongly **biased**



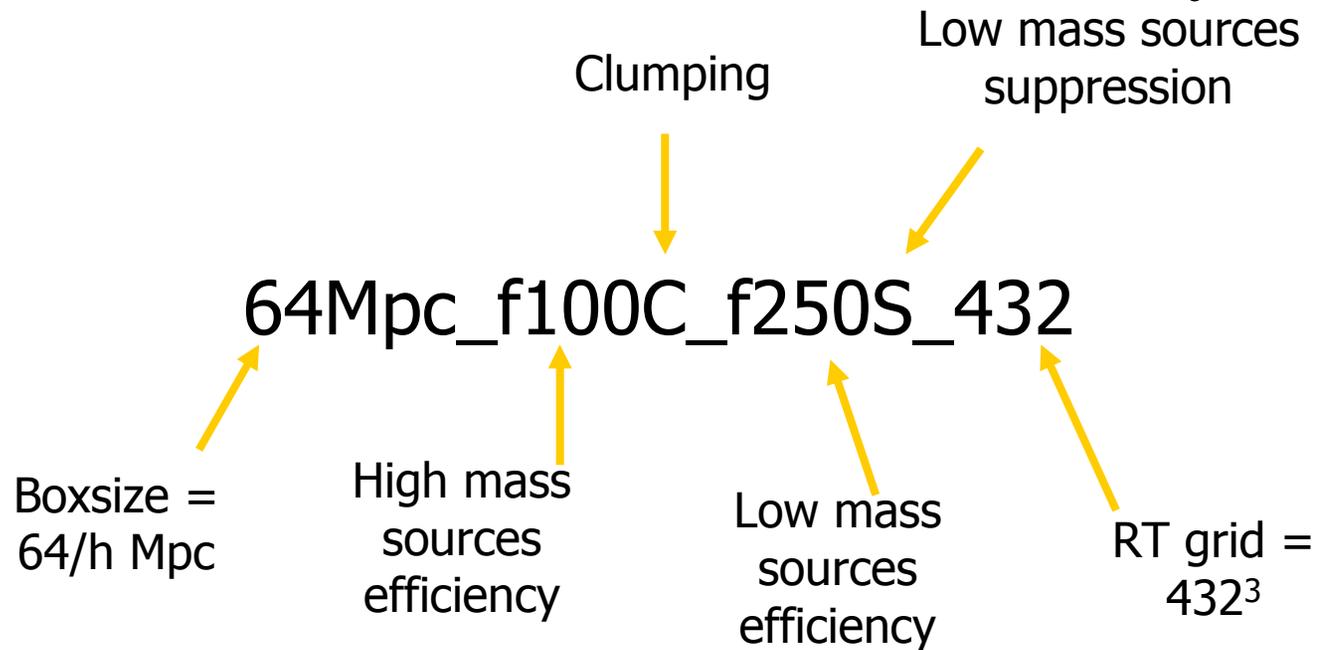
# Evolution of the Mean Ionized Fraction of the Universe

- self-regulated reion. (i.e. small-mass halos resolved) starts earlier, but ends about the same time →
- high-mass halos dominate the end of EOR



# Notation

- Our simulations are characterized by



# The Fluctuating H<sub>2</sub> Dissociating Background During Reionization

Ahn, Shapiro, Iliev, Mellema, & Pen 2008, ApJ, submitted (astro-ph/0807.2254; 0807.0920)

- Simulations suggest first stars formed inside minihalos of mass  $\sim 10^{5-6}$  solar masses at redshift  $z > \sim 20$ , when H<sub>2</sub> molecules cooled the primordial, metal-free gas and gravitational collapse ensued.
- **But** H<sub>2</sub> Lyman-Werner (“LW”) band photons (11.2 – 13.6 eV) dissociate H<sub>2</sub>, so too much LW background intensity (i.e.  $J_{\text{LW}} > (J_{\text{LW}})_{\text{threshold}}$ )
  - ➔ star formation inside minihalos suppressed

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- **But** during EOR, sources of reionization also emit continuum below 13.6 eV Lyman limit, in the H<sub>2</sub> LW bands → *rising LW background inevitable!*

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• **How high does it get?**

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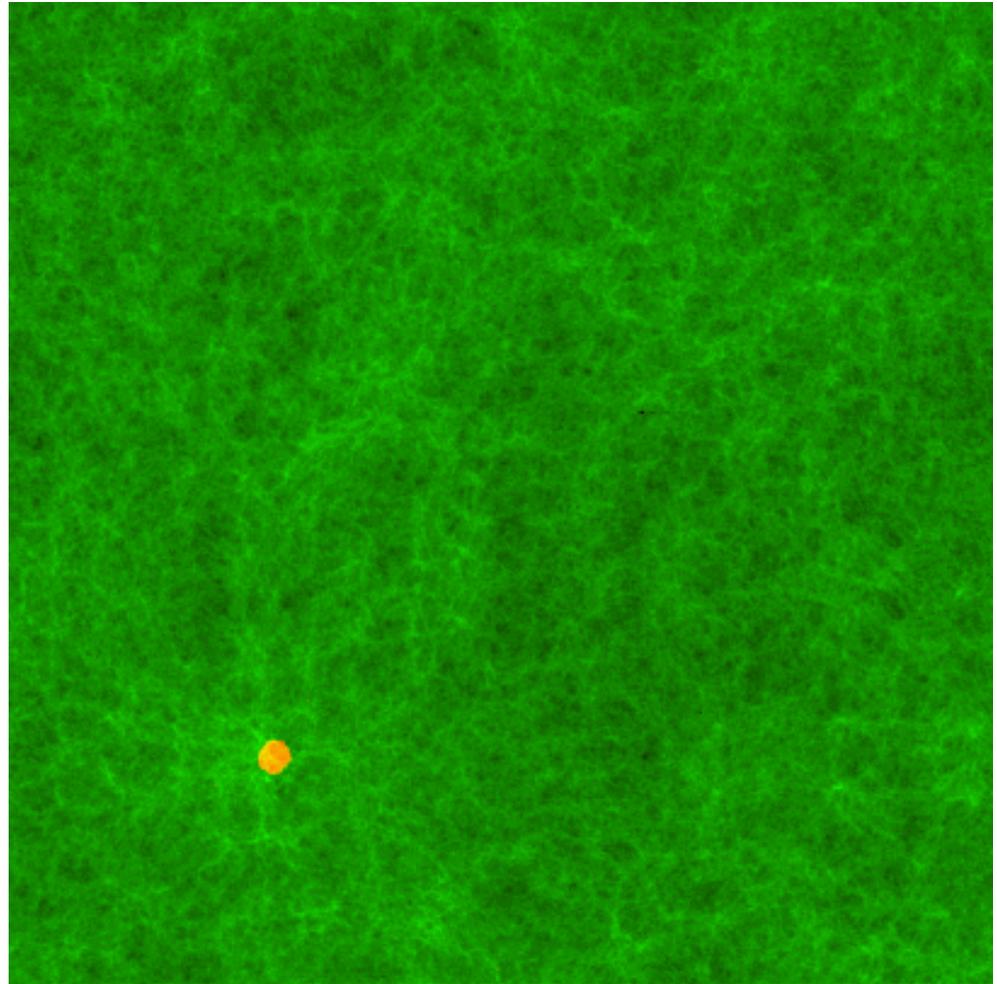
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- Ionization sources also emit continuum below Lyman limit, in the H<sub>2</sub> Lyman-Werner bands (11.2 – 13.6 eV).
- In IGM, this radiation is attenuated by scattering in H Lyman series lines and downgrading to lower energy photons.
- By transferring this radiation from each source halo thru the IGM, we compute the inhomogeneous LW band intensity field during reionization.
- e.g. Pop II sources,  
 $f_{\text{esc}} = 0.2$ ,  $f_* = 0.2$ ,  
 $f_{\gamma} = 250$ .

