

# **Simulating the Early Structure Formation and the Epoch of Reionization**

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with

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# The Formation of Early Cosmic Structures

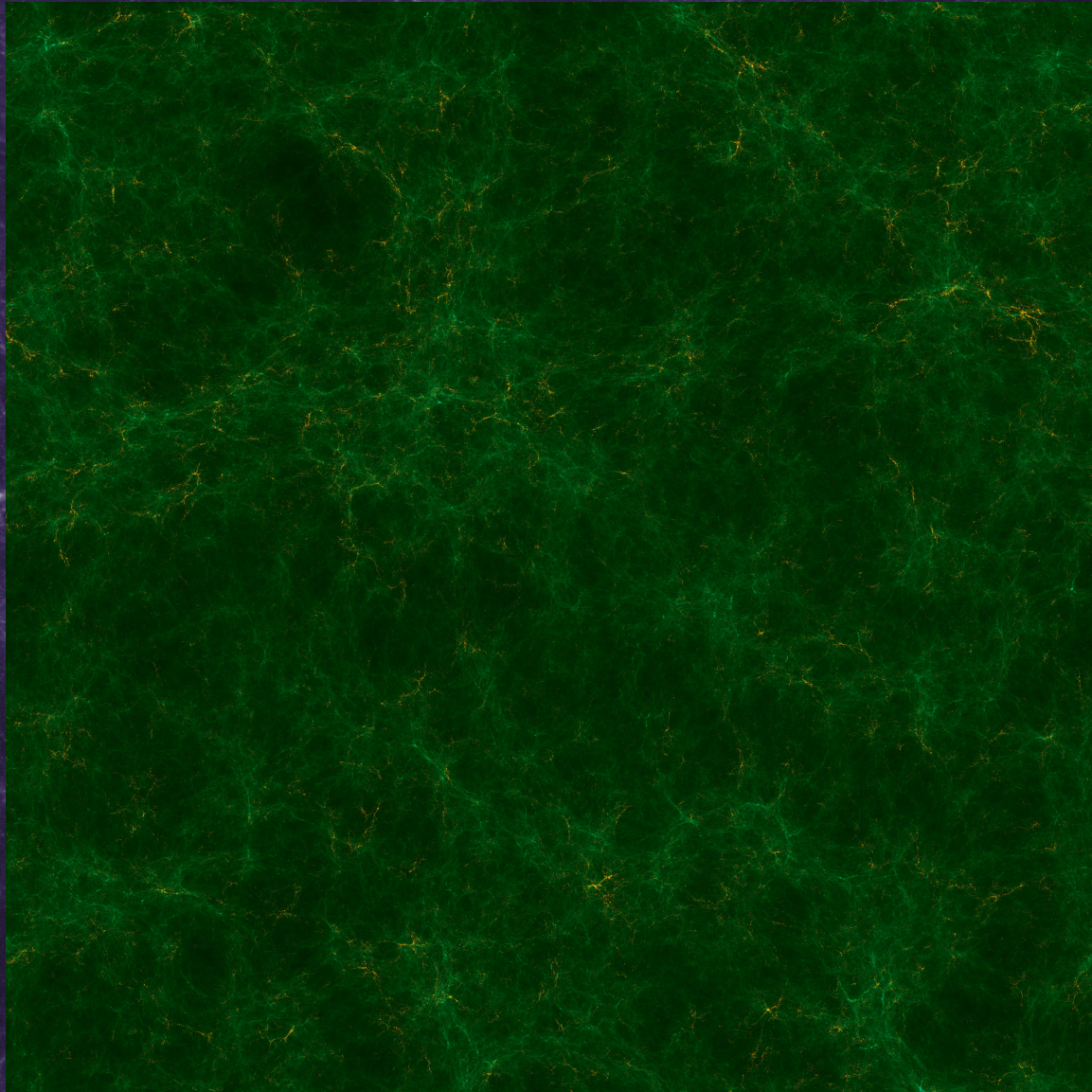
Iliev, Mellema, Pen, Merz, Shapiro, Alvarez 2006a, MNRAS, 369, 1885, and in progress)

114/h Mpc box @  $z=6$   
3072<sup>3</sup> particles (29 billion),  
6144<sup>3</sup> cells, P<sup>3</sup>M simulation  
density=green, halos=orange

We have now ran simulations with  
1024<sup>3</sup>, 1500<sup>3</sup>, 1728<sup>3</sup>, 2048<sup>3</sup> and 3072<sup>3</sup>  
particles in boxes of 37/h-114/h Mpc.

These sizes allow us to resolve all  
halos down to the atomically-cooling  
limit ( $10^8 M_{\text{str}}$ ) in 100-150/h Mpc  
boxes - the ultimate goal for  
this type of simulations.

Still larger simulations are possible  
on current hardware, with  
64-300 billion particles  
(6x-30x the Millenium simulation)  
165 billion (5488<sup>3</sup>; on 10,976 cores)  
was recently finished (see next);  
10<sup>12</sup> (10,000<sup>3</sup>=trillion)-particle  
simulations are now within reach..



Simulations ran at Texas Advanced  
Computing Facility on up to 2,048 cores.



# The Formation of Early Cosmic Structures: The Very Small Scales

(Iliev, et al., work in progress)

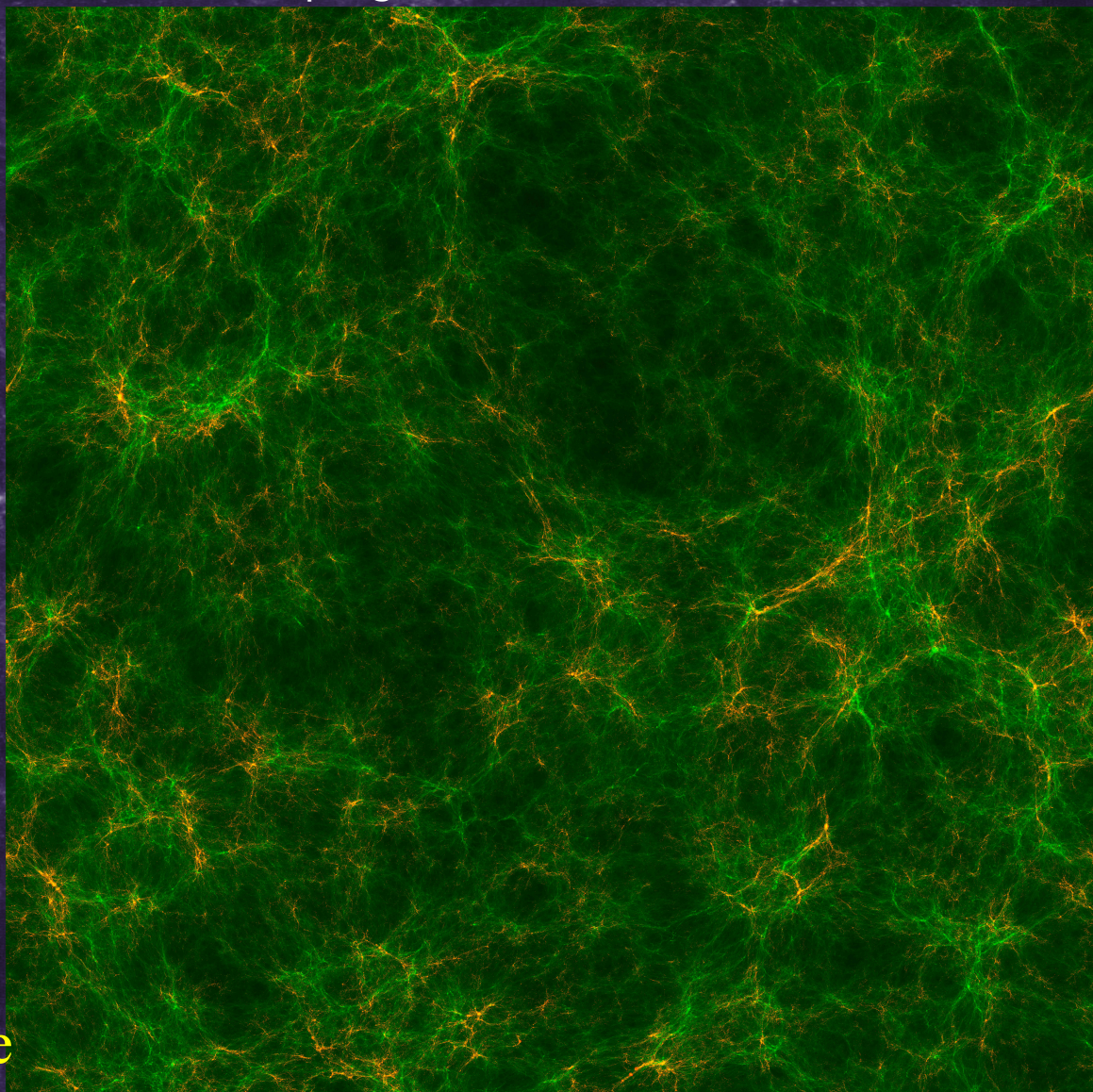
20/h Mpc box @  $z=8$   
5488<sup>3</sup> particles (165 billion),  
10976<sup>3</sup> cells, P<sup>3</sup>M simulation

Resolves all halos down to small minihalos ( $10^5 M_{\text{sdg}}$ ). We also ran 11.4/h Mpc and 6.3/h Mpc boxes with same min resolution.

Structures are highly biased. Extend to extremely small scales (resolution of this simulation is 182 pc!)

First halos form at  $z=43$ .  
>112 million halos at  $z=8$ .

Very useful for modelling the effects of small-scale structure and 21-cm absorption.



Simulations ran at Texas Advanced Computing Center on 864-21,952 cores.



# The high- $z$ halo mass function

(work in progress)

Rich statistics ( $z=8$ ):

20/h Mpc box: 114 million halos

2/h Mpc box: 5M+ (mini)halos

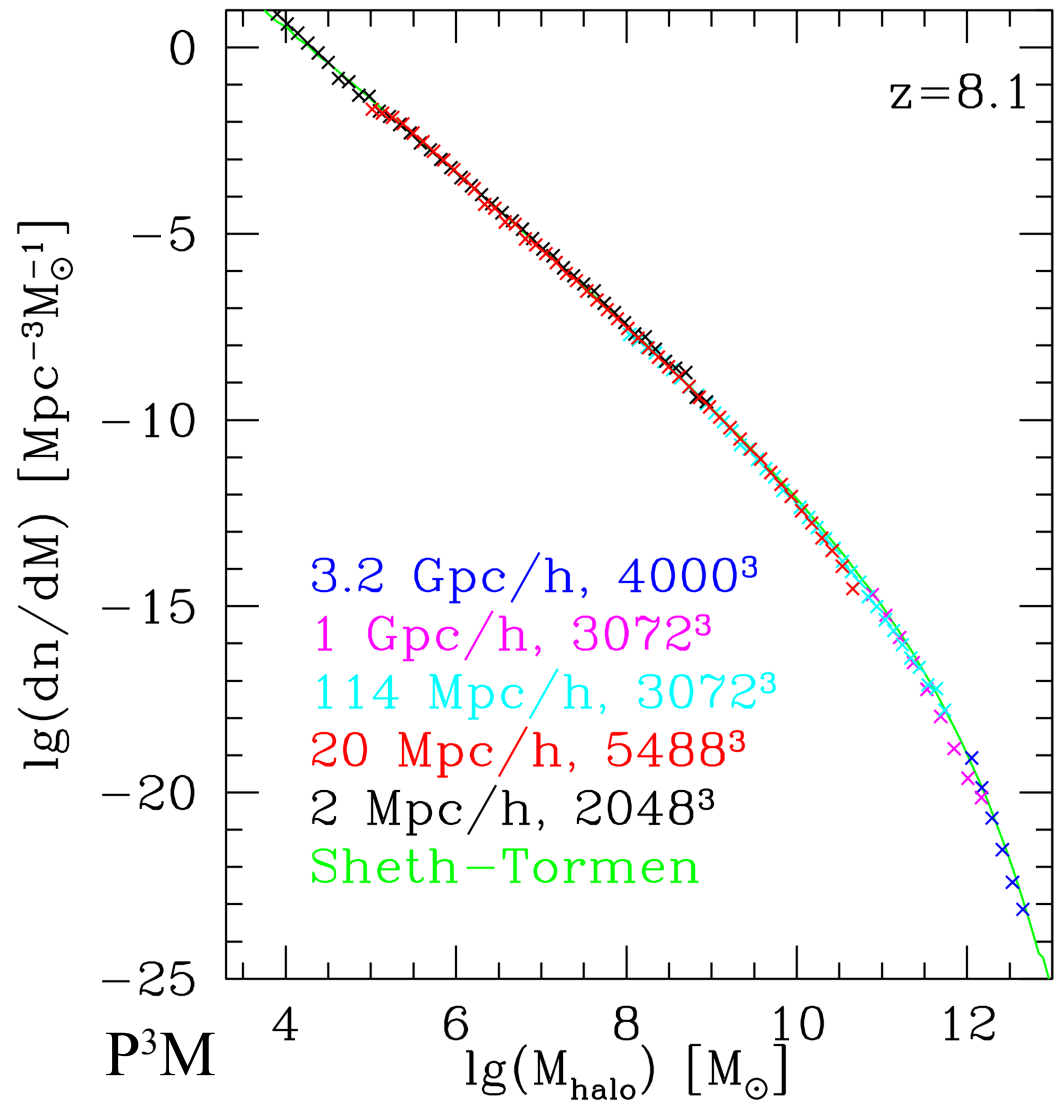
114/h Mpc box: 12M+ halos

1 Gpc/h box: 330k+ halos

3.2 Gpc/h box: 3600+ halos

(MW-sized or larger!)

Results show good agreement with each other, but differ from the Sheth-Tormen mass function (green) at the high-mass end.





# The high- $z$ halo mass function

(work in progress)

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20/h Mpc box: 114 million halos

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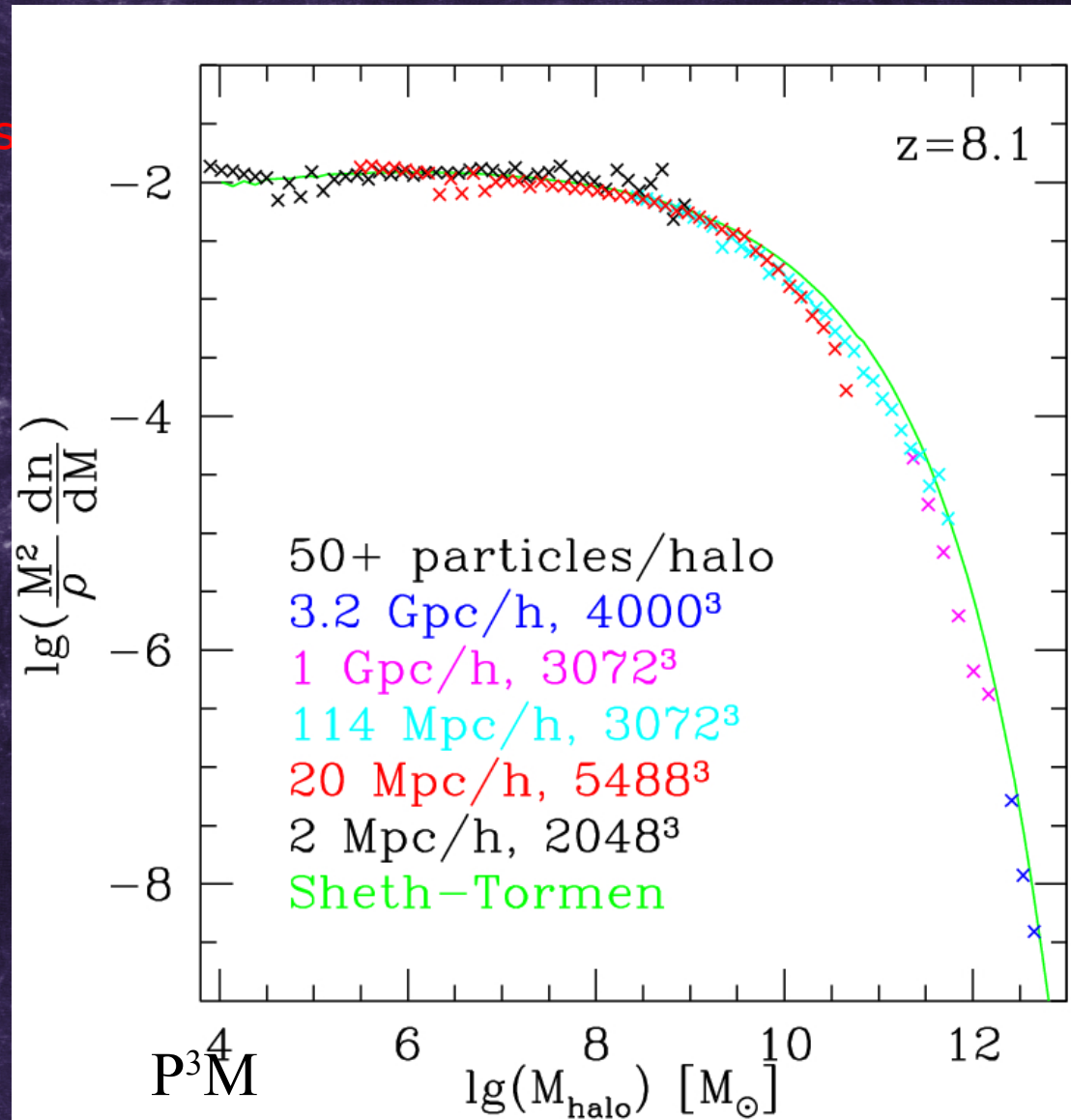
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(MW-sized or larger!)

Results show good agreement with each other, but differ from the Sheth-Tormen mass function (green) at the high-mass end.





# The high- $z$ halo mass function

(work in progress)

$z=16.6$ , 100+ particles/halo

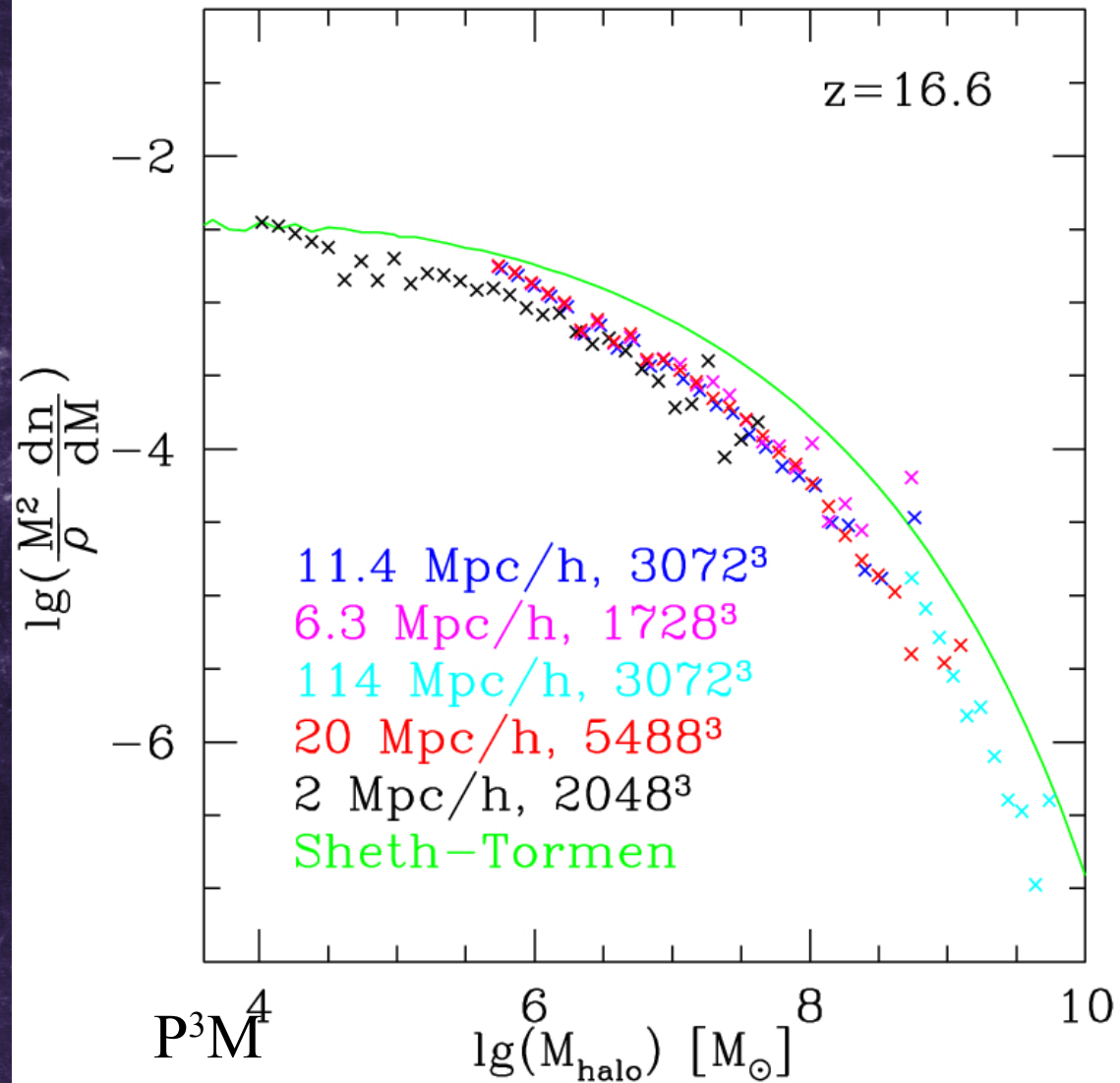
20/h Mpc box: 25 million halos

2/h Mpc box:  $\sim 2$ M (mini)halos

114/h Mpc box: 150k+ halos

6.3 Mpc/h box: 760k+ halos

Results show good agreement with each other, but differ from the Sheth-Tormen mass function (green) for rare halos (i.e. everywhere).



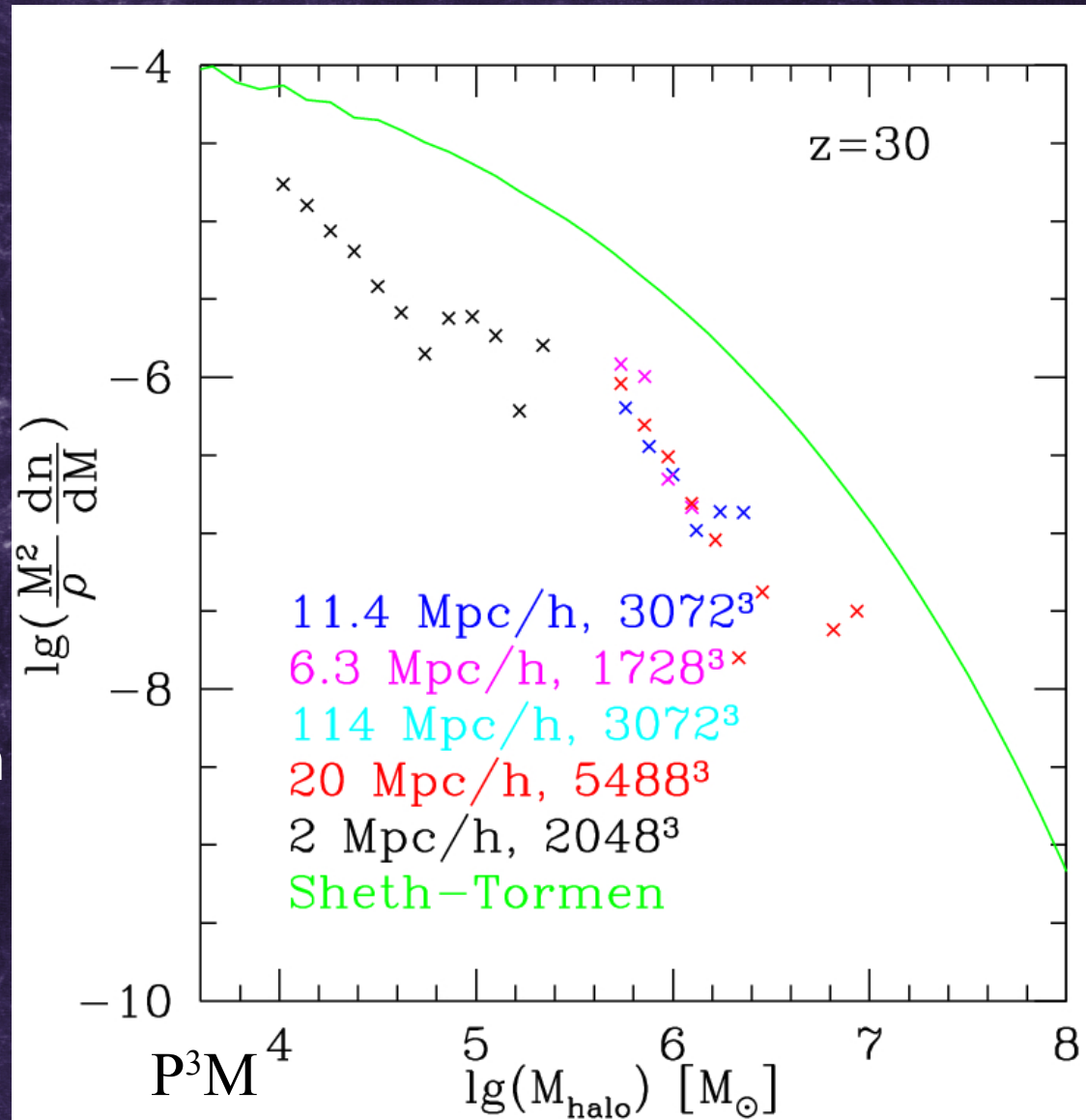


# The high- $z$ halo mass function

(work in progress)

$Z=30$ , 100+ particles/halo  
20/h Mpc box:  $\sim 100k$  halos  
2/h Mpc box: 30k+ (mini)halos  
6.3 Mpc/h box: 3k+ halos

Results show good agreement with each other, but differ by an order of magnitude from the Sheth-Tormen mass function (green) for all halos.

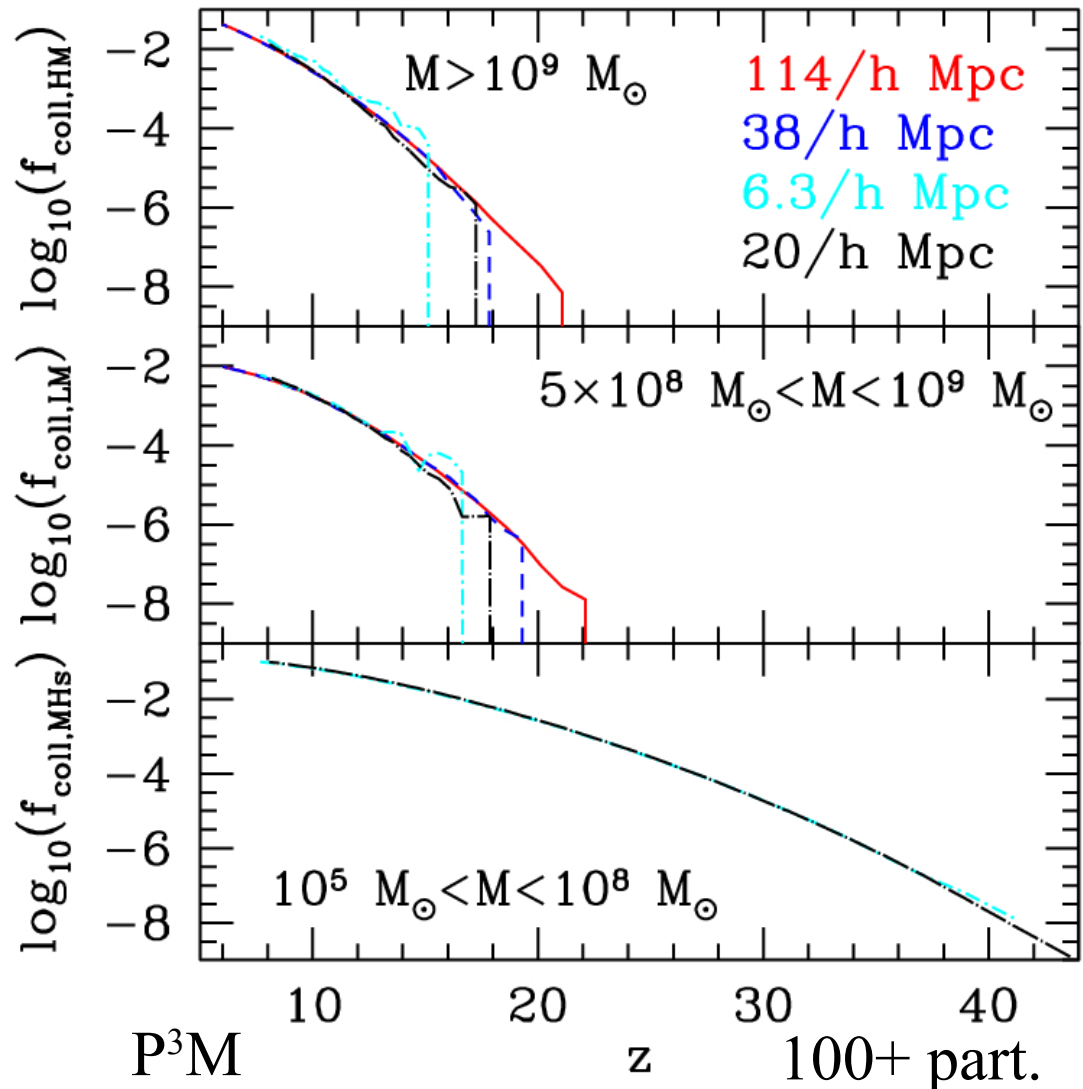




# The high- $z$ collapsed fractions

(work in progress)

Halo collapsed fractions agree quite well for a range of box sizes from 114 Mpc/h to 6.3 Mpc/h. Cut-off and noise at high mass is due to poor statistics (i.e. cosmic variance).

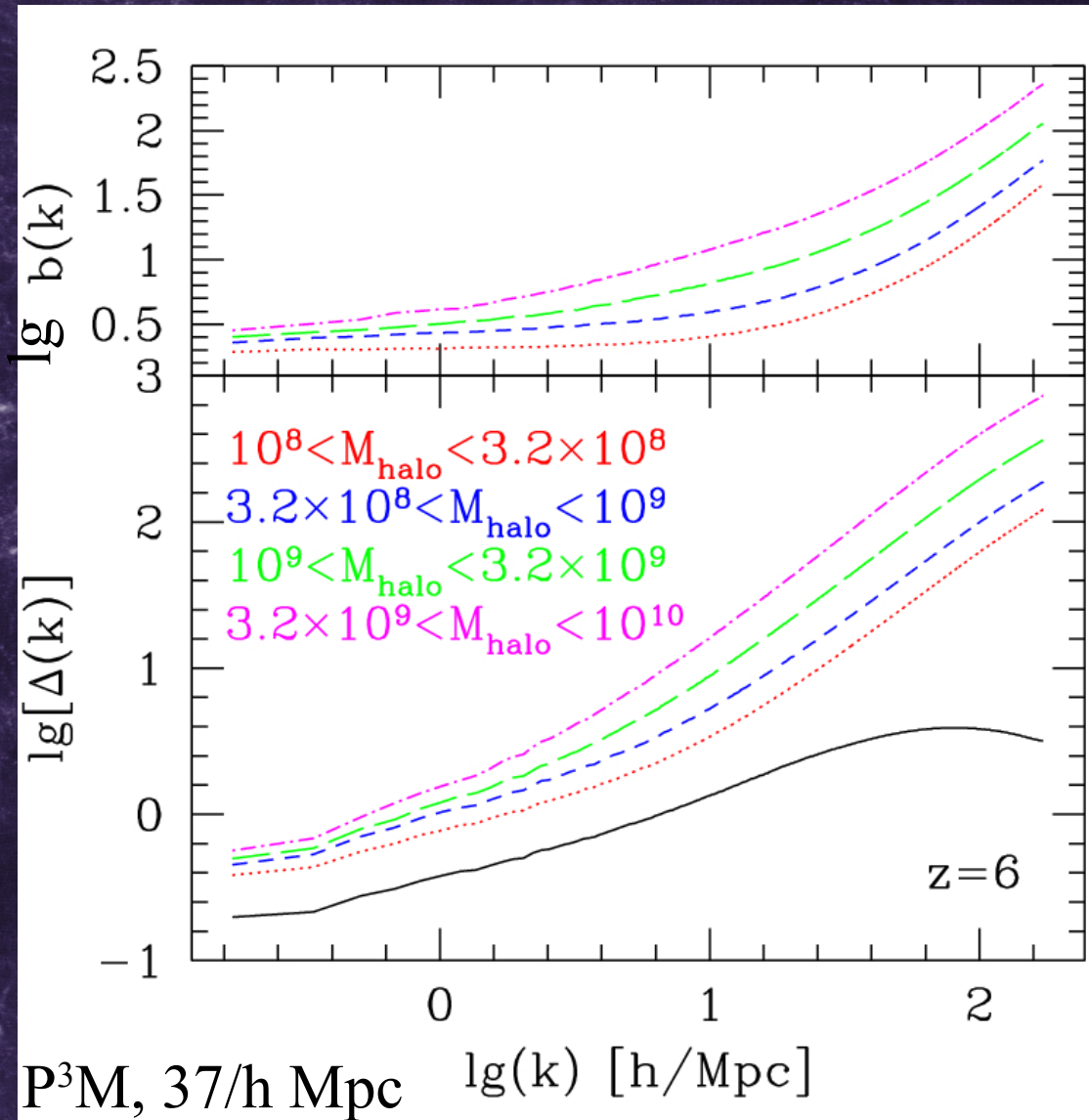




# The high- $z$ halo bias

(work in progress)

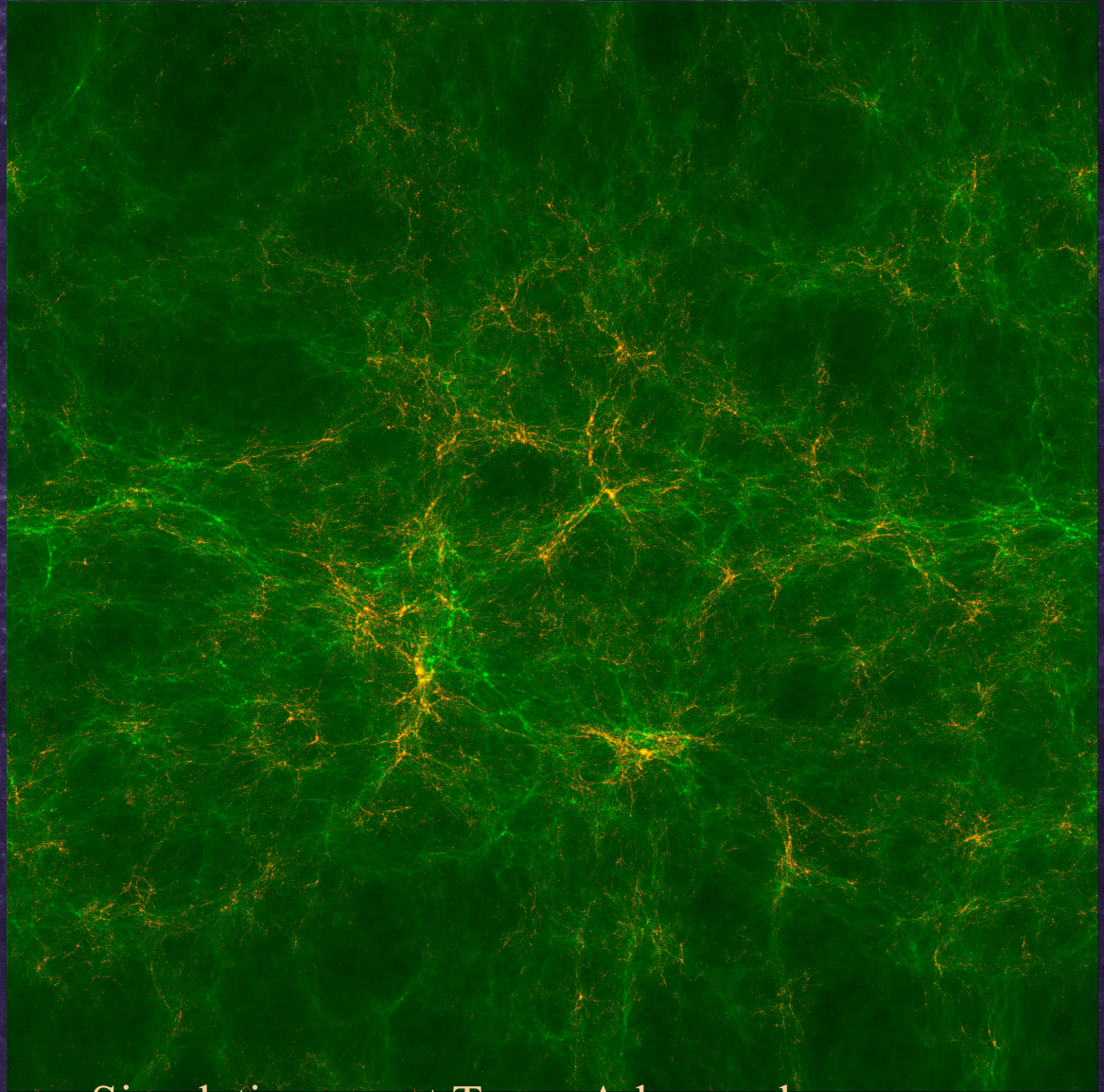
- Halos at high- $z$  are strongly biased.
- Bias increases strongly with halo mass and can reach a few hundred in the nonlinear regime.
- Scale at which bias becomes linear varies significantly with halo mass.