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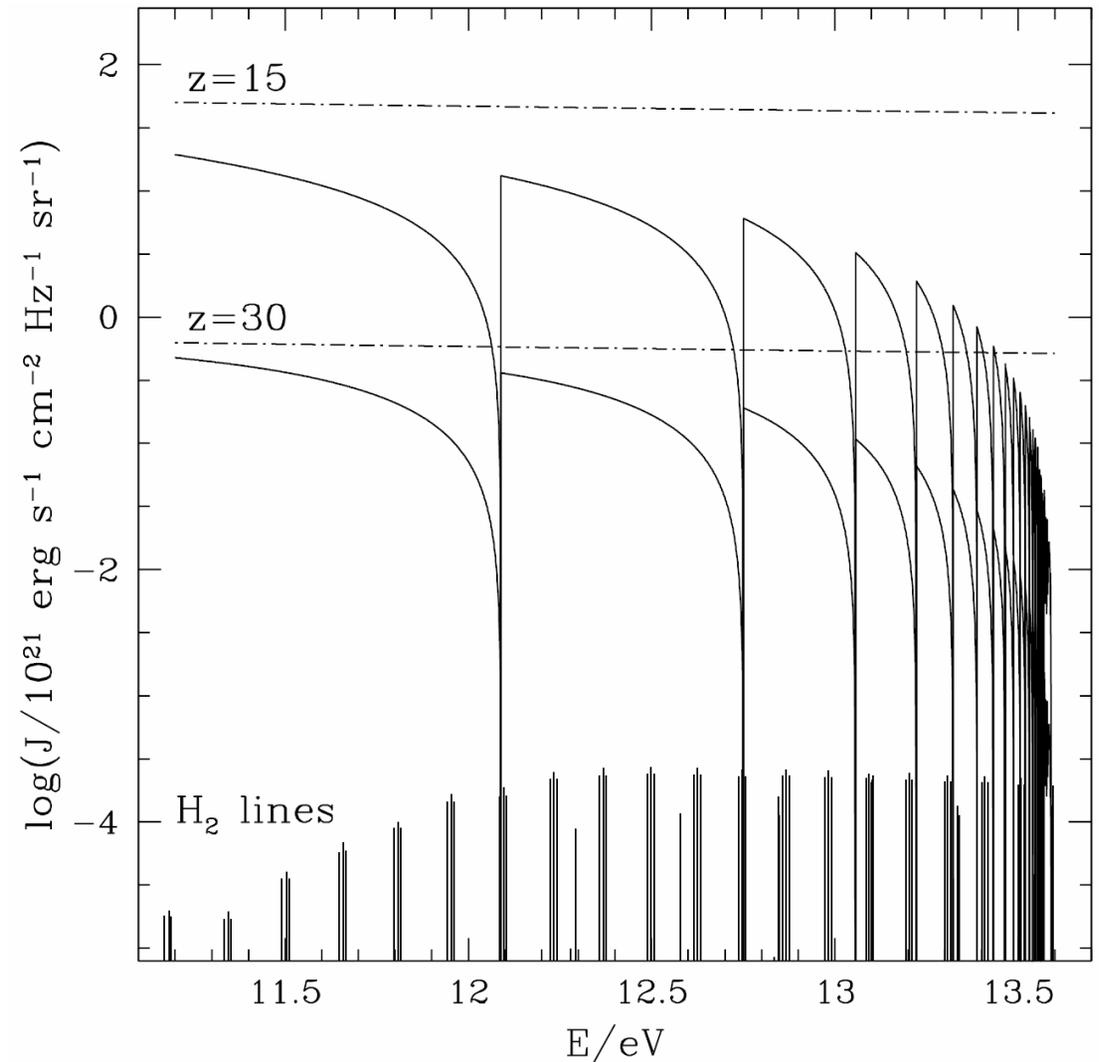
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35/h Mpc box

# Previous approximation for cosmic mean LW Background during EOR: homogeneous universe $\rightarrow$ “saw-tooth” modulation

- assume sources of UV emissivity *uniformly* distributed in space (e.g. Haiman et al. 2000; Ricotti et al. 2002; Yoshida et al. 2003)
- assume  $H_2$  dissociating photons, emitted below H Lyman limit, are removed whenever they redshift into an H Lyman series line and are resonantly scattered by the IGM, down-converting them out of LW bands
- uniform IGM opacity filters uniformly distributed LW emitters by “saw-tooth” modulation.

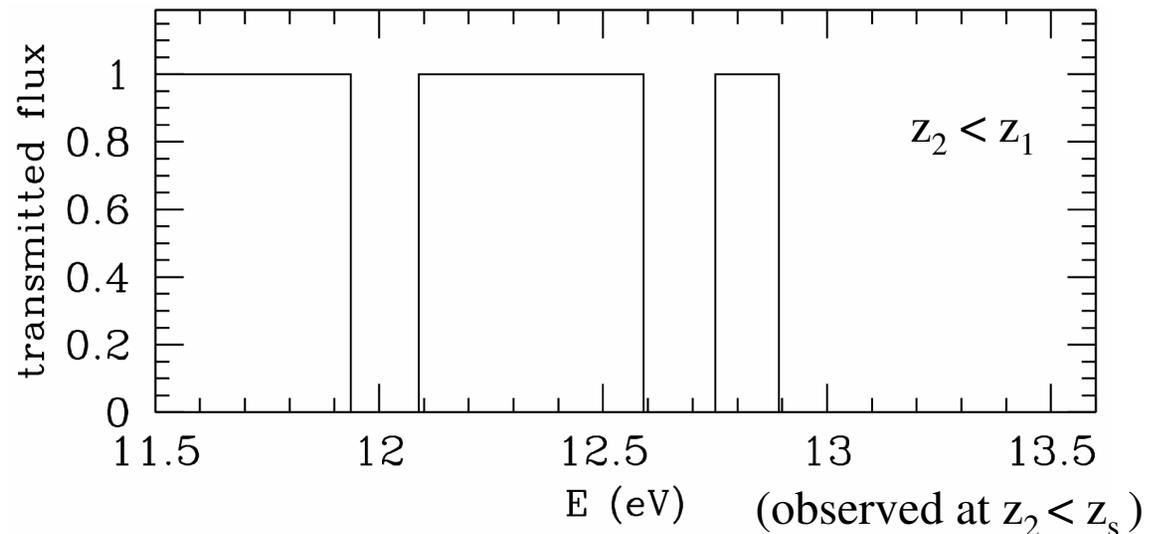
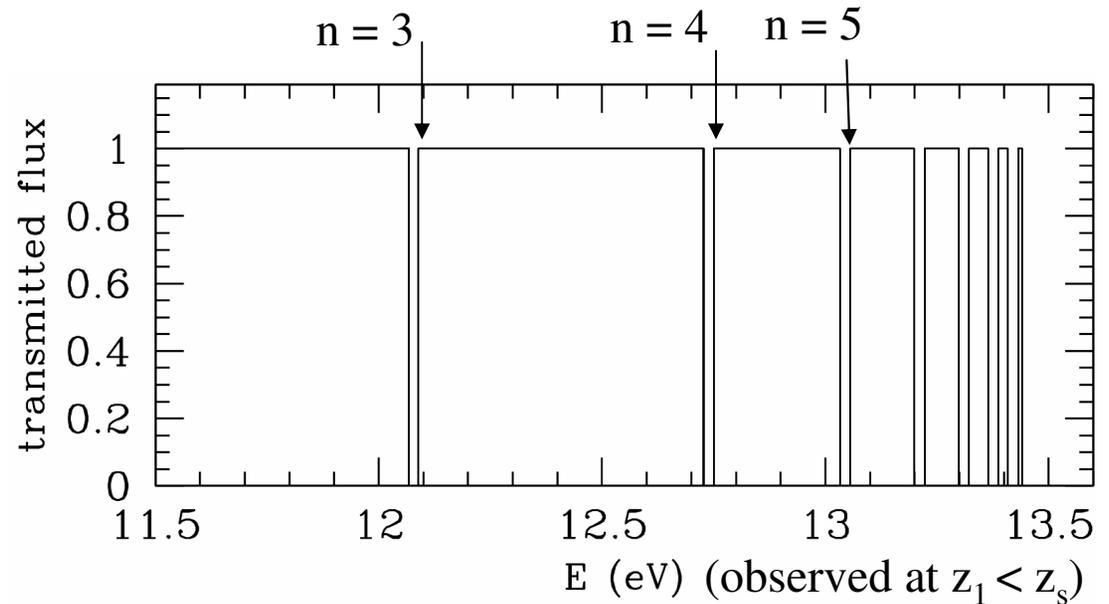


(Haiman, Abel, and Rees 2000)

## Attenuation of LW photons from a single source: “picket-fence” modulation

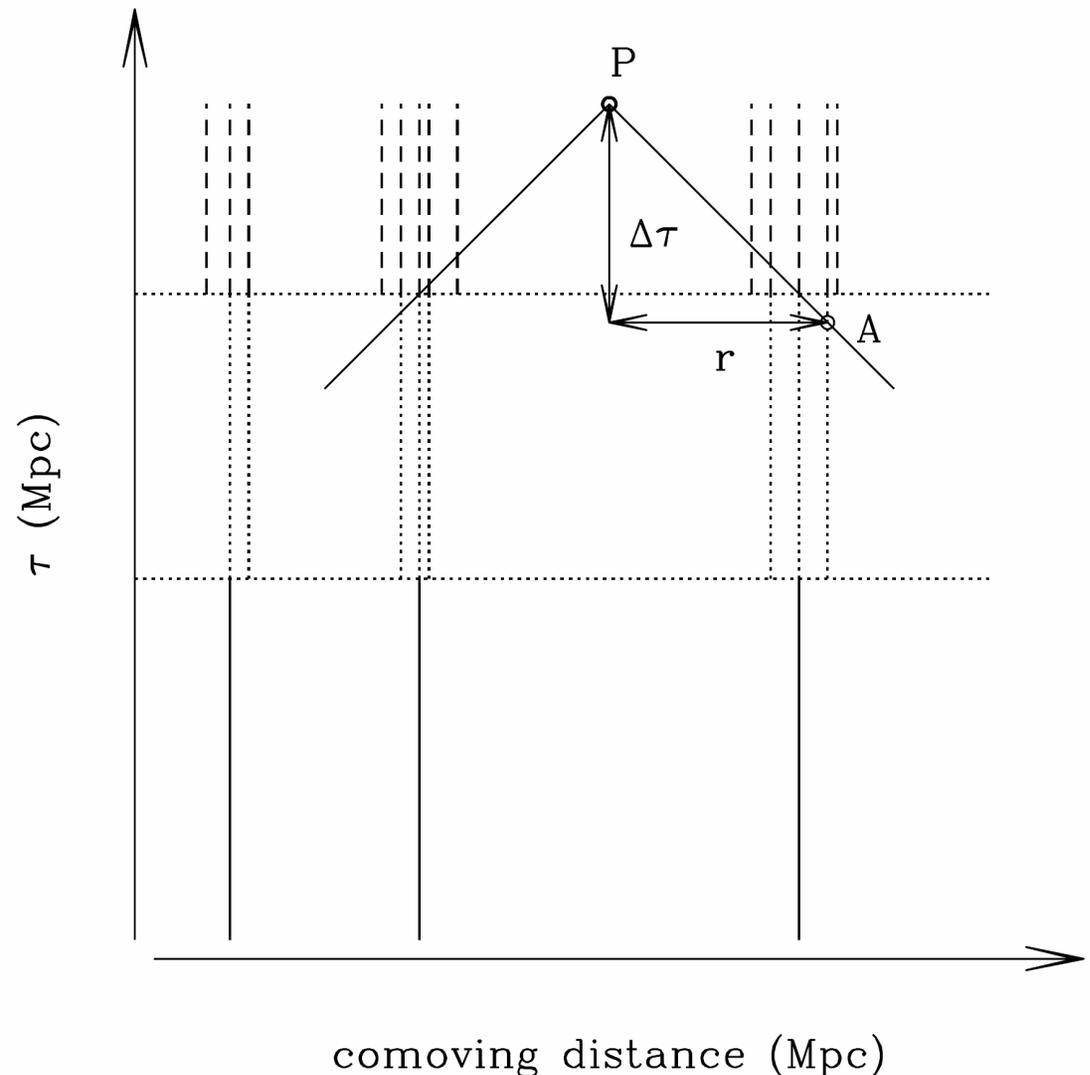
- A source at redshift  $z_s$  observed at different distances suffers different amounts of attenuation, dilution, and redshift
- When LW photon redshifts into the nearest lower H Lyman series line, it is scattered and destroyed (converted to lower energy photon).
- Source is completely attenuated at comoving distance

$$r_{\text{cMpc}} = 97 [(1 + z)/21]^{-0.5}$$



LW background radiative transfer is intrinsically cosmological : sources along the “past light-cone” of every point in space

- Space-time diagram of radiation sources and observer at point P at conformal time  $\tau$
- luminosity of each halo source is constant during finite time-step
- observer at point P will see sources whose world lines intersect the past light-cone
- must determine the attenuation, dilution, and redshift of the LW photons emitted at A and received at P



# Computational Challenge

$J_\nu(\mathbf{x}_{\text{obs}}, z_{\text{obs}}, \nu_{\text{obs}})$  at observed frequency  $\nu_{\text{obs}}$  at some comoving position  $\mathbf{x}_{\text{obs}}$  at redshift  $z_{\text{obs}}$  is given by

$$J_\nu(\mathbf{x}_{\text{obs}}, z_{\text{obs}}, \nu_{\text{obs}}) = \frac{1}{4\pi} \sum_s F_{\nu,s}(\mathbf{x}_{\text{obs}}, z_{\text{obs}}, \nu_{\text{obs}}), \quad (5)$$

where  $F_{\nu,s}$  is the flux received at  $(\mathbf{x}_{\text{obs}}, z_{\text{obs}}, \nu_{\text{obs}})$  that was emitted at  $(\mathbf{x}_s, z_s, \nu_s)$  by a source (denoted by subscript  $s$ ), where

$$\frac{\nu_s}{\nu_{\text{obs}}} = \frac{1 + z_s}{1 + z_{\text{obs}}}. \quad (6)$$

# Computational Challenge

The position and redshift,  $(\mathbf{x}_s, z_s)$ , of a source are related to those of the observer at  $(\mathbf{x}_{\text{obs}}, z_{\text{obs}})$  by the fact that the signal emitted at the epoch  $z_s$  must reach the position  $\mathbf{x}_{\text{obs}}$  at the epoch  $z_{\text{obs}}$ , travelling at the speed of light while the universe expands. We express this implicitly by writing the comoving separation,  $r_{\text{os}}$ , of the source and observer as follows:

$$r_{\text{os}} = |\mathbf{x}_{\text{obs}} - \mathbf{x}_s| = \int_{t(z_s)}^{t(z_{\text{obs}})} \frac{cdt}{a(t)} = - \int_{z_{\text{obs}}}^{z_s} c \frac{dz}{H(z)}. \quad (7)$$

## Computational Challenge

The differential flux,  $F_{\nu,s}$ , received at  $(\mathbf{x}_{\text{obs}}, z_{\text{obs}}, \nu_{\text{obs}})$  from a source of differential luminosity  $L_\nu$  emitted at  $(\mathbf{x}_s, z_s, \nu_s)$  is given by

$$F_{\nu,s}(\mathbf{x}_{\text{obs}}, z_{\text{obs}}, \nu_{\text{obs}}) = \frac{L_\nu(\nu = \nu_s)}{4\pi D_L^2(z_{\text{obs}}, z_s)} \cdot \left( \frac{1 + z_s}{1 + z_{\text{obs}}} \right) \cdot \exp[-\tau_{\nu_{\text{obs}}}], \quad (9)$$

Here  $D_L(z_{\text{obs}}, z_s)$  is

the luminosity distance given by

$$D_L(z_{\text{obs}}, z_s) \equiv \left( \frac{r_{\text{os}}}{1 + z_{\text{obs}}} \right) \left( \frac{1 + z_s}{1 + z_{\text{obs}}} \right), \quad (10)$$

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the luminosity distance given by

$$D_L(z_{\text{obs}}, z_s) \equiv \left( \frac{r_{\text{os}}}{1 + z_{\text{obs}}} \right) \left( \frac{1 + z_s}{1 + z_{\text{obs}}} \right), \quad (10)$$

- Expected number of computational operations :  $\sim N_{\text{sources}} * N_{\text{cells}} * N_{\text{frequencies}}$ 
    - where  $N_{\text{sources}} >\sim 10^7$  within the LW horizon of  $r_{\text{LW}} \sim 100$  cMpc
    - $N_{\text{cells}} >\sim 10^6$  grid cells for sufficient resolution and statistical accuracy
    - $N_{\text{frequencies}} \gg 1$  for multi-frequency transfer of optically thick Lyman series lines
- ➔ *full 3D, multi-frequency radiative transfer would be prohibitive!!*

# Computational Challenge

The differential flux,  $F_{\nu,s}$ , received at  $(\mathbf{x}_{\text{obs}}, z_{\text{obs}}, \nu_{\text{obs}})$  from a source of differential luminosity  $L_{\nu}$  emitted at  $(\mathbf{x}_s, z_s, \nu_s)$  is given by

$$F_{\nu,s}(\mathbf{x}_{\text{obs}}, z_{\text{obs}}, \nu_{\text{obs}}) = \frac{L_{\nu}(\nu = \nu_s)}{4\pi D_L^2(z_{\text{obs}}, z_s)} \cdot \left( \frac{1 + z_s}{1 + z_{\text{obs}}} \right) \cdot \exp[-\tau_{\nu_{\text{obs}}}], \quad (9)$$