# Halo bias at high redshift: illustration (work in progress)

6.3/h Mpc box @  $z=10$   
1728<sup>3</sup> particles (5.2 billion),  
3456<sup>3</sup> cells, P<sup>3</sup>M simulation

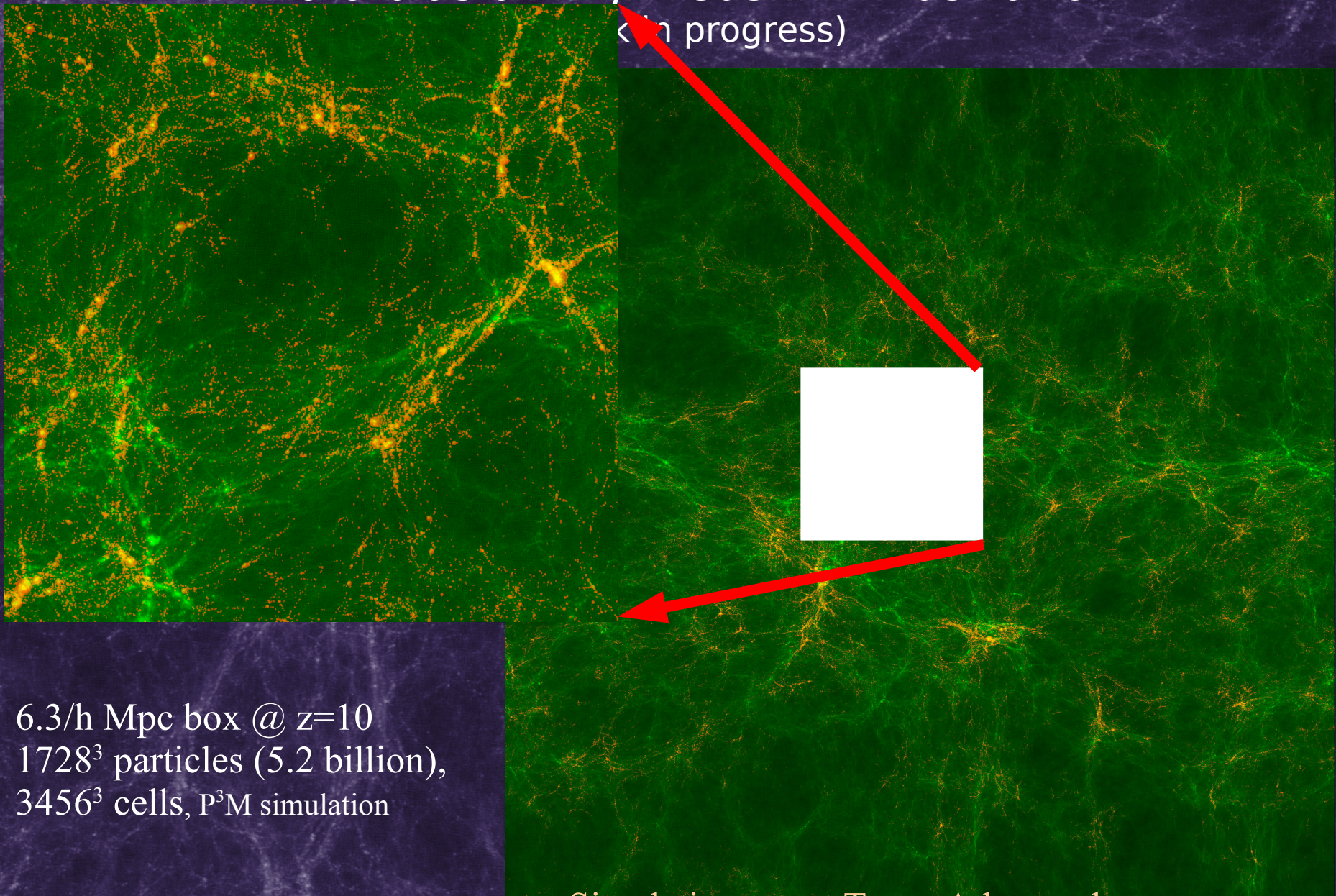


Simulation ran at Texas Advanced  
Computing Facility on 864 cores.



# Halo bias at high redshift: illustration

(in progress)



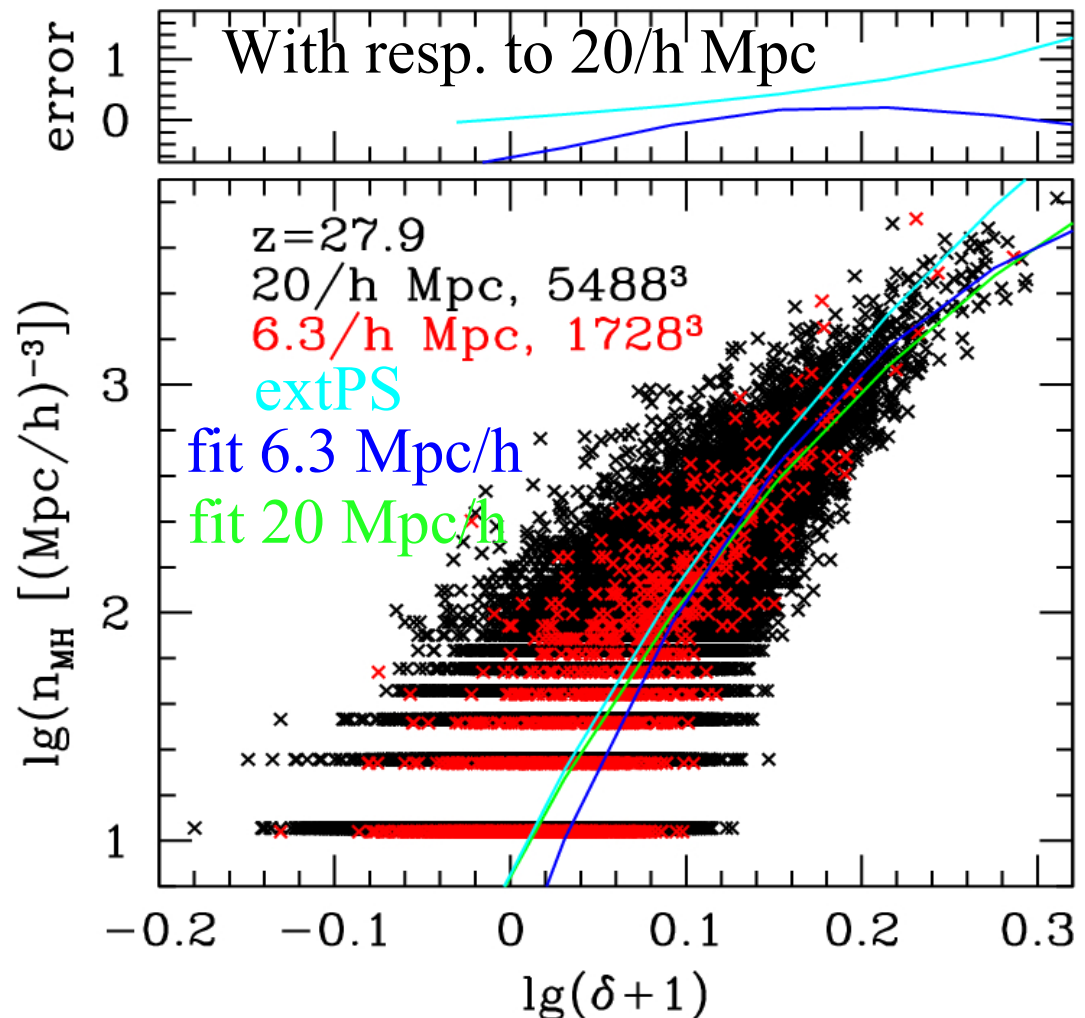
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# Conditional mass functions

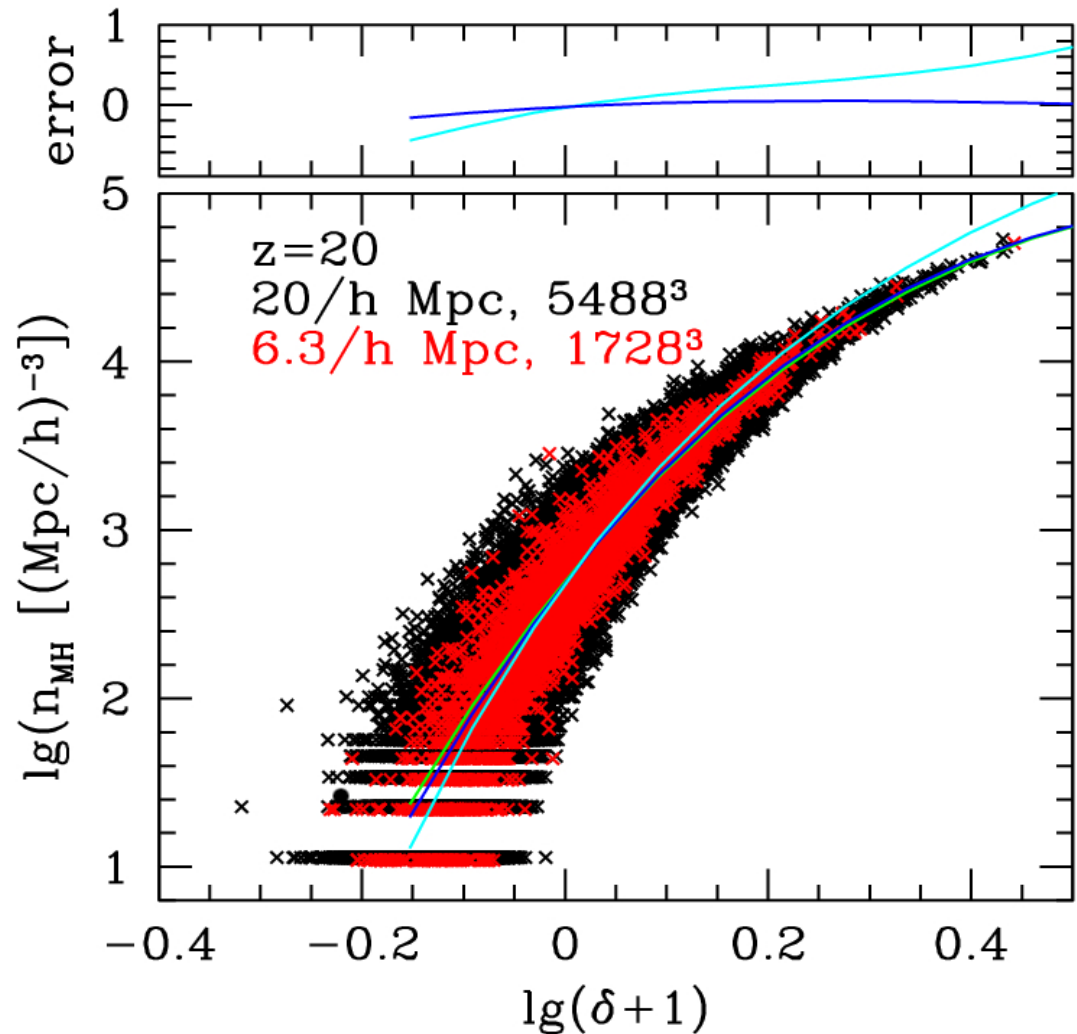
- Locally, the halo mass function depends strongly on the over/under-density.
- Extended PS-type models are often used for modelling this effect.
- Direct comparison to simulations shows this is not a very good approximation to actual structures.
- Scatter is also very significant.





# Conditional mass functions

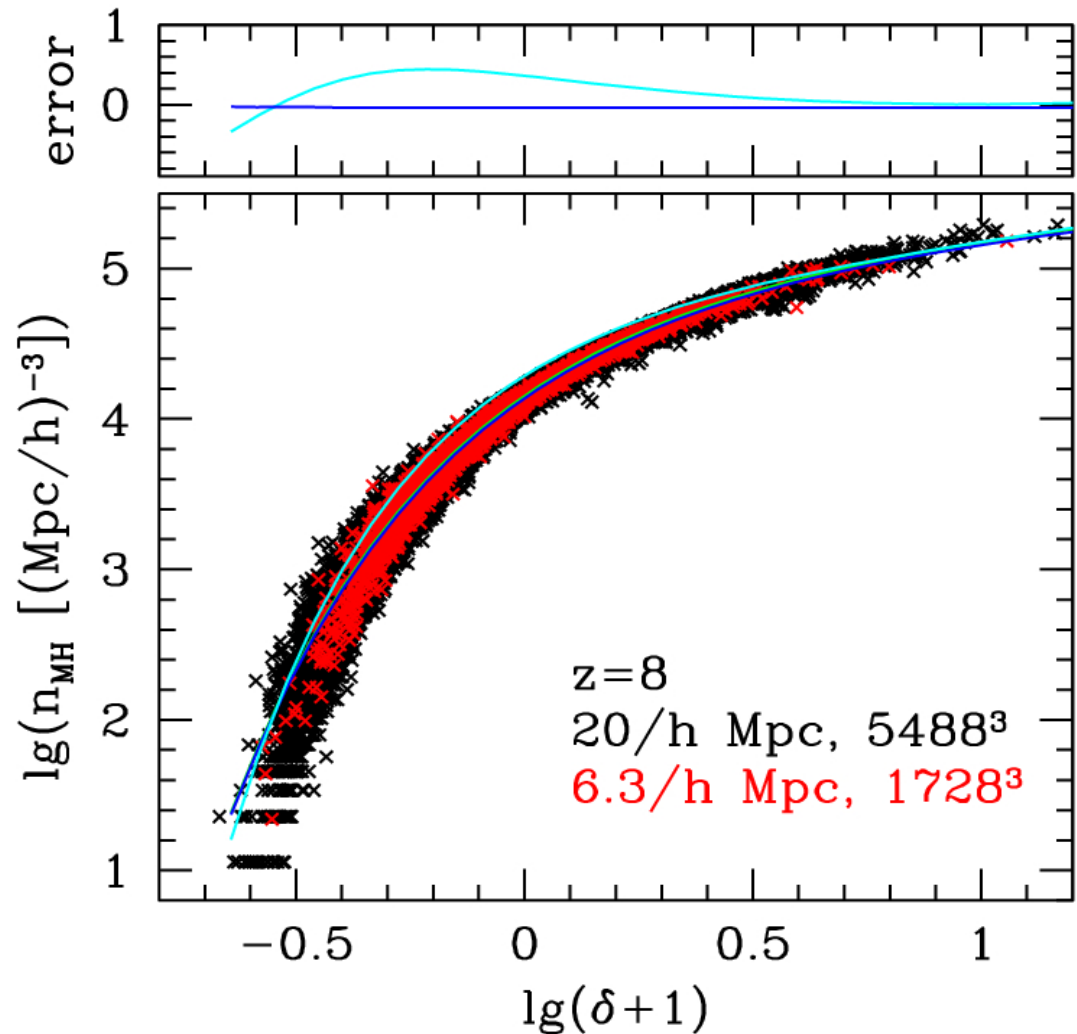
- As we go to lower redshifts, the extended PS model does somewhat better, but is still very significantly different, by up to factor of 2, especially in the highest and lowest density regions.
- Scatter remains high.
- Boxsize has almost no effect on mean fit.





# Conditional mass functions

- As we go to lower redshifts, the extended PS model does much better for dense regions, but still overpredicts the number of minihalos for mean and low density by up to 60%.
- Scatter remains high.
- Boxsize has no effect on mean fit.





# The high- $z$ halo mass functions: effect of primordial non-Gaussianity

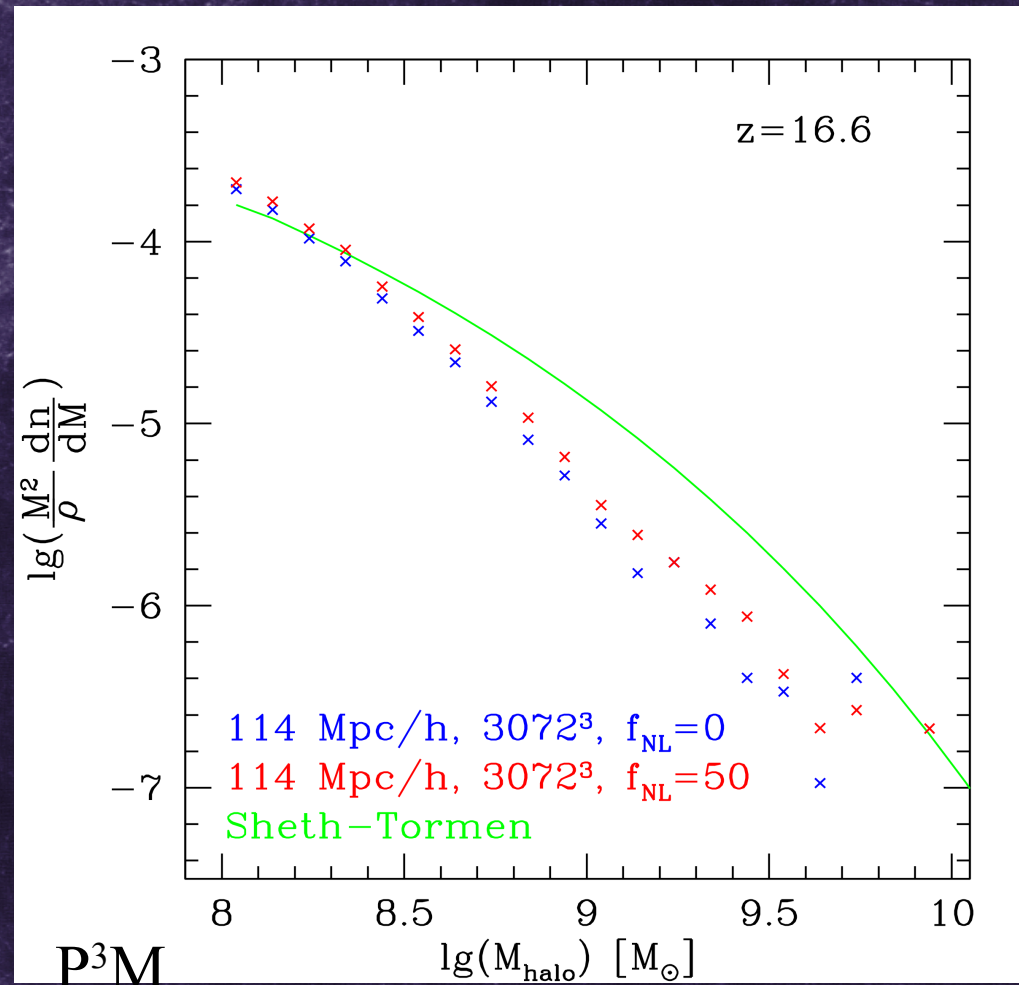
(work in progress)

Many inflationary theories predict the possibility of non-Gaussianity in the primordial density fluctuations.

Usually characterized by parameter  $f_{\text{NL}}$  (quadratic term in potential). Current observational limits suggest  $0 < f_{\text{NL}} < 50$ .

Important effects on very large scales at  $z=0$  (e.g. Dalal et al 2008, Desjacques et al. 2009, Pillepich et al., 2009)

Can it also affect reionization?



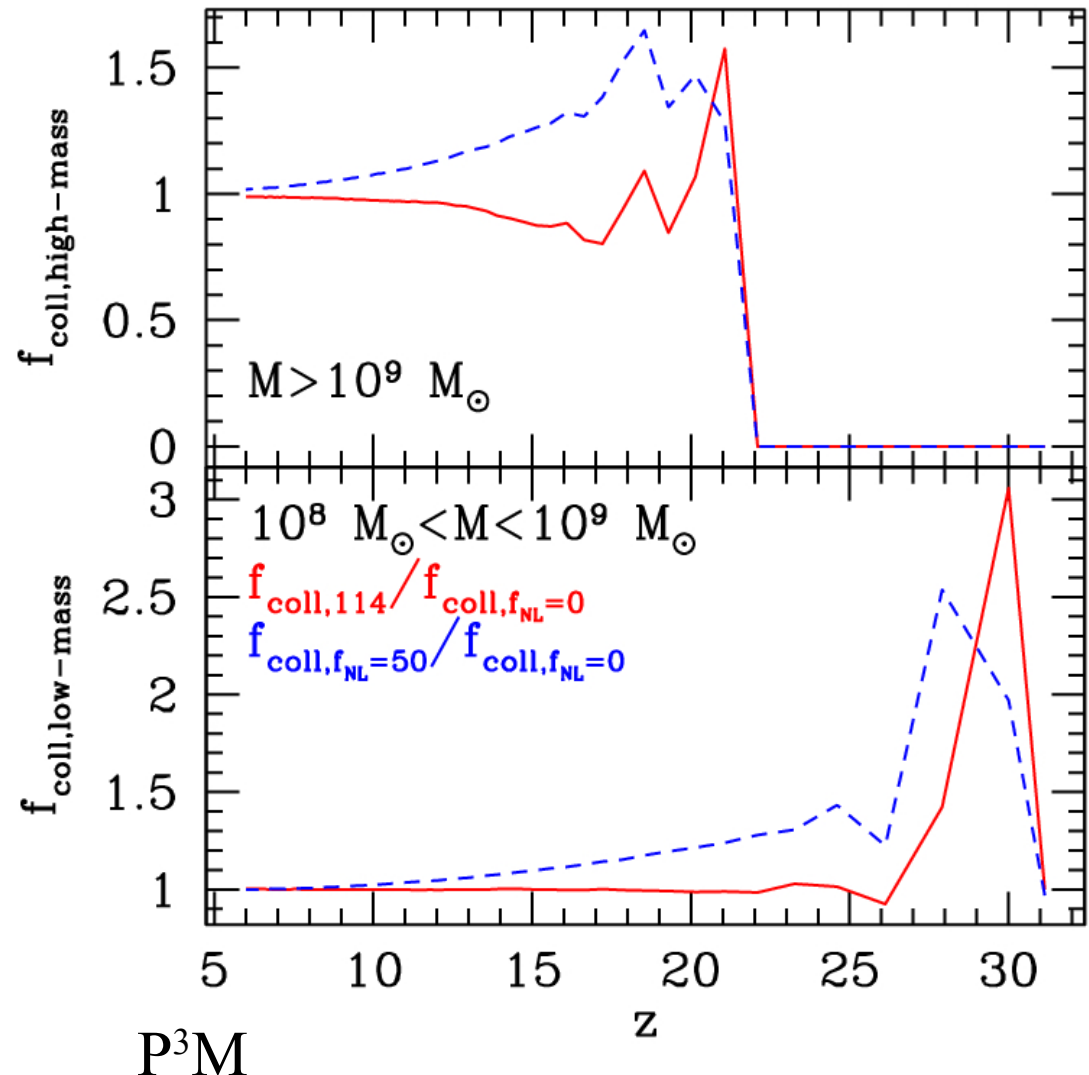


# The high- $z$ collapsed fractions: effect of primordial non-Gaussianity

(work in progress)

Effect of non-Gaussianity is largest at for very rare halos and gradually diminishes as halos become more common (blue).

Initial 'peak' is in fact due to cosmic variance (present also for 2 random realizations without Non-Gaussianity (red)).



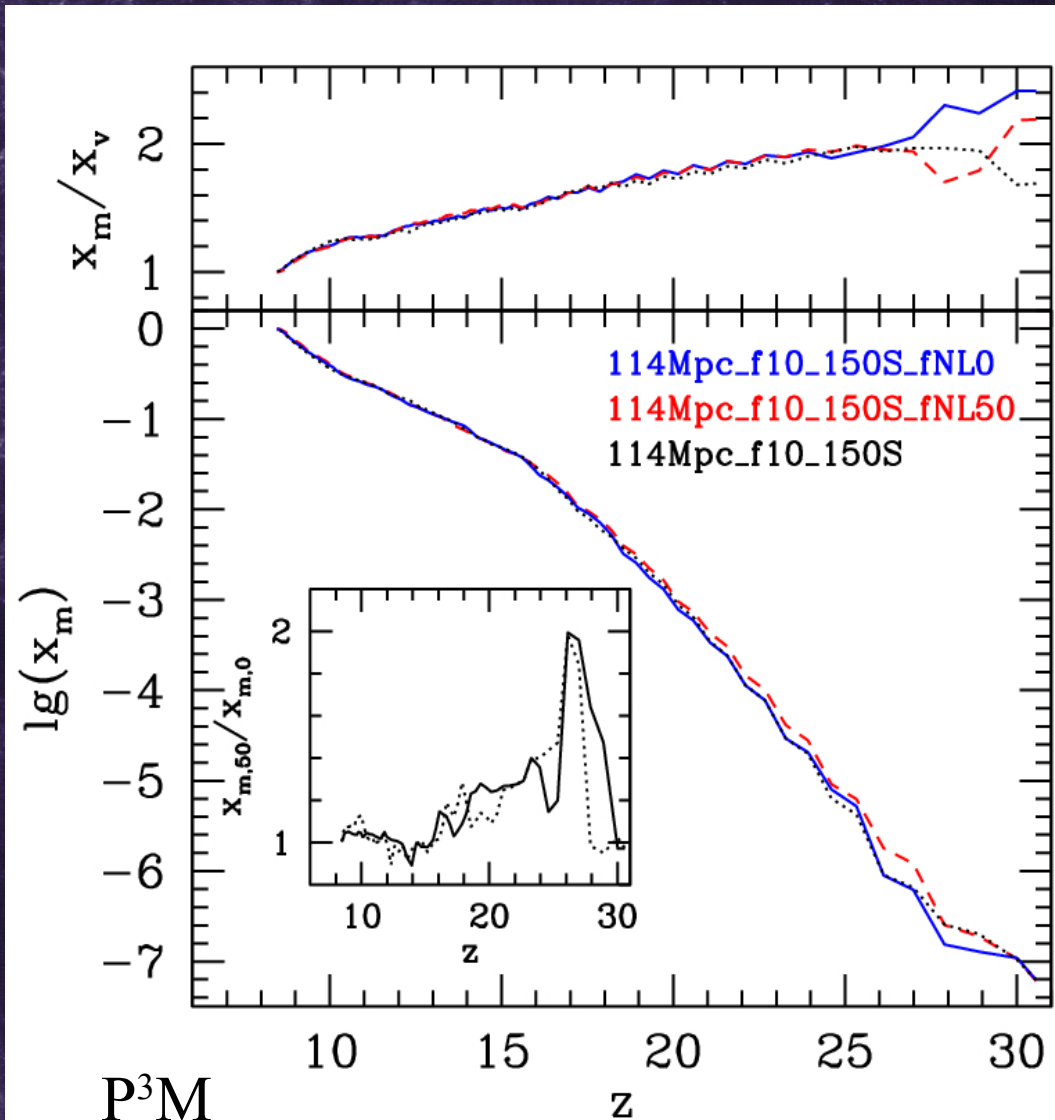


# Effect of primordial non-Gaussianity: reionization history

(work in progress)

Effect on mean reionization history is significant ( $>20\%$ ) at high- $z$  ( $z > 16$ ), when reionization is dominated by rare sources and largely disappears at lower redshifts.

Non-Gaussianity affects most the halo clustering, thus this could be a stronger effect on HII region sizes, 21-cm fluctuations, etc. Stay tuned...



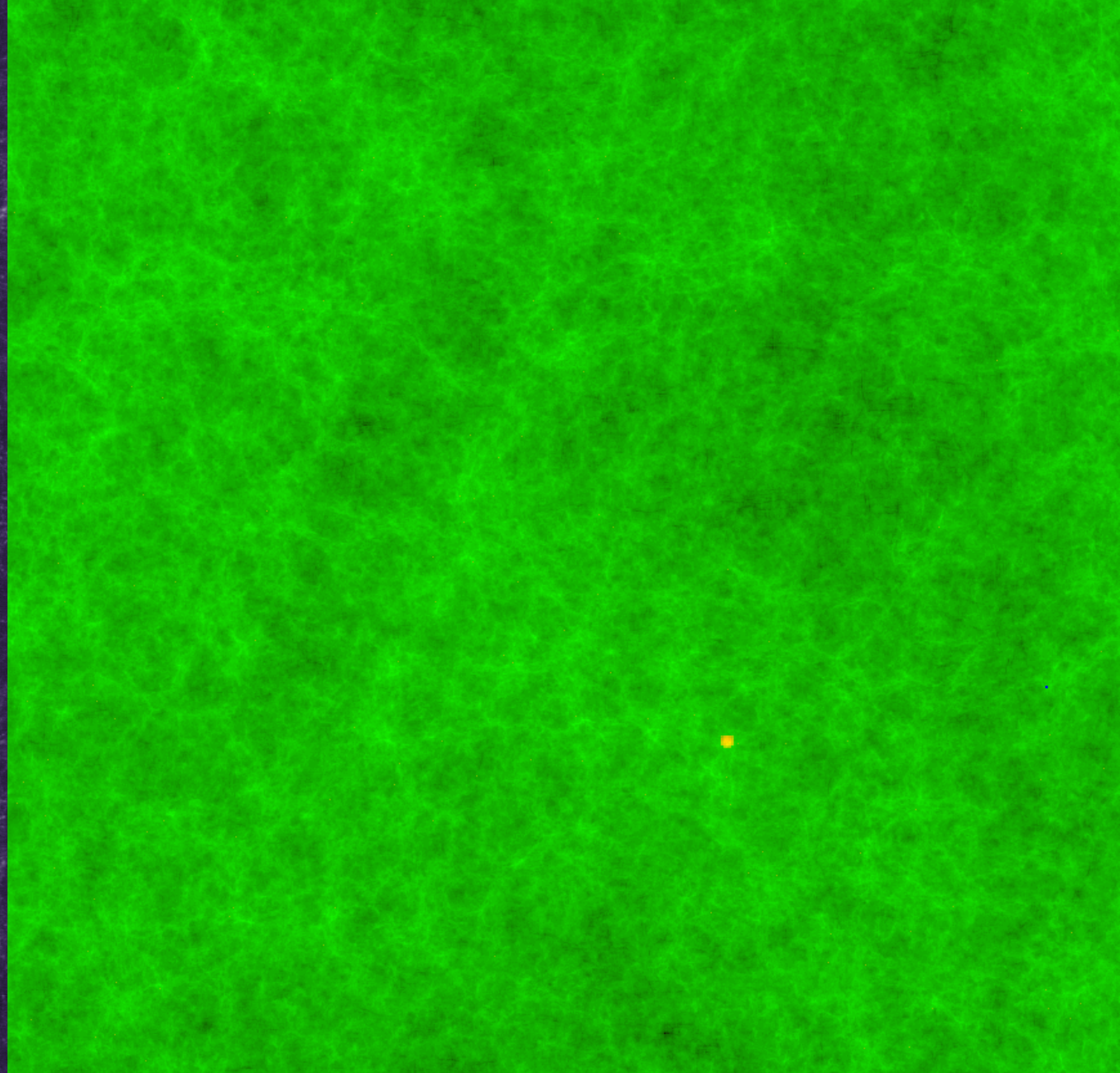


# Reionization in Action: From the Dark Ages to Reionized Universe

- Strong halo clustering
- quick local percolation
- large H II regions with complex geometry.

64/h Mpc box,  
WMAP3+ cosmology,  
432<sup>3</sup> radiative transfer  
simulation. Evolution:  
z=30 to 7.

>10<sup>8</sup> solar mass halos  
resolved



Simulations ran at Texas Supercomputing Center on up to 10,000 cores

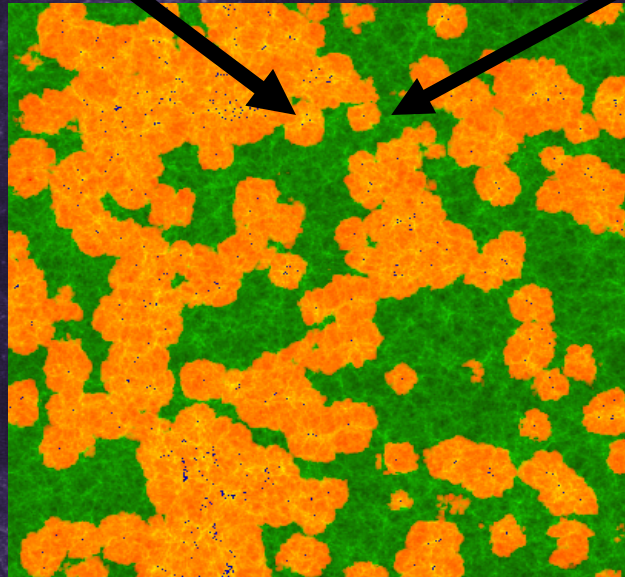


# Large-Scale Simulations of Reionization

[Iliev et al. 2006a, 2007a; Mellema, Iliev, et al. 2006; and in prep.]

- N-body: CubeP<sup>3</sup>M  
1728<sup>3</sup>-3072<sup>3</sup> part.  
(5.2 to 29 billion) or more -  
4000<sup>3</sup>-5488<sup>3</sup> (64-165 billion)
- density slices
- velocity slices
- halo catalogues-sources
- Scales well at least up to  
21,952 cores

35-114/h Mpc (CubeP<sup>3</sup>M)  
resolving  $10^8 M_{\text{star}}$  halos  
up to  $21 \times 10^6$  sources  
50-100 dens. snapshots  
simple source models  
sub-grid clumping  
no hydro – large scales.



- C<sup>2</sup>-Ray code  
(Mellema, Iliev, et al. 2006)
- radiative transfer
  - noneq. chemistry
  - precise
  - highly efficient
  - coupled to gasdynamics
    - massively parallel  
(scales well up to  
10,240 cores).