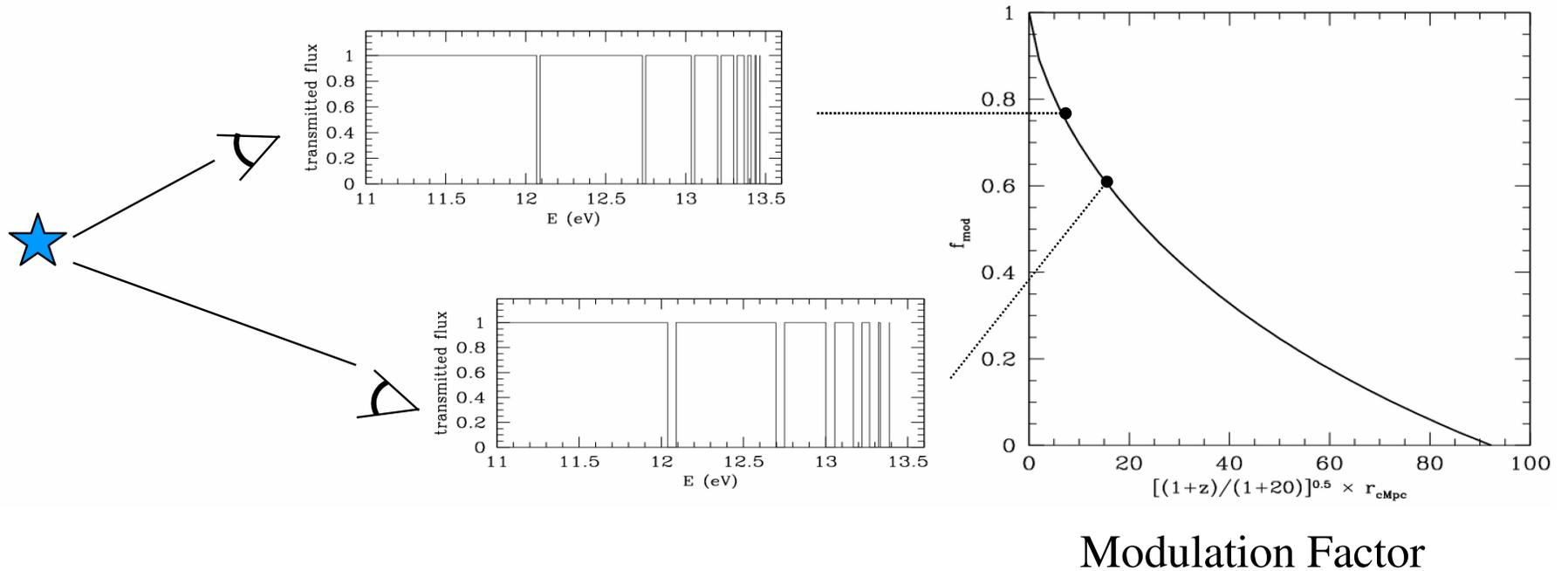
Here  $D_L(z_{\text{obs}}, z_s)$  is

the luminosity distance given by

$$D_L(z_{\text{obs}}, z_s) \equiv \left( \frac{r_{\text{os}}}{1 + z_{\text{obs}}} \right) \left( \frac{1 + z_s}{1 + z_{\text{obs}}} \right), \quad (10)$$

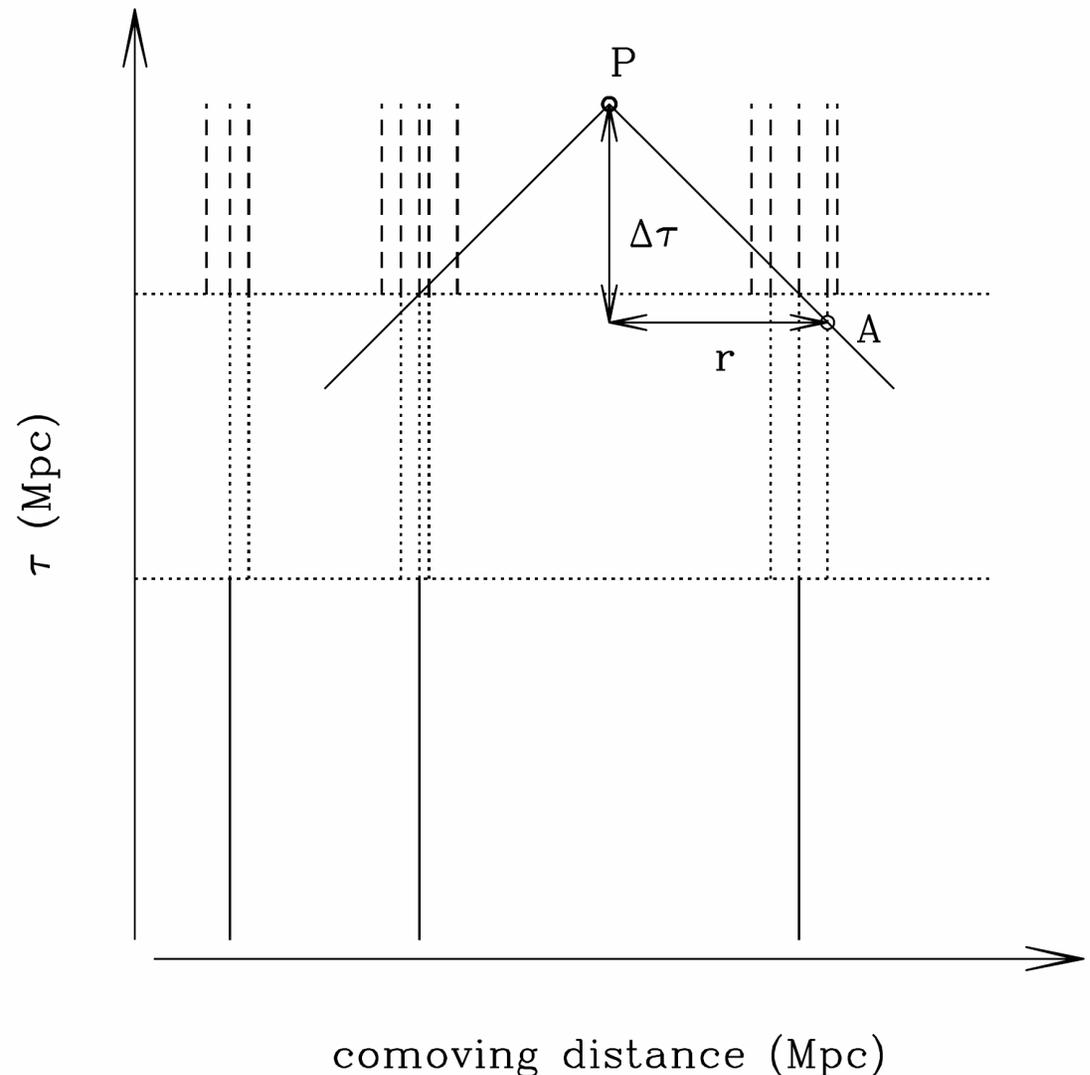
- Expected number of computational operations :  $\sim N_{\text{sources}} * N_{\text{cells}} * N_{\text{frequencies}}$   
 where  $N_{\text{sources}} >\sim 10^7$  within the LW horizon of  $r_{\text{LW}} \sim 100$  cMpc  
 $N_{\text{cells}} >\sim 10^6$  grid cells for sufficient resolution and statistical accuracy  
 $N_{\text{frequencies}} \gg 1$  for multi-frequency transfer of optically thick Lyman series lines  
 → *full 3D, multi-frequency radiative transfer would be prohibitive!!*  
 → **We solve this by making a grey opacity approximation equivalent to multi-frequency...**

# Attenuation of LW photons from a single source: “picket-fence” modulation factor



LW background radiative transfer is intrinsically cosmological : sources along the “past light-cone” of every point in space