Coupled to hydro

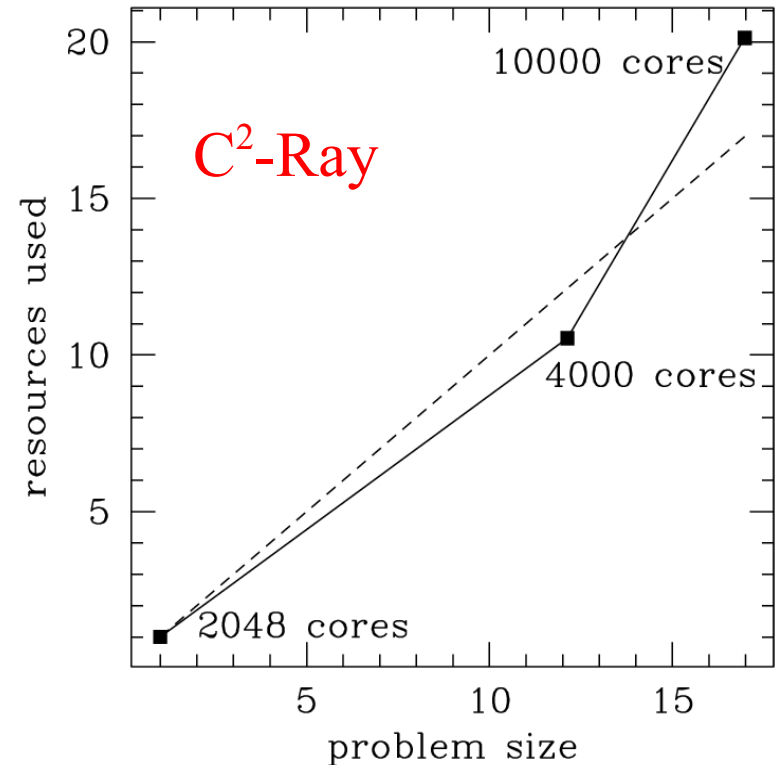
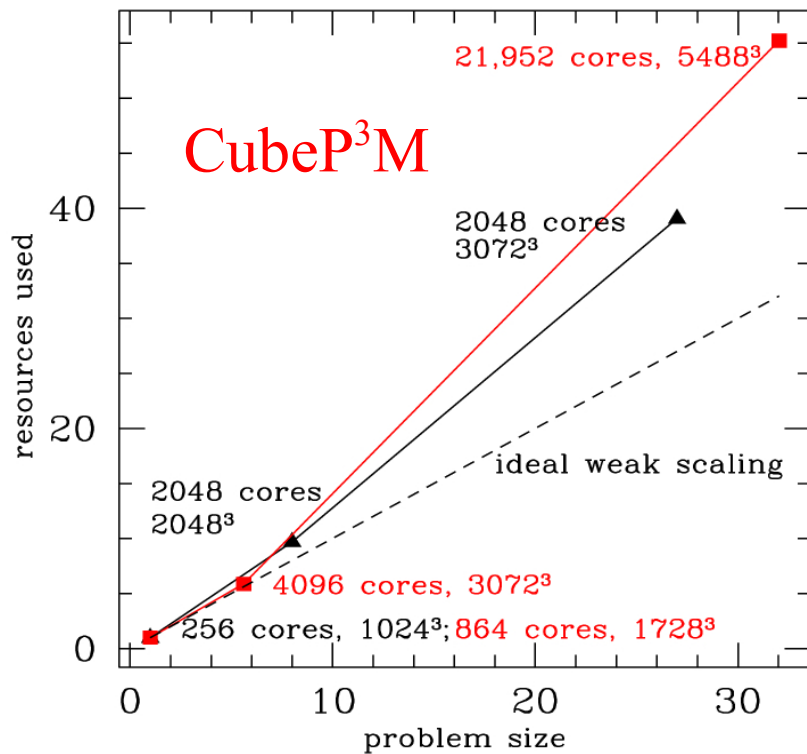


# Code Scaling

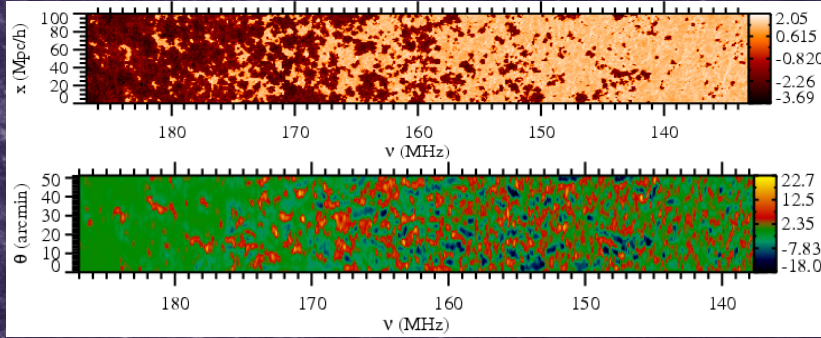
(Iliev, Mellema, Merz, Shapiro, Pen 2008 in TeraGrid08 proceedings)

Both N-body and radiative transfer codes are massively parallel and scale (weakly) up to thousands of processors.

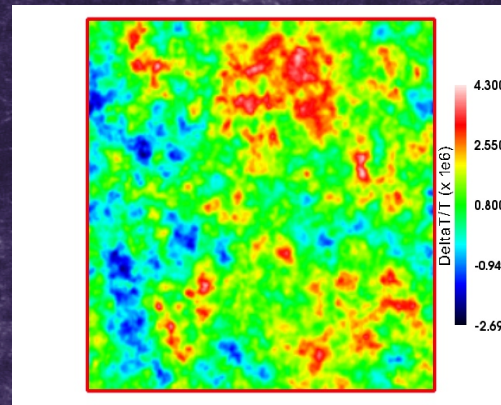
Full, detailed radiative transfer: Petascale-size problem!



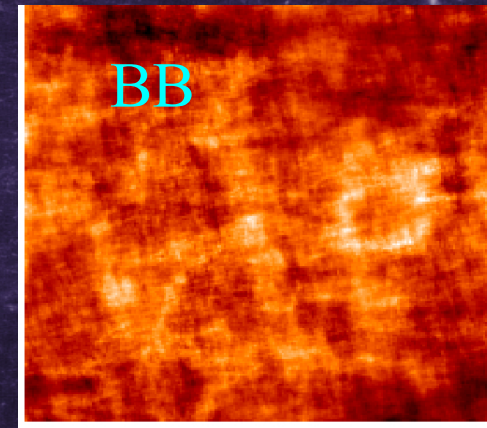




redshifted 21-cm



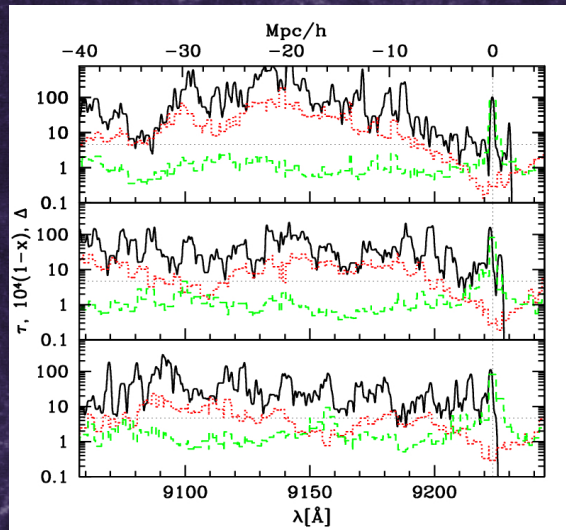
kinetic Sunyaev-Zeldovich  
effect (kSZ)



CMB polarization

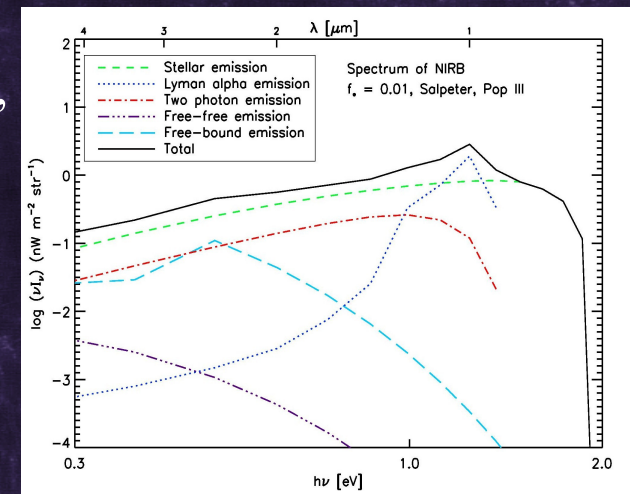
# Observing the Reionization Epoch

Ly- $\alpha$  sources



Iliev et al. 2006a, MNRAS;  
2007(a,b,c,d), 2008 MNRAS,  
ApJ, Mellema et al. 2006,  
MNRAS; Dore et al., 2006,  
Phys. Rev. D; Holder, Iliev  
& Mellema 2006 ApJ,  
Fernandez et al. 2010, ApJ  
Tilvi et al. 2010, ApJ

NIR fluctuations





# Kine(ma)tic SZ effect

- Temperature variations given by LOS integral:

$$\frac{\Delta T}{T}(\hat{\mathbf{n}})_{\text{kSZ}} = \sigma_T \int d\eta e^{-\tau(\eta)} a n_e \hat{\mathbf{n}} \cdot \mathbf{v},$$

- Spectrum is black-body (no spectral distortions of original CMB).
- Both density and velocity distributions are important, with ionization imposing additional fluctuations during EoR.
- Dominated by IGM during EoR and by clusters later-on.



# kSZ from patchy reionization: extraction from simulations

- (Iliev, Pen, Mellema, Bond, Shapiro, 2007)

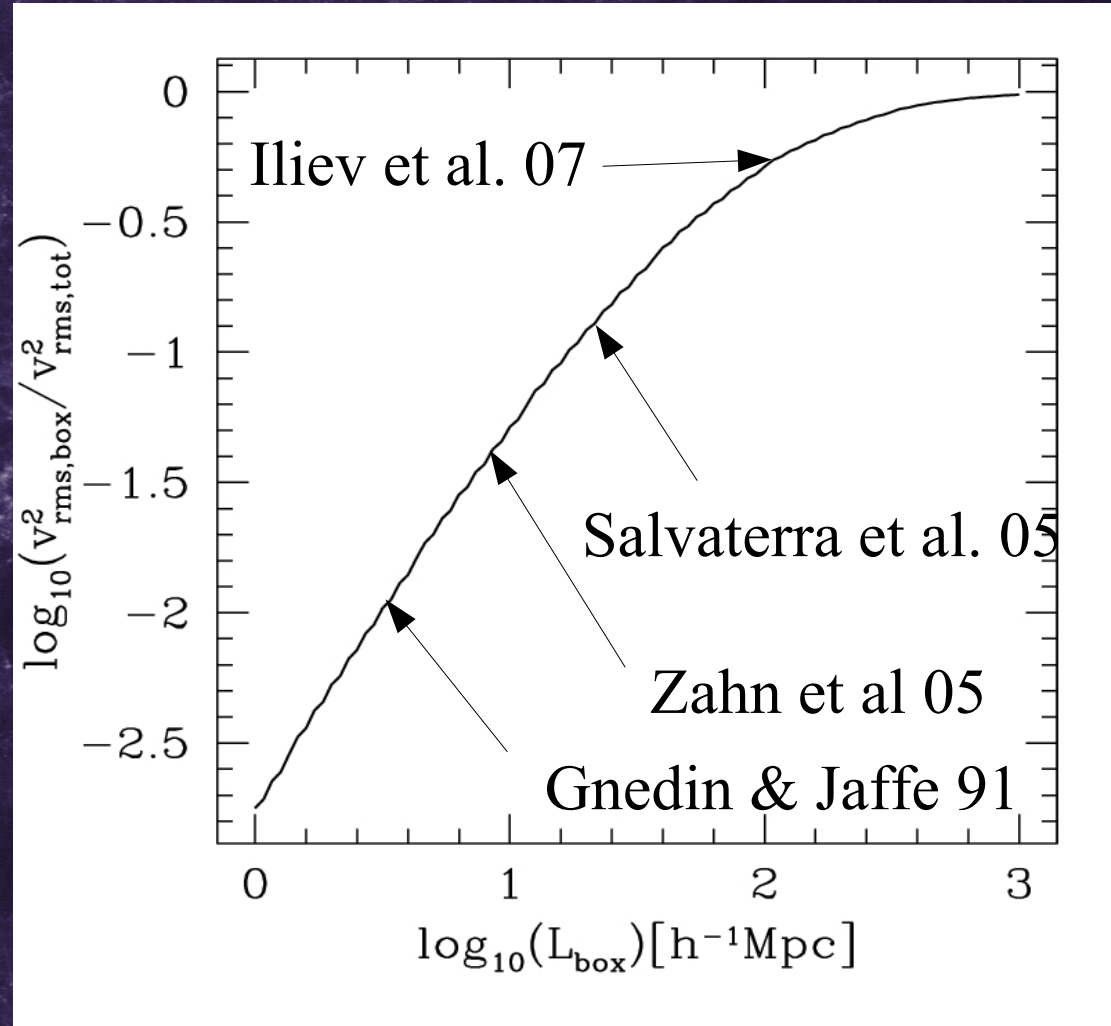
$$\frac{\Delta T}{T}(\hat{\mathbf{n}})_{\text{kSZ}} = \sigma_T \int d\eta e^{-\tau(\eta)} a n_e \hat{\mathbf{n}} \cdot \mathbf{v},$$

- Method:
  - find all integrals along LOS for available outputs
  - every light-crossing time interpolate between closest two outputs
  - to avoid periodicity artefacts change directions (x-y-z) and do random shifts (using box periodicity) and/or 90 degree rotations.



# Large-scale velocities

- The coherent bulk motions due to cosmic structure formation peak at very large scales — hundreds of Mpc (missing rms power vs. boxsize shown).
- Fortunately, those large-scale motions are linear and can be (statistically) corrected for (Iliev et al. 2007).





# Large-scale velocities correction:algorithm

(Iliev, Pen, Bond, Mellema & Shapiro 2007)

- First, the missing velocity power is calculated based on the linear theory for the simulation boxsize and cosmology.
- Then, the full computational volume is assumed to be moving with the same coherent velocity,  $v_{\text{box}}$ , in which case:

$$\left(\frac{\Delta T}{T_{\text{CMB}}}\right)_{\text{tot}}(z) = \left(\frac{\Delta T}{T_{\text{CMB}}}\right)_{\text{box}}(z) + \tau_{\text{es}}(z) \frac{\bar{v}_{\text{box}}(z)}{c}$$

- Here, the velocity  $v_{\text{box}}$  is chosen with random amplitude and direction using

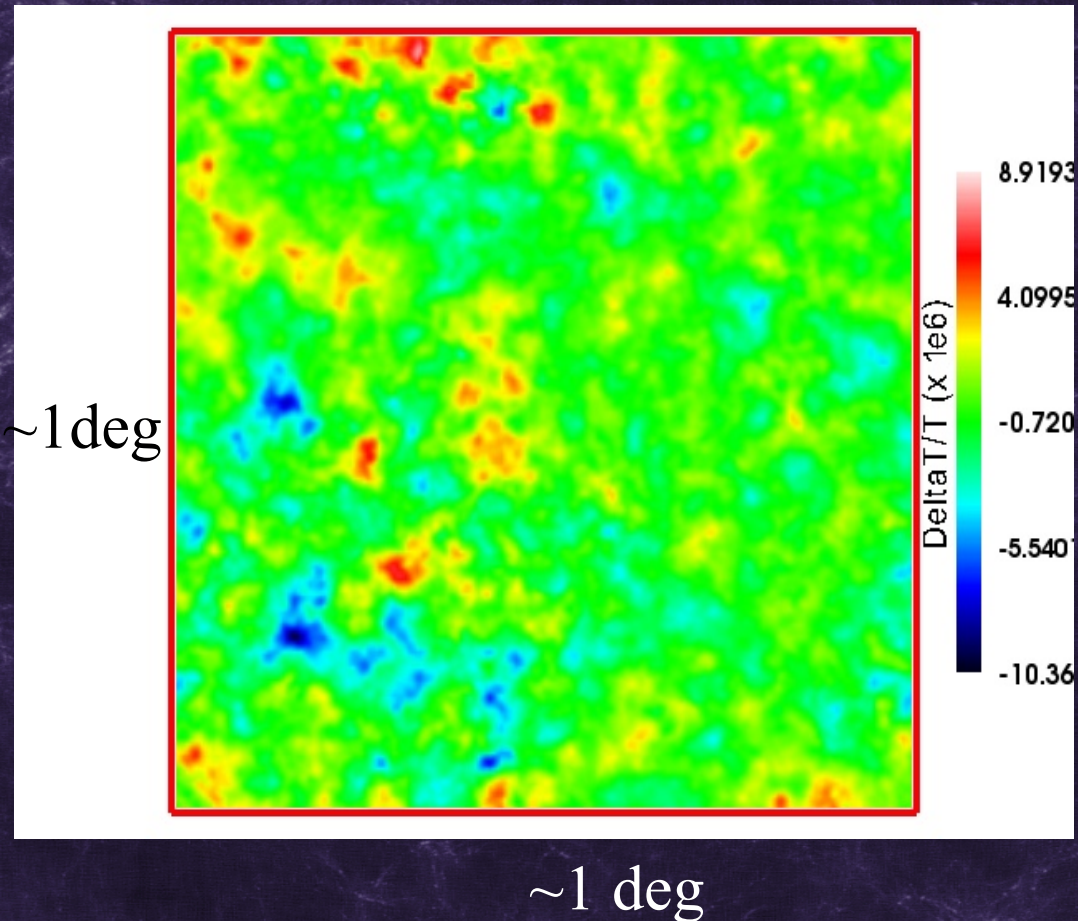
$$\bar{v}_{\text{box}}(z) = v_{\text{rms,missing}}(-2 \ln q)^{1/2} \cos(2\pi\theta)$$

where  $q$  and  $t$  are uniformly-distributed random numbers between 0 and 1, which guarantees Gaussian-distributed  $v_{\text{box}}$  with zero mean (Box & Mueller 1958).



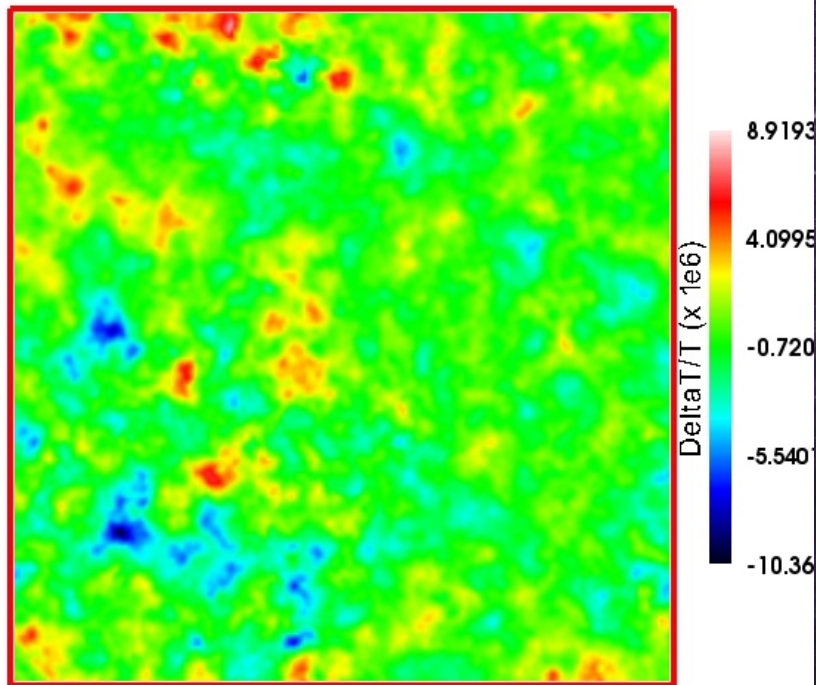
# Sample kSZ map from patchy reionization

- Sample kSZ map (run f250).
- range of pixel values is  $\Delta T/T = -10^{-5}$  to  $10^{-5}$ , i.e.  $\Delta T$  max/min are in the tens of  $\mu\text{K}$  at  $\sim$  arcmin scales.