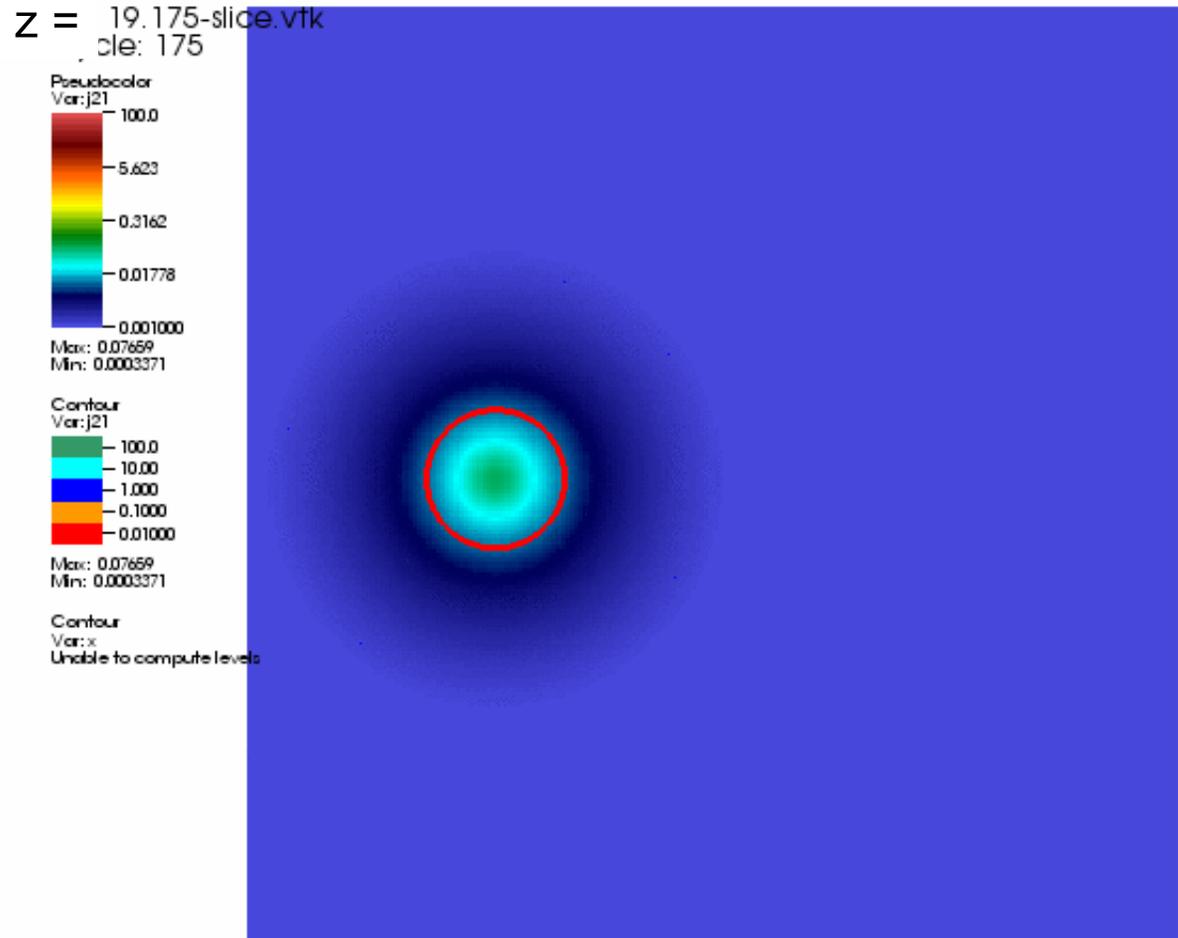
- Space-time diagram of radiation sources and observer at point P at conformal time  $\tau$
- luminosity of each halo source is constant during finite time-step
- observer at point P will see sources whose world lines intersect the past light-cone
- must determine the attenuation, dilution, and redshift of the LW photons emitted at A and received at P



# The Fluctuating H<sub>2</sub> Dissociating Background During Reionization

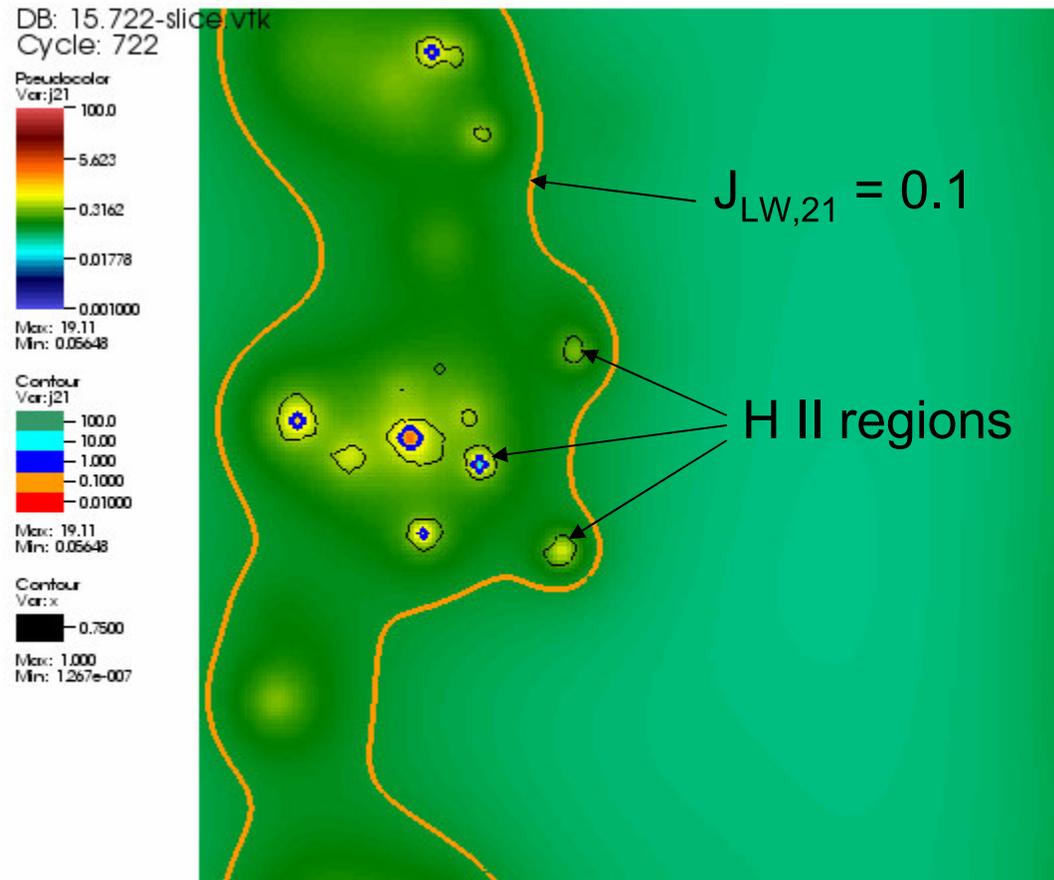
Ahn, Shapiro, Iliiev, Mellema, & Pen 2008, MNRAS, submitted (astro-ph/0807.0920)

- LW background radiative transfer code parallelized using MPI for distributed-memory parallel computers;
- e.g. 35/h Mpc reionization simulation has  $(203)^3$  cells,  $N_{\text{sources}} = 200,000$  by  $z = 8$ , but must do LW transfer in  $5^3$  boxes stacked around the central box to fill 100 Mpc LW horizon →  $N_{\text{sources}}$ , total > 20 million!
- Ran for 22 hours, on 320 computing cores, 1.5 GB memory per core, Texas supercomputer *Lonestar* (5200 cores of dual-core Intel Xeon processors, with 11.6 TB aggregate memory).

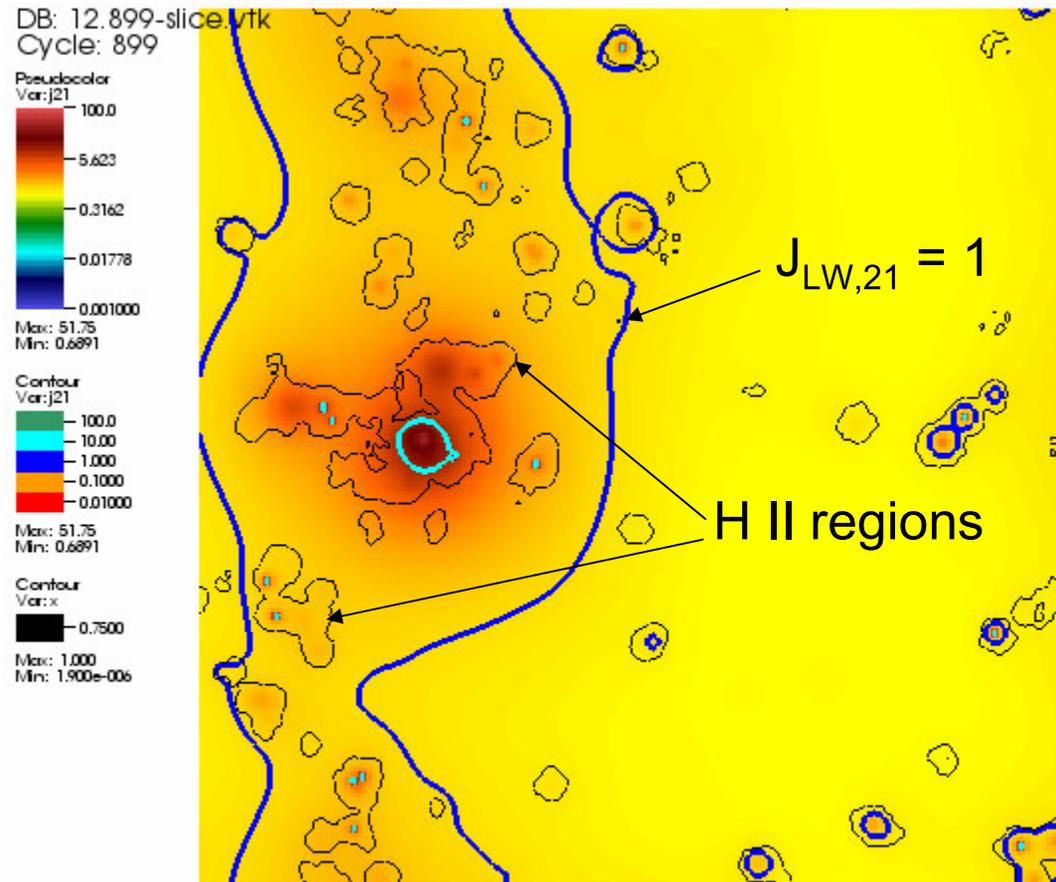


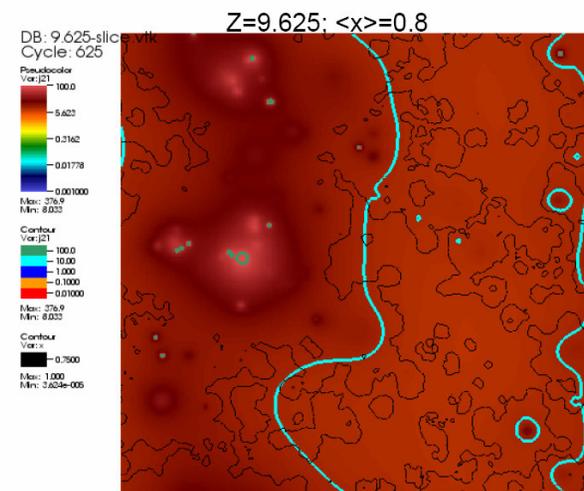
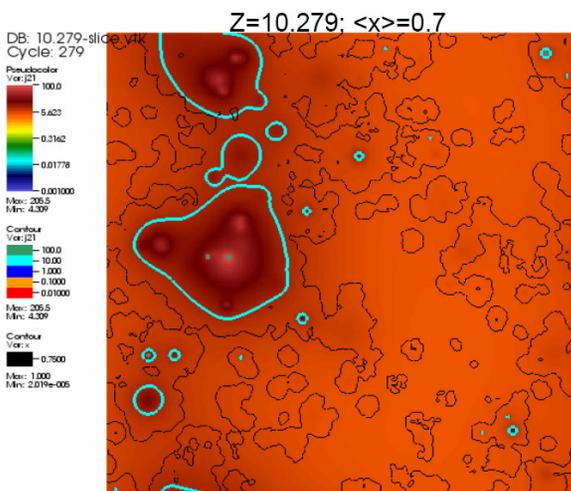
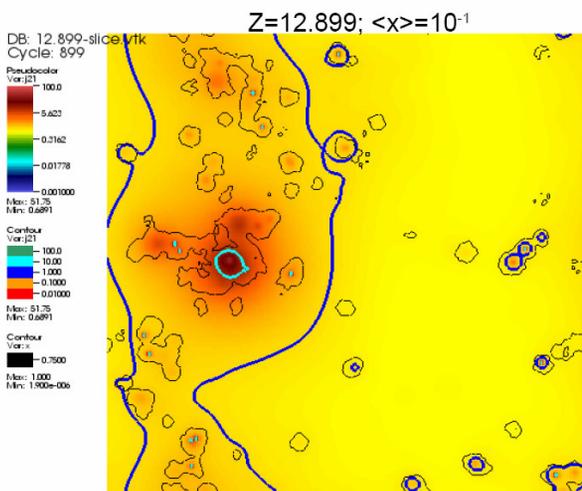
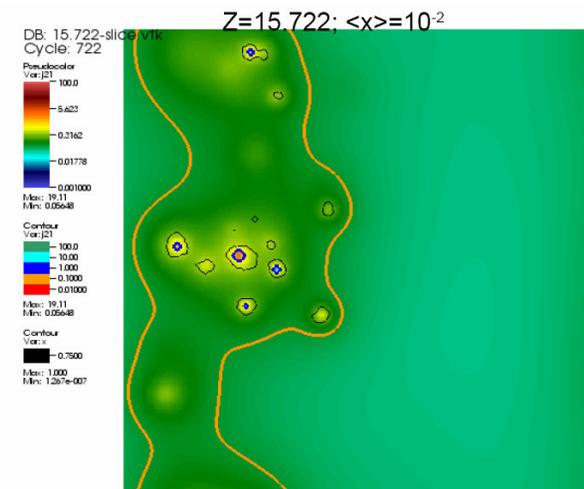
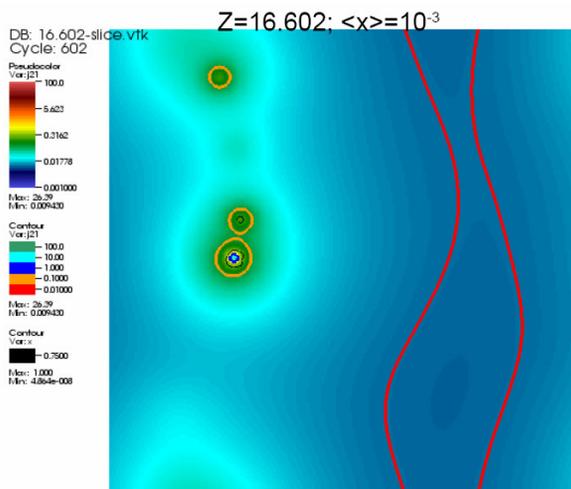
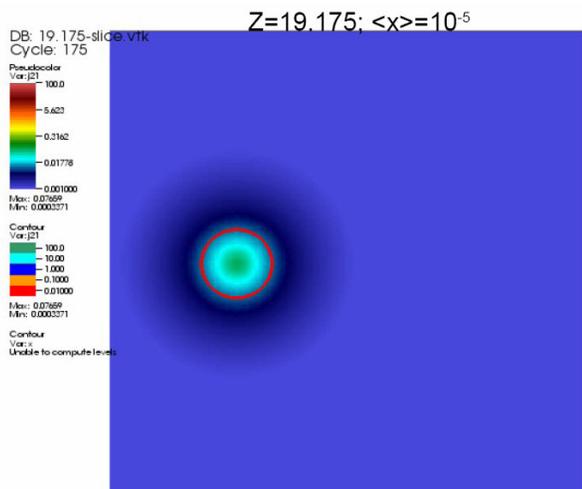
35/h Mpc box