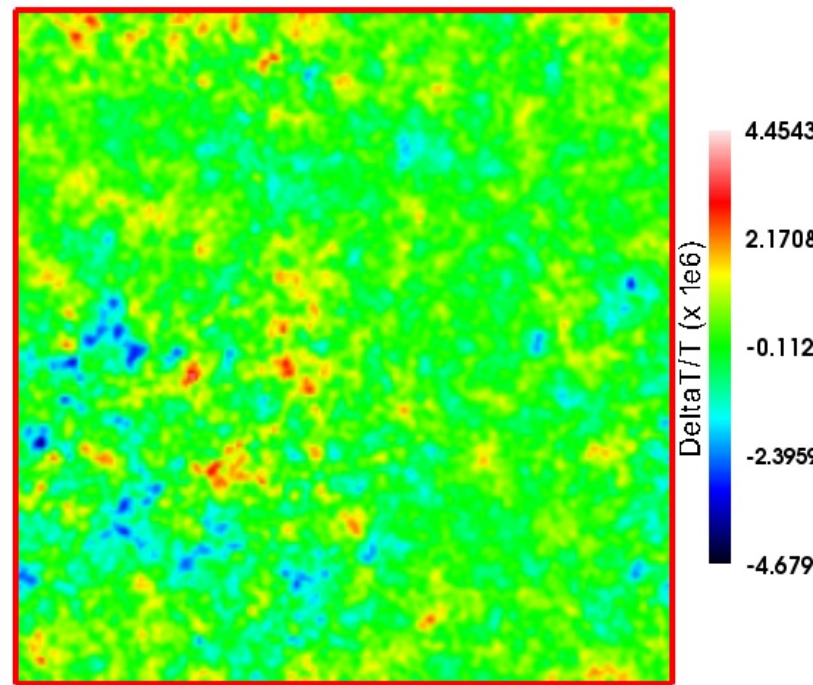




# kSZ sky maps: extended vs. instant reionization



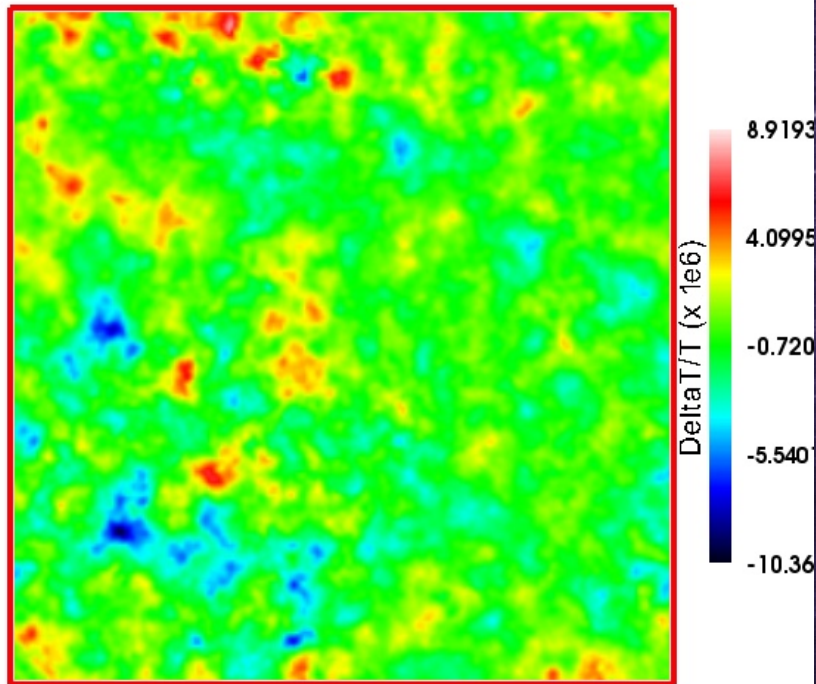
$f250$



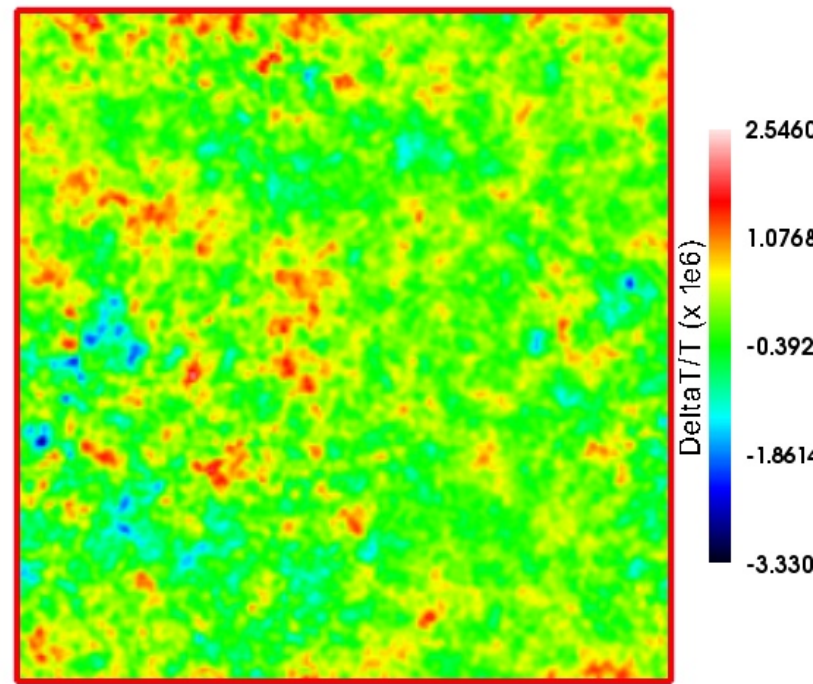
instant reionization, same  $\tau$



# kSZ sky maps: patchy vs. uniform reionization



f250

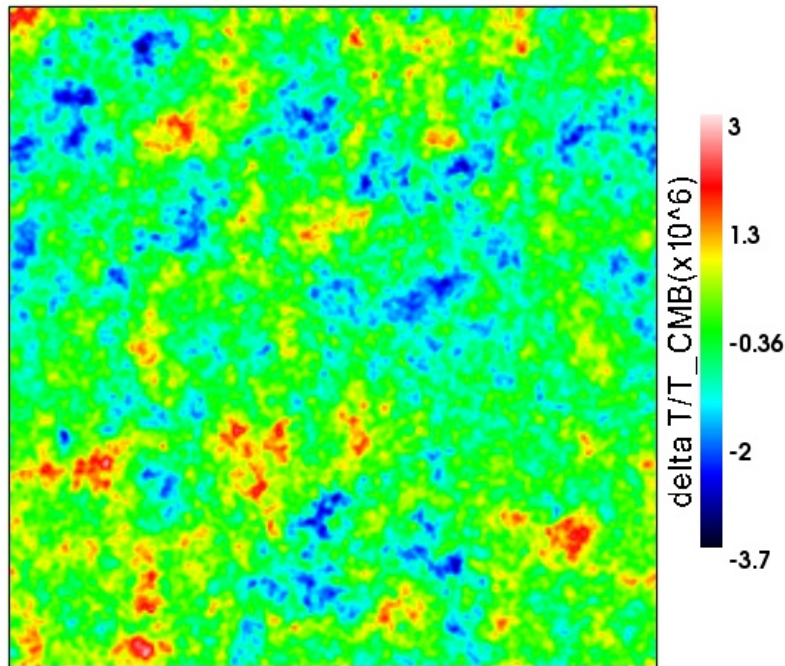


uniform reionization, same  $x_m$  (and, thus  $\tau$ )

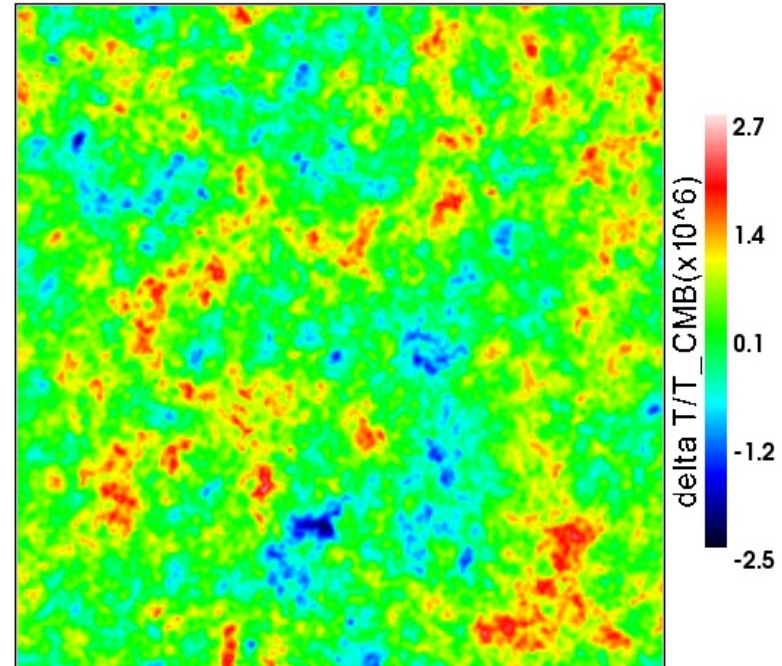


# kSZ sky maps: self-regulated reionization

(work in progress)



Early reionization scenario



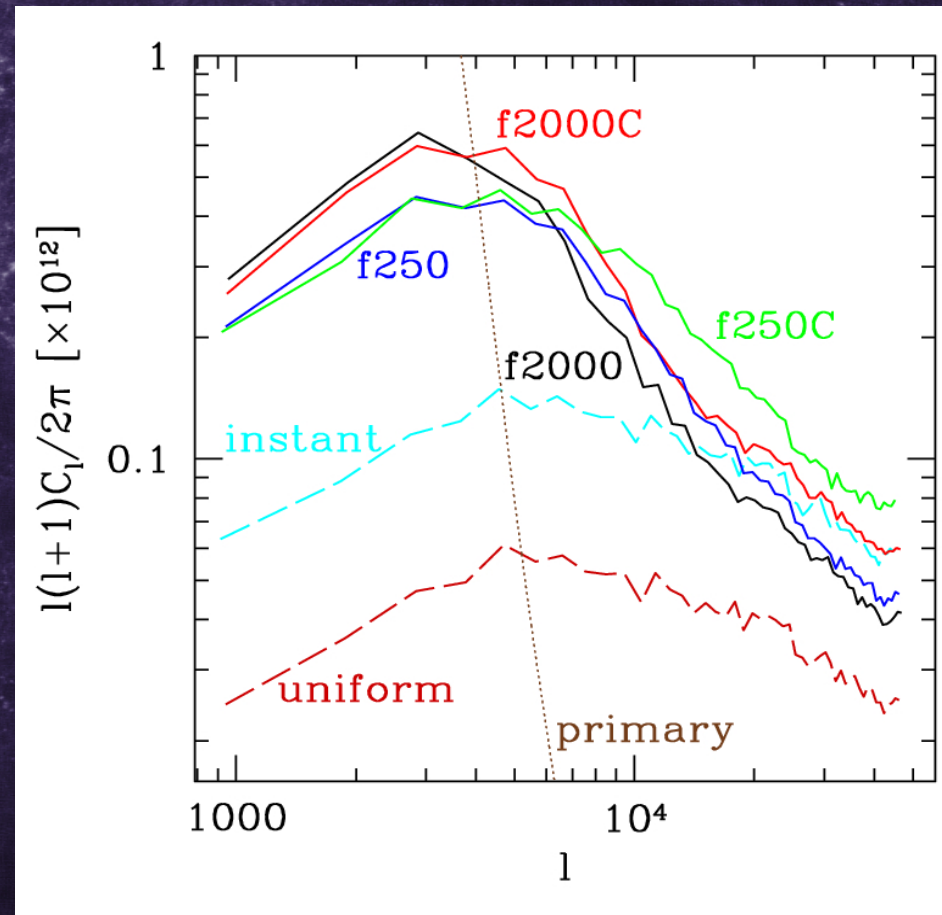
Extended reionization scenario

114/h Mpc box, overlap at  $z \sim 8.3$  (early) and  $z \sim 6.5$  (extended),  
 $\tau = 0.08$  (early) and  $\tau = 0.06$  (extended).



# kSZ sky power spectra

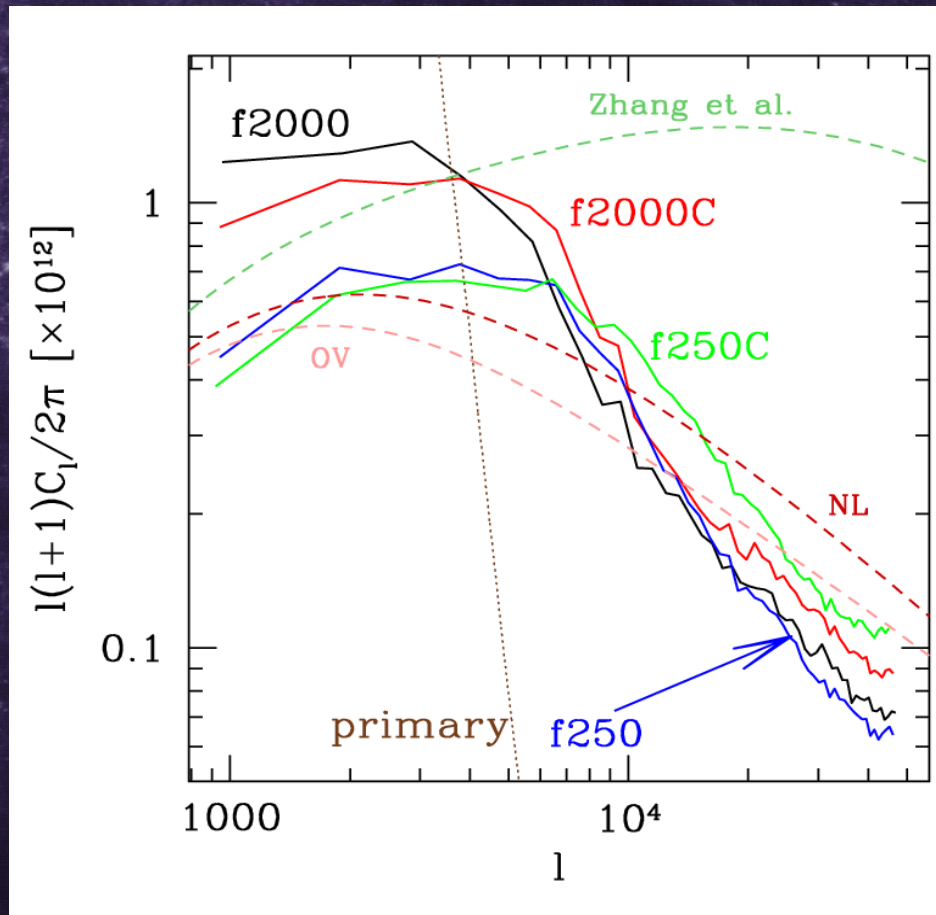
- Power spectra peak at  $l \sim 3000$ - $5000$ , with a peak value  $> 1 \mu\text{K}$
- Early and late reionization scenarios (f2000 and f250) would be difficult to distinguish (some differences for  $l \sim 3000$ - $20,000$ )
- Instant reionization (at  $z \sim 13$ , same  $\tau$  as f250) has  $\sim$  order of magnitude less power for  $l \sim 2000$ - $8000$ , but same large- $l$  behaviour.
- Uniform reionization (same  $x_m$  as f250) has much less power on all scales.





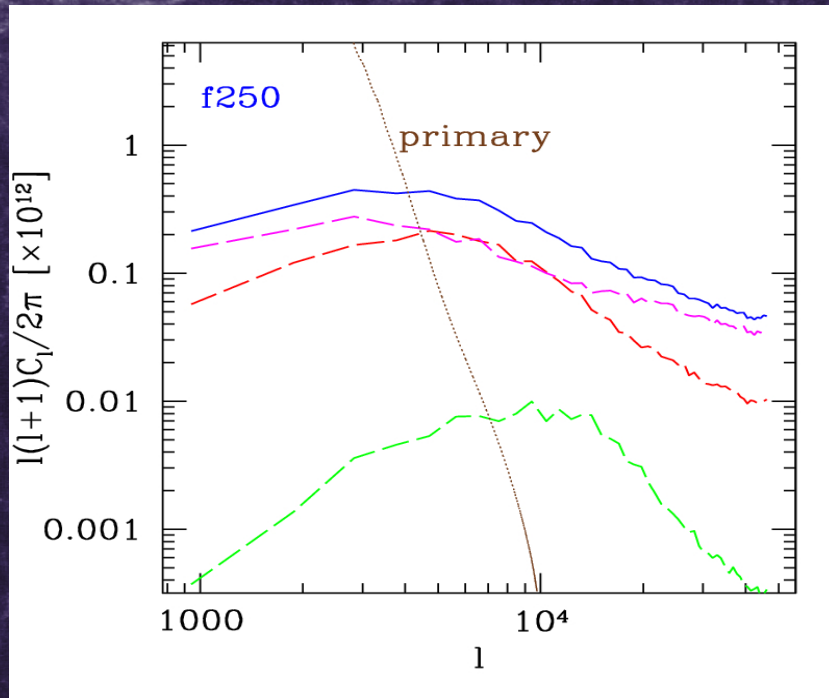
# kSZ sky power spectra with large-scale velocity correction

- Power spectra peak at  $l \sim 3000$ - $5000$ , with a peak value  $> 1 \mu\text{K}$
- Early and late reionization scenarios (f2000 and f250) would be difficult to distinguish (some differences for  $l \sim 3000$ - $20,000$ )

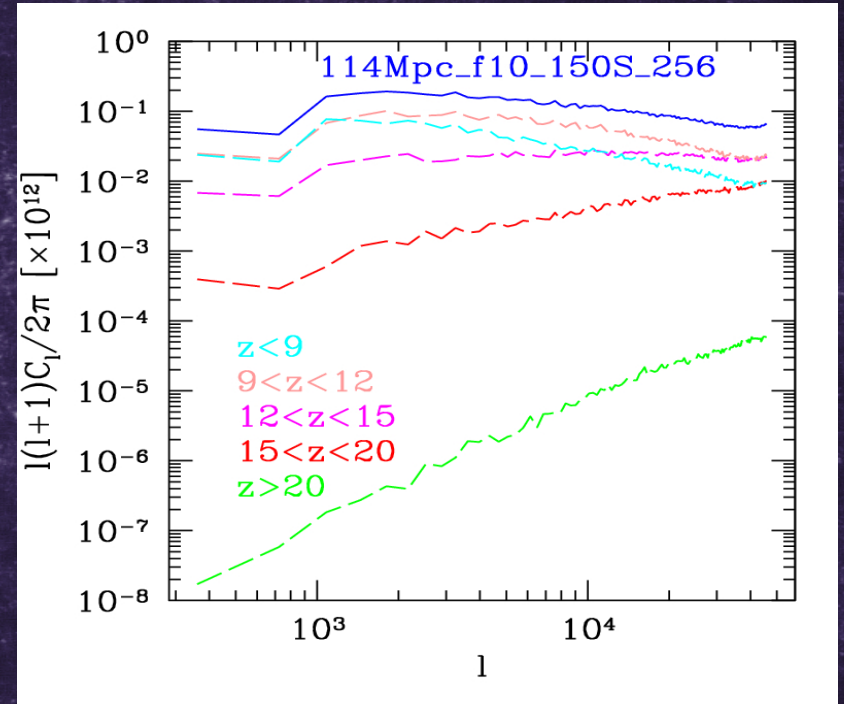




# kSZ sky power spectra: contributions by epoch



Not self-regulated



Self-regulated

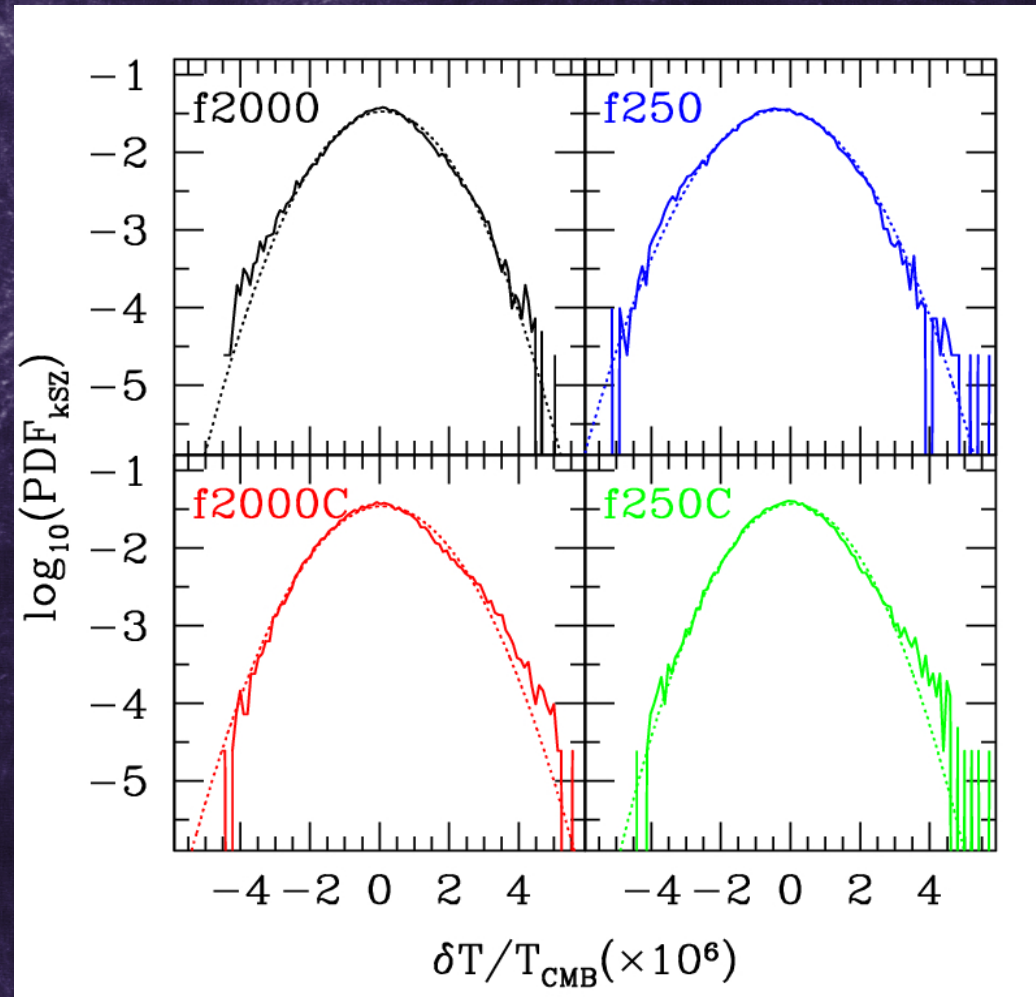


# kSZ non-Gaussianity?

- Not really! Maps are highly Gaussian

solid: f250  
simulation

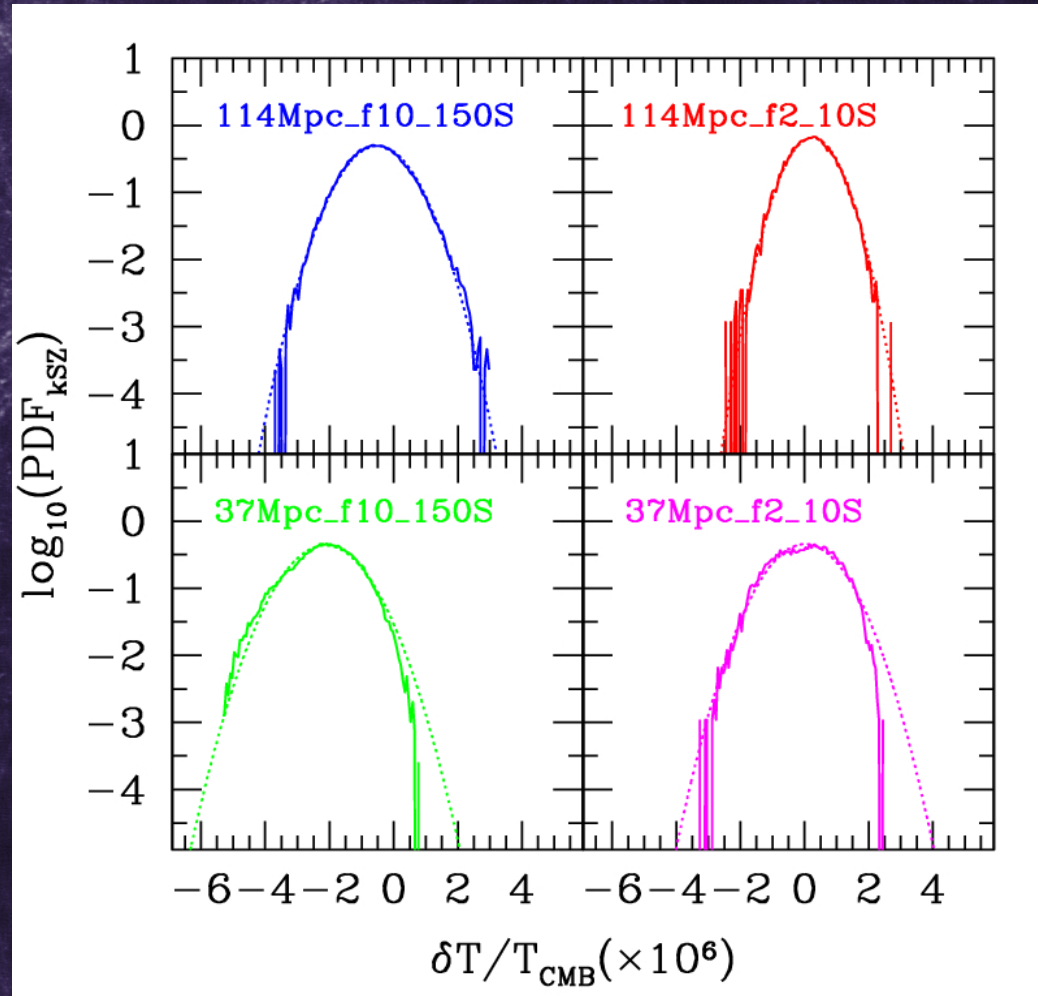
dotted: Gaussian  
with same mean  
and rms





# KSZ PDFs: self-regulated models

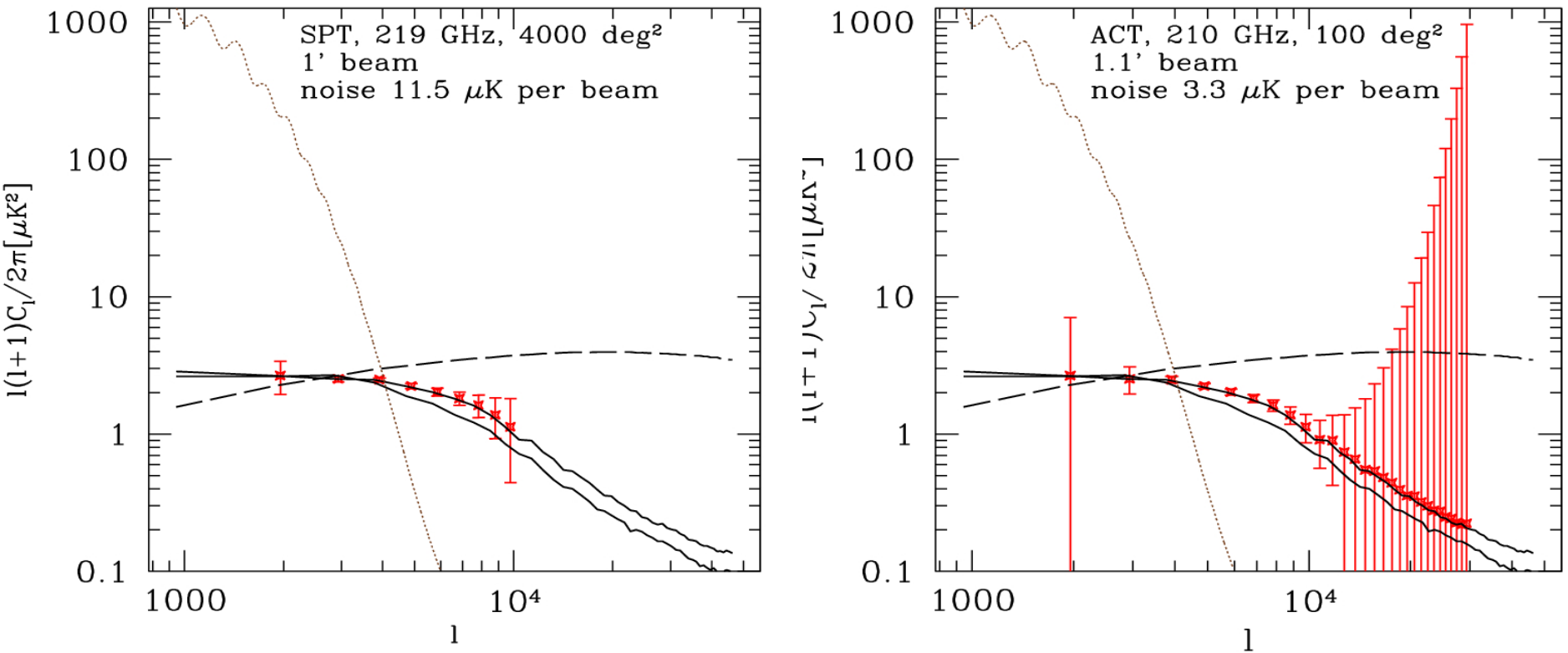
Maps are still largely Gaussian, with some departures at wings. Extended reionization scenarios yield somewhat less wide PDFs.





# Detectability of kSZ

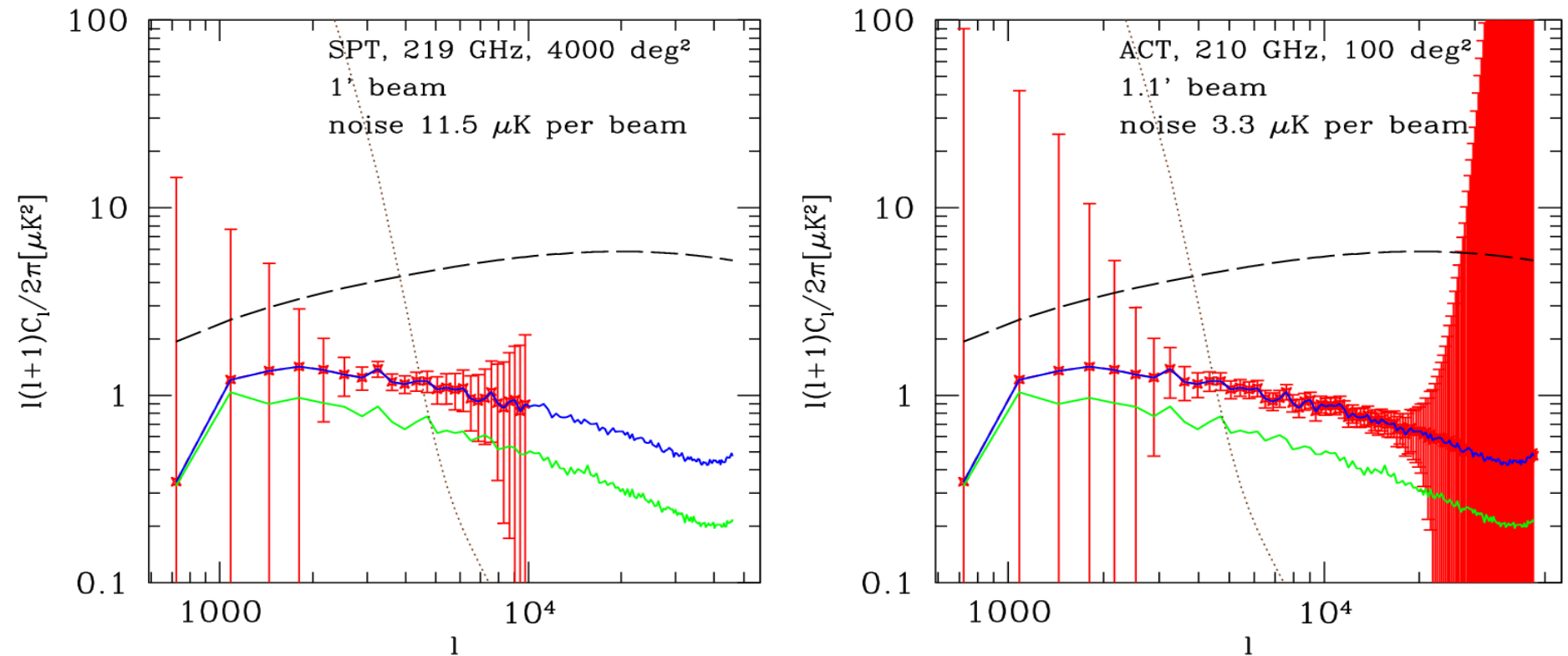
(Iliev, Mellema, Pen, Bond, Shapiro, 2008, MNRAS, 384, 863)



Sky power spectra of patchy EoR kSZ vs. expected noise levels of SPT and ACT. Includes noise from primary CMB and post-EoR kSZ (shown). tSZ is assumed subtracted.