# H<sub>2</sub> Dissociating Background during EOR

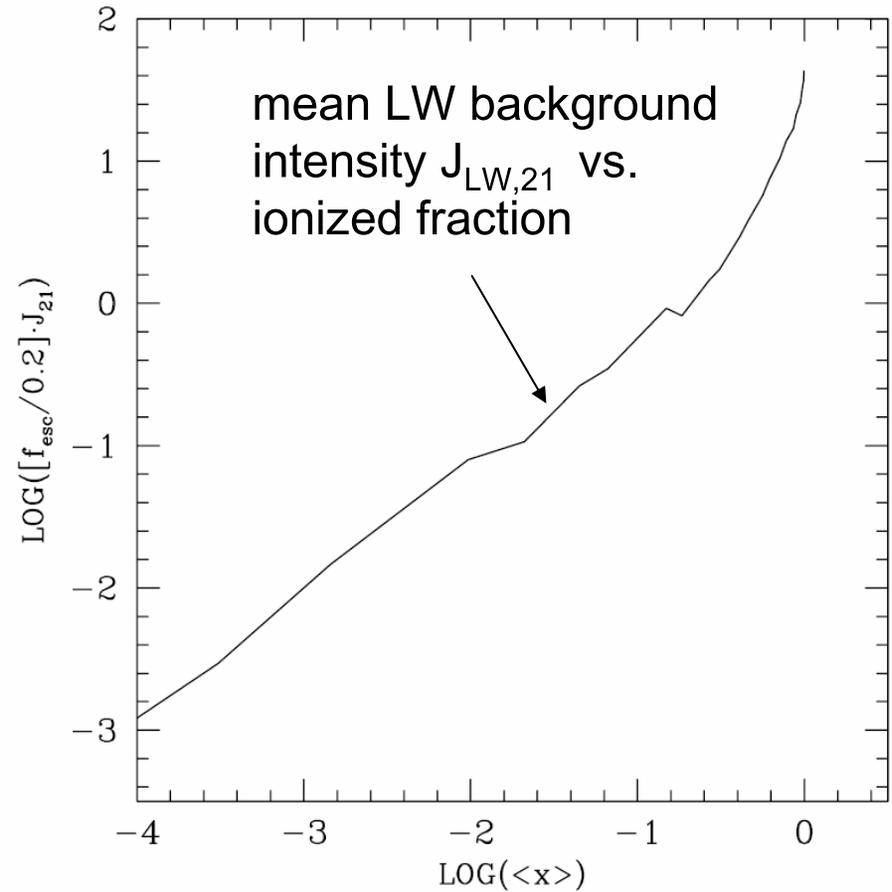
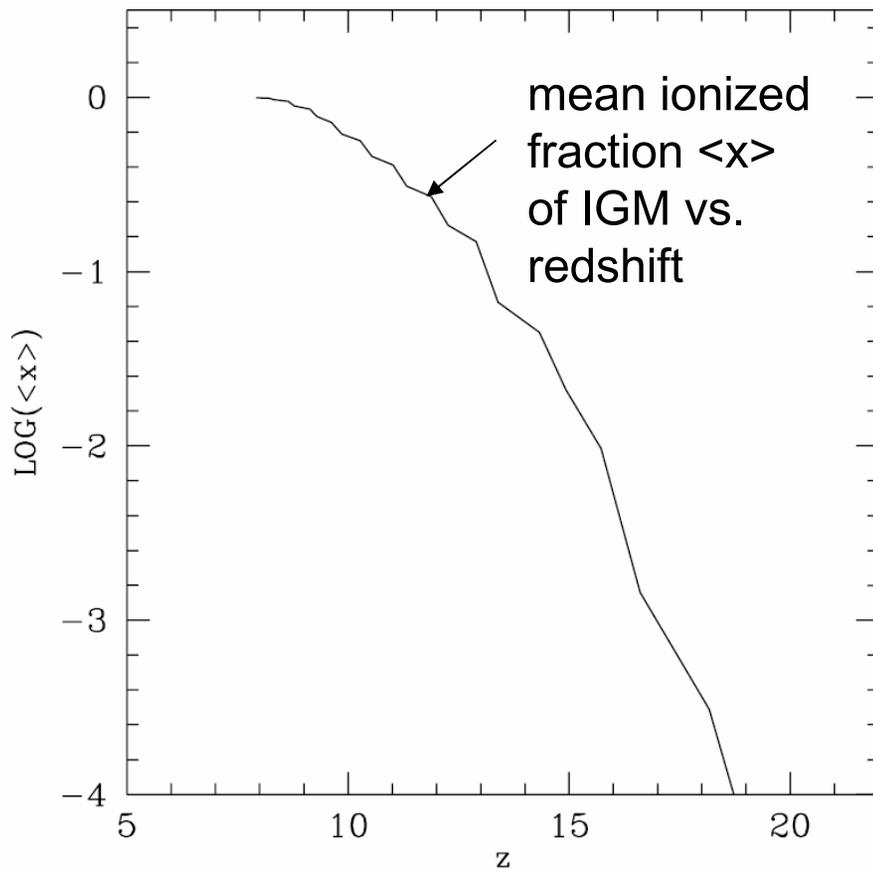


# H<sub>2</sub> Dissociating Background during EOR



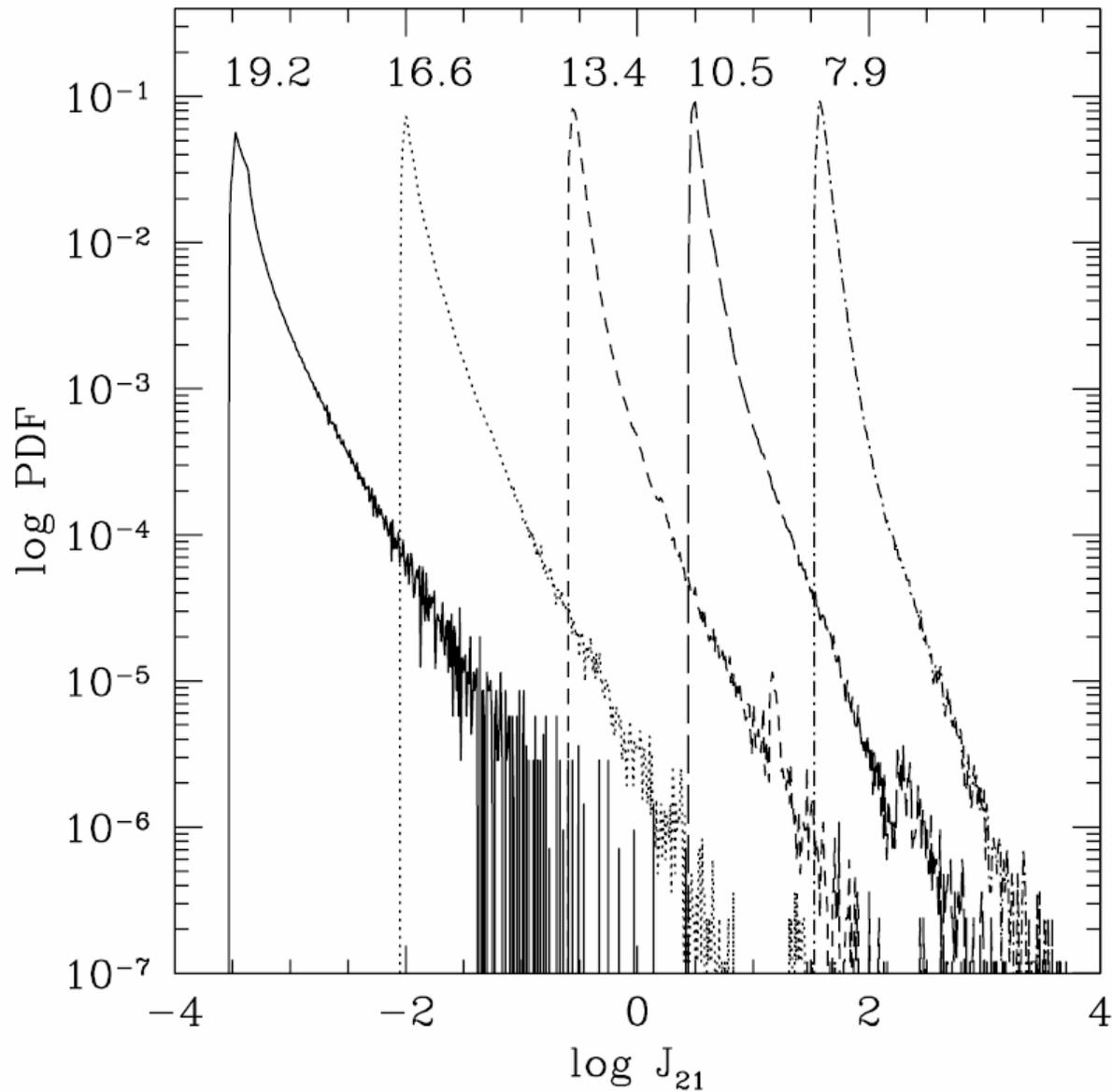


# The Mean $H_2$ Dissociating UV Background During EOR



$$J_{LW,21} = J / (10^{-21} \text{ erg s}^{-1} \text{ cm}^{-2} \text{ Hz}^{-1} \text{ ster}^{-1})$$

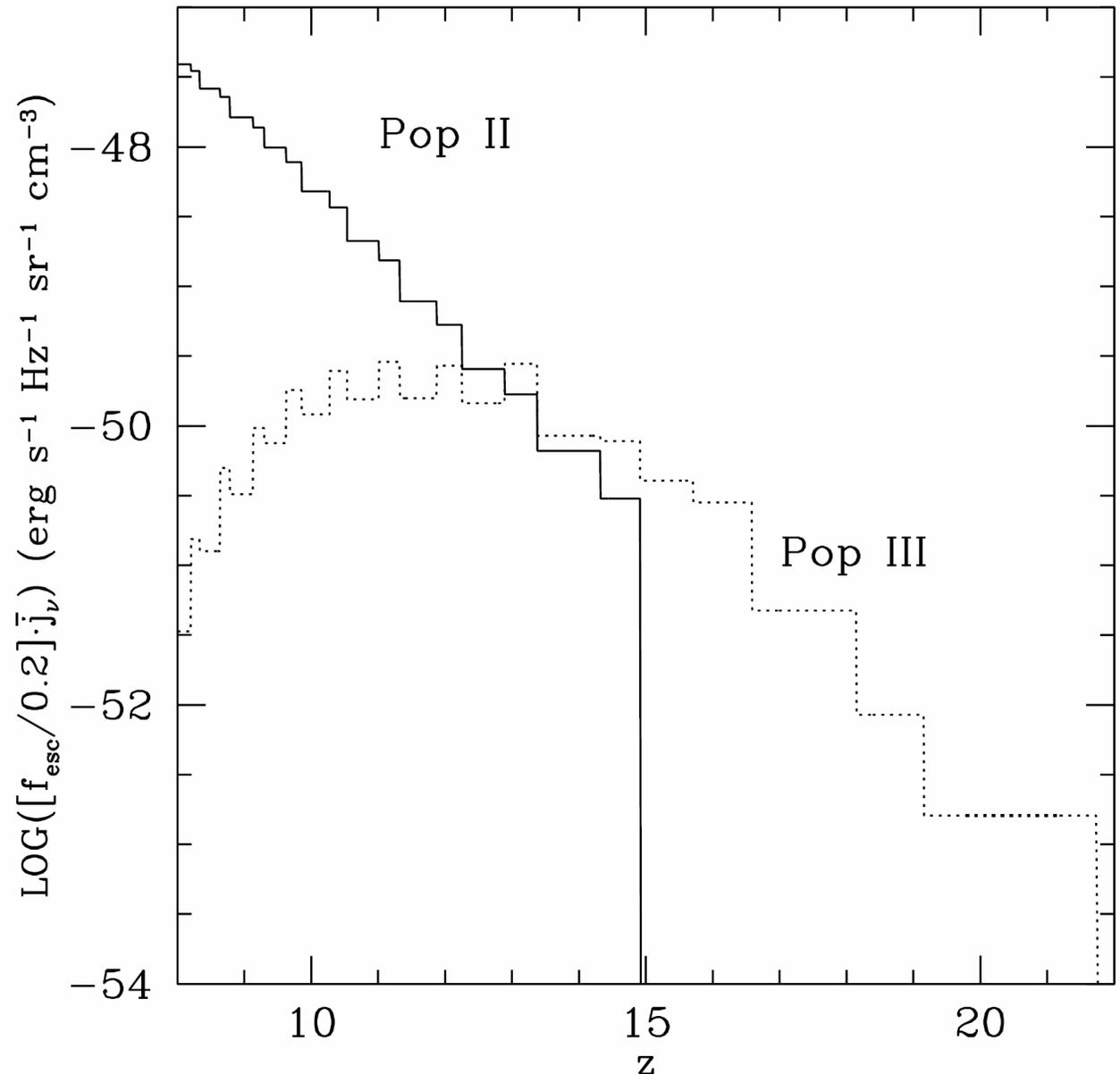
# Distribution of Intensity Fluctuations for the LW Background During Reionization



(35/h Mpc box)

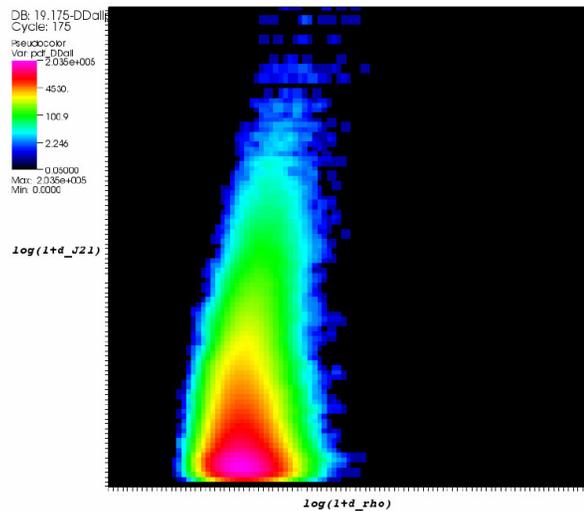
# What are the dominant sources of the LW background during the EOR?

- Self-regulation of reionization
  - ➔ early LW background is dominated by low-mass sources that are suppressed if they form inside H II regions,
  - BUT the rise of the small-mass sources saturates long before end of EOR
  - ➔ the high-mass sources eventually dominate the LW background

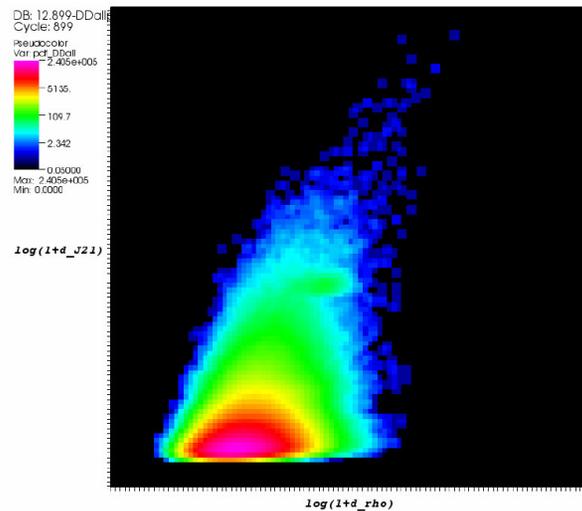


# LW background intensity fluctuations in space are correlated with matter density fluctuations

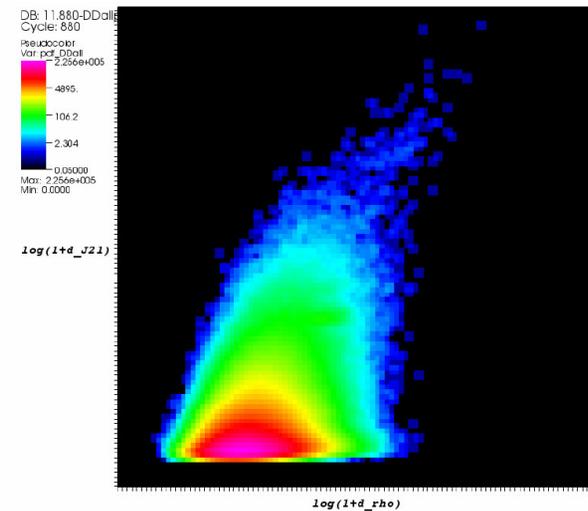
$z = 19$



$z = 13$



$z = 12$



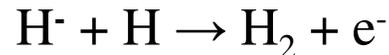
## LW Background Conclusions

- Picket-fence modulation of LW background photons
  - makes computation of inhomogeneous LW background tractable
- LW rises above the threshold for suppressing star formation in minihalos long before end of the EOR → supports the idea that MHs, on average, not significant reionization source, but
- LW intensity fluctuates significantly in space → may be “safe spots” early on, to form Pop III stars in minihalos where LW background minima occur, far from the large-scale H II regions made by clustered dwarf galaxies.
- Fluctuation in LW background comes from source clustering, at a scale of ~10 comoving Mpc
- May contribute to NIR background fluctuations
- Understanding radiative feedback on Pop III star formation in minihalos may be important to complete the theory of reionization

# More Feedback From First Radiation Sources: H<sup>-</sup> Photodissociation

Chuzhoy, Kuhlen, & Shapiro (2007), *ApJL*, 665, L85 (astro-ph/0704.0426)

- Rate for H<sub>2</sub> formation in primordial gas,



is proportional to abundance of H<sup>-</sup> ==> destroying H<sup>-</sup> will reduce H<sub>2</sub> formation rate;

- Photodissociation can destroy H<sup>-</sup>,



- **During reionization, as sources release ionizing radiation, they also cause a background of H<sup>-</sup> dissociating radiation to build up, which reduces the H<sub>2</sub> formation rate by factor F<sub>s</sub>,**

$$F_s \sim 1 + 1000 k_s x / (f_{\text{esc}} \delta),$$

where **x = cosmic mean ionized fraction**, **δ = local baryon gas overdensity**,

and **k<sub>s</sub> = a constant of order unity which depends on type of radiation source**

(e.g. recombination radiation, direct stellar or quasar emission, or secondary emission by nonthermal electrons following X-ray background ionization) ;

- **Hence, by the time  $x \gtrsim 0.1$ , H<sup>-</sup> photodissociation may significantly reduce H<sub>2</sub> abundance and cooling, and the rate of primordial star formation.**