# Detectability of kSZ: self-regulated (work in progress)

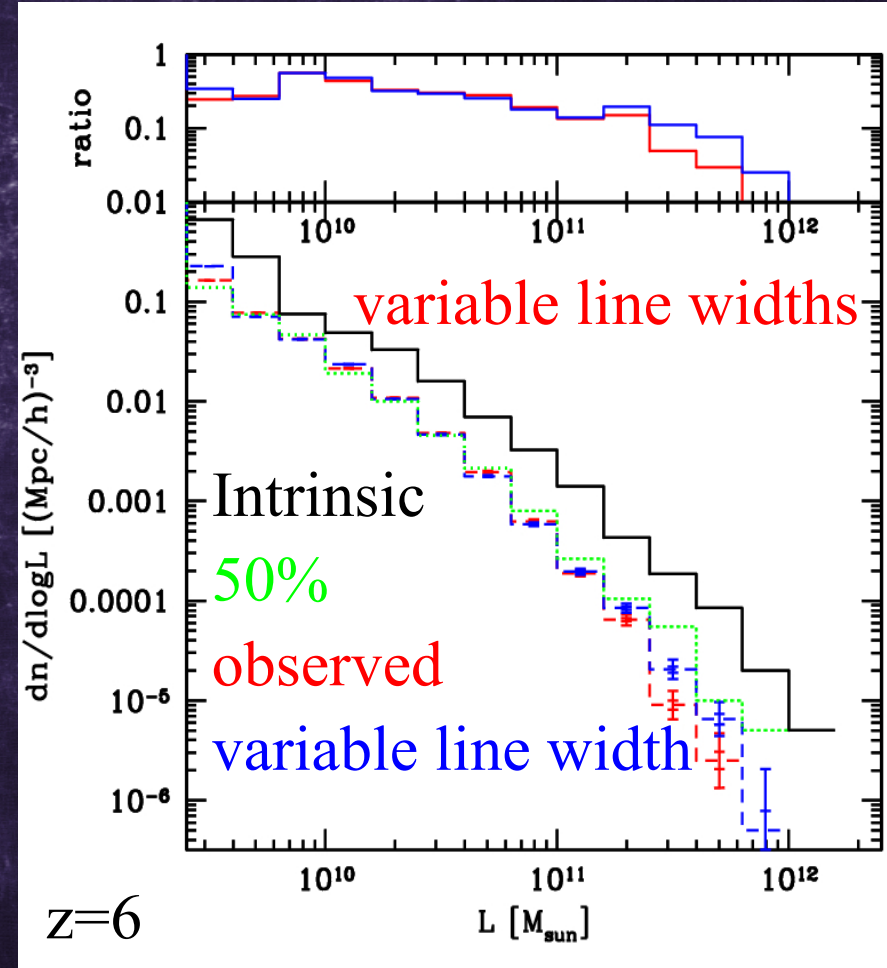
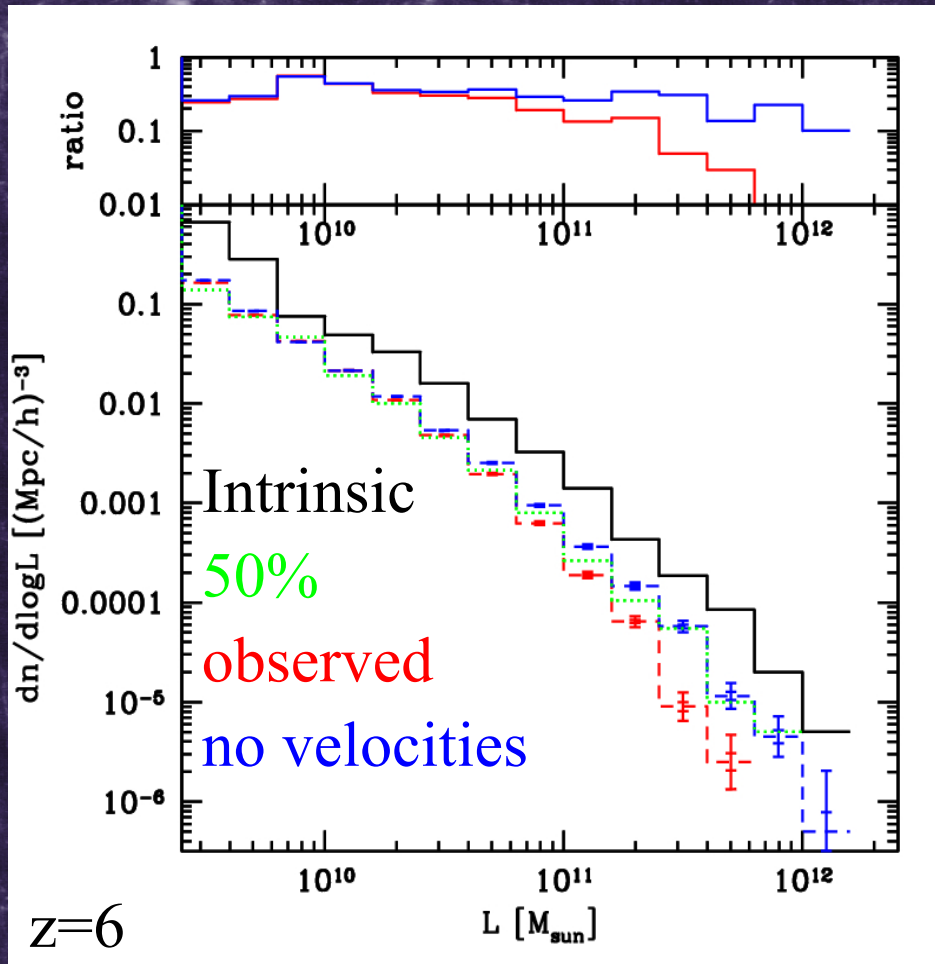


Sky power spectra of patchy EoR kSZ with expected noise levels of SPT and ACT. Includes noise from primary CMB and post-EoR kSZ (shown). tSZ is assumed subtracted. Early and extended scenarios are clearly distinguishable for  $l > 5000$ .



# Ly- $\alpha$ Luminosity Functions: effects of velocities and the assumed line widths

(Iliev et al. 2008 MNRAS, 391, 63)



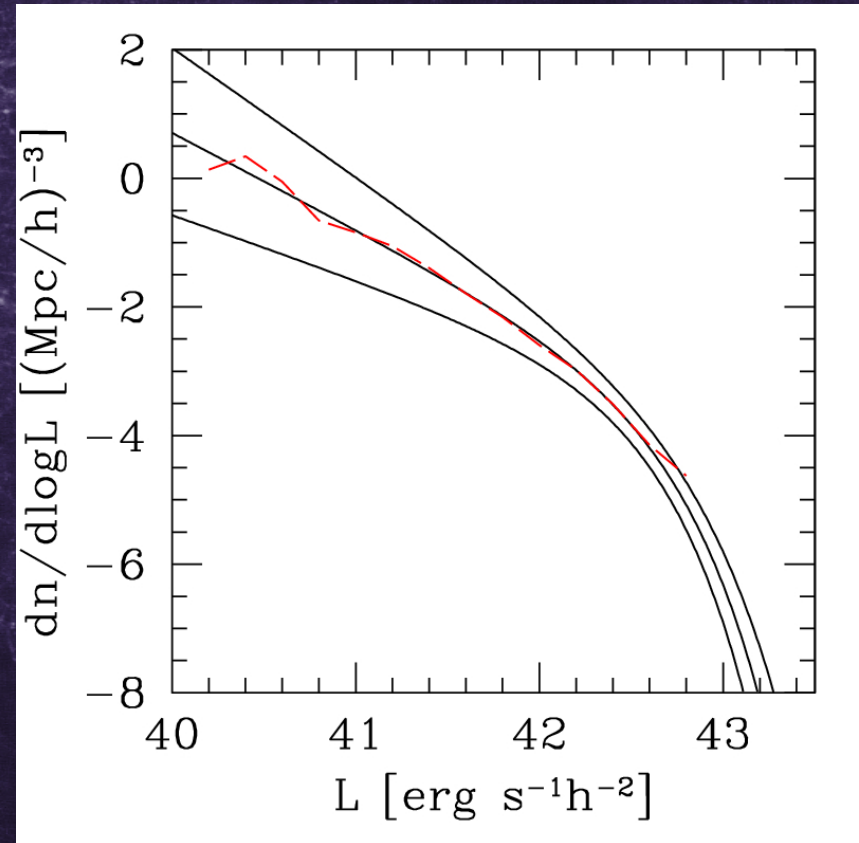


# Luminosity function: simulations vs. observations

(**Iliev** et al. 2008, MNRAS, 391, 63)

LF normalization: set by matching the number density of sources in simulations to the observed one (by Kashikawa et al. 2006).  
Excellent match of the shape, for an assumed faint-end slope of -1.5 for the fit to the observations.

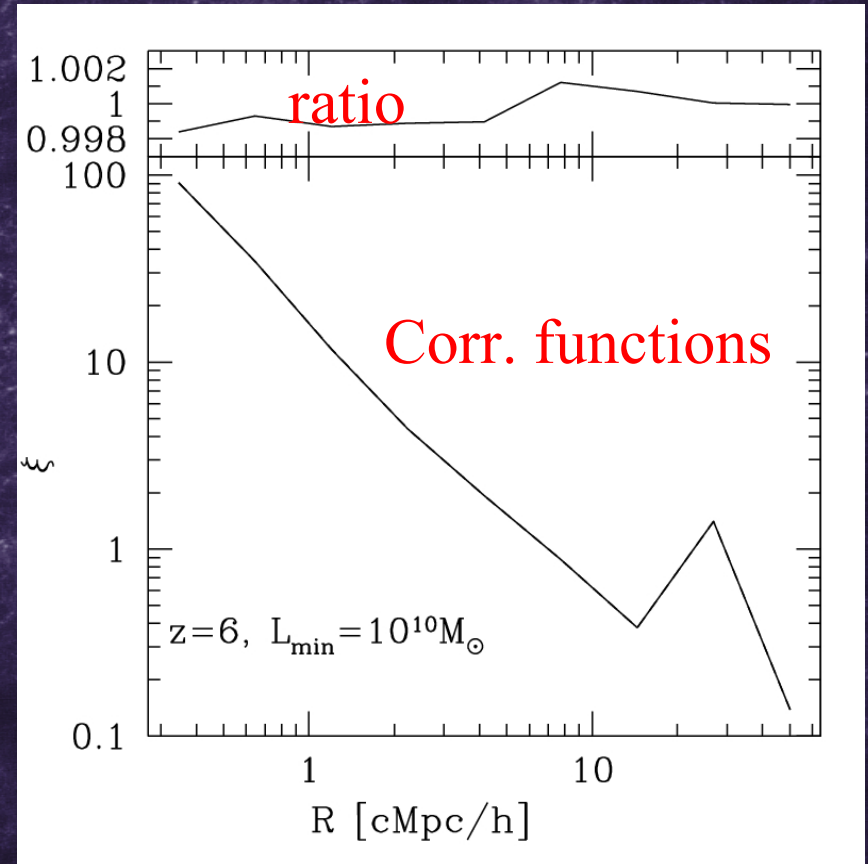
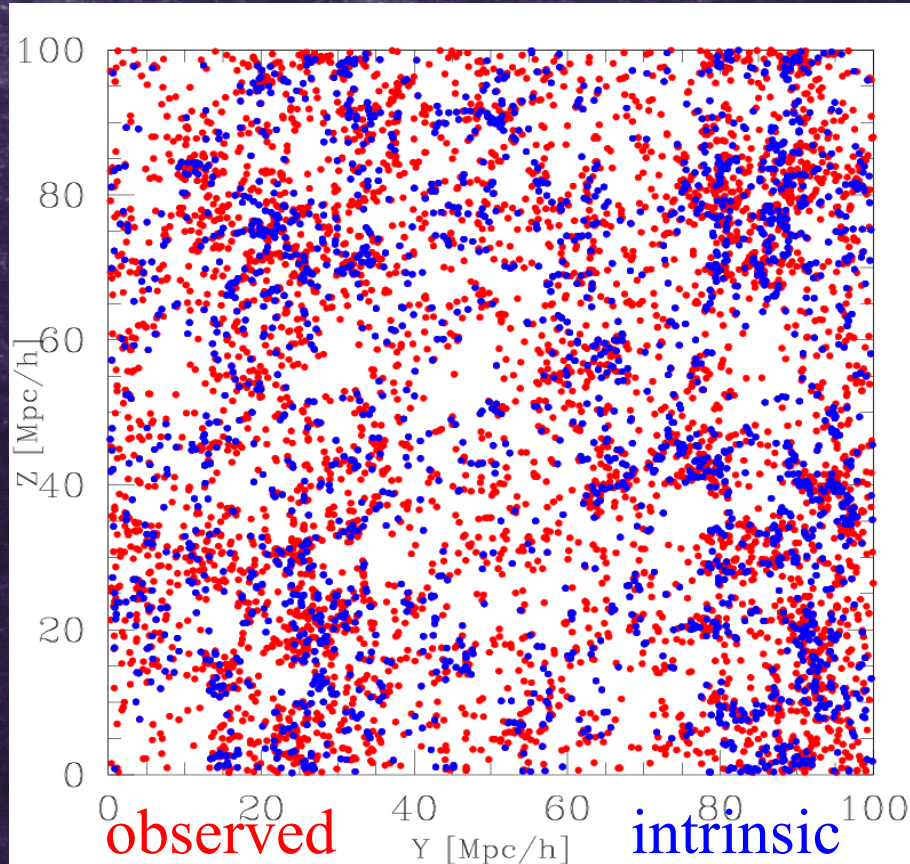
→ the **majority** of sources responsible for reionization are **too faint** to be observed at present.





# Correlation functions of Ly- $\alpha$ sources

(Iliev et al. 2008, MNRAS, 391, 63)



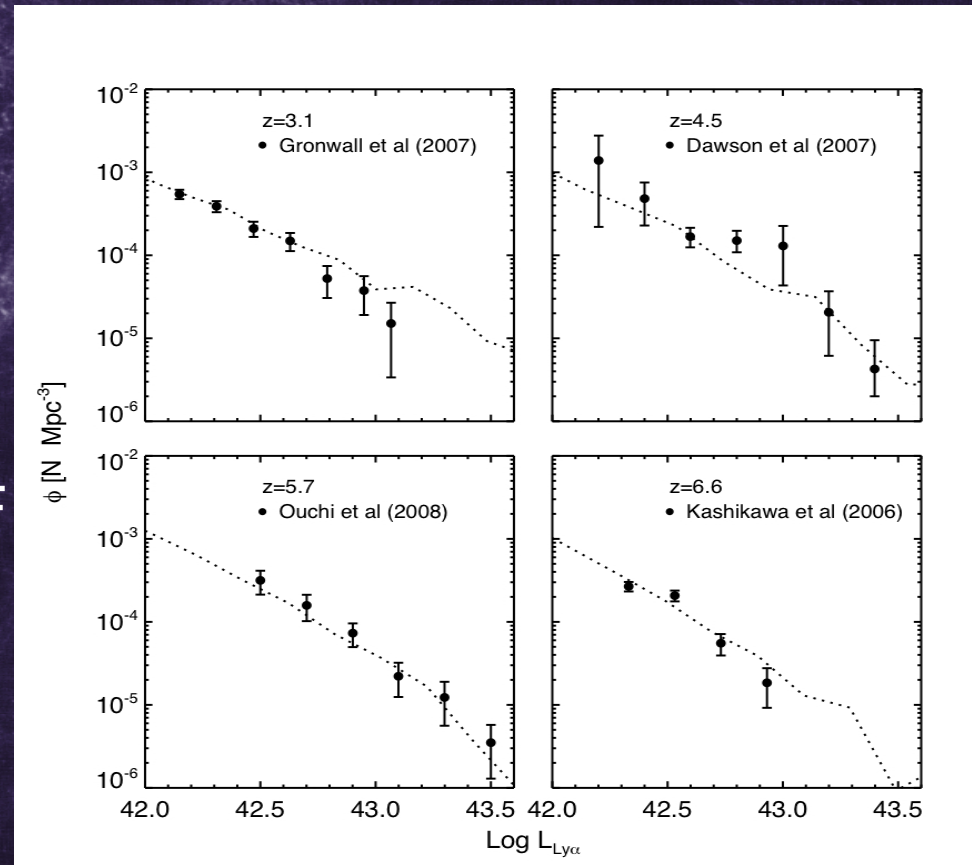
For a given (e.g. observed) **number density** of sources their clustering is largely **unaffected** by reionization patchiness (max 10% difference at small scales and at high- $z$ , decreasing later).



# A simple physical model for the luminosity function of Ly- $\alpha$ sources

(Tilvi, Malhotra, Rhoads, Scannapieco, Thacker, Iliev & Mellema, 2009, ApJ, 704, 724)

- A simple, 1-parameter model, based on assumption that Ly- $\alpha$  luminosity is proportional to halo mass growth.
- Matches well the Ly- $\alpha$  LF data at  $z=3-6.6$ .

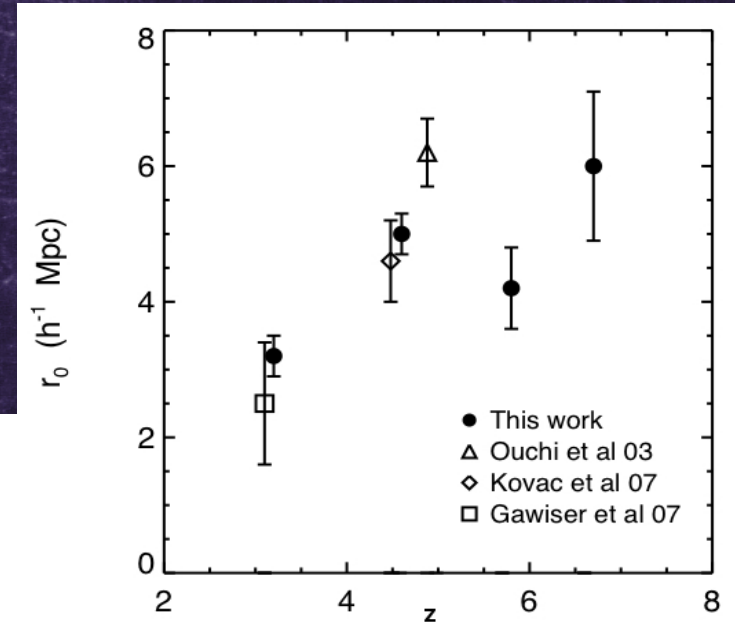
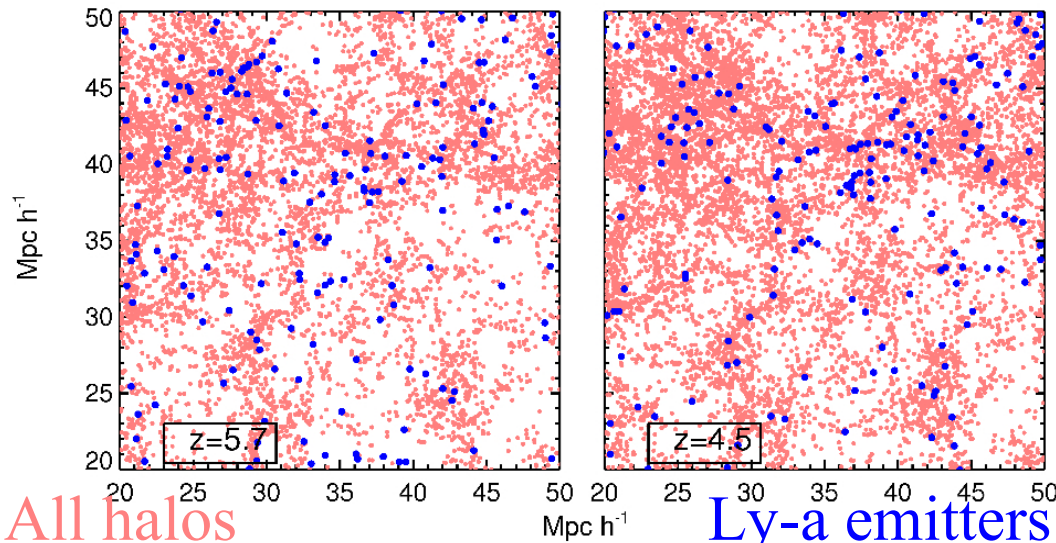




# A simple physical model for the luminosity function of Ly-a sources: source clustering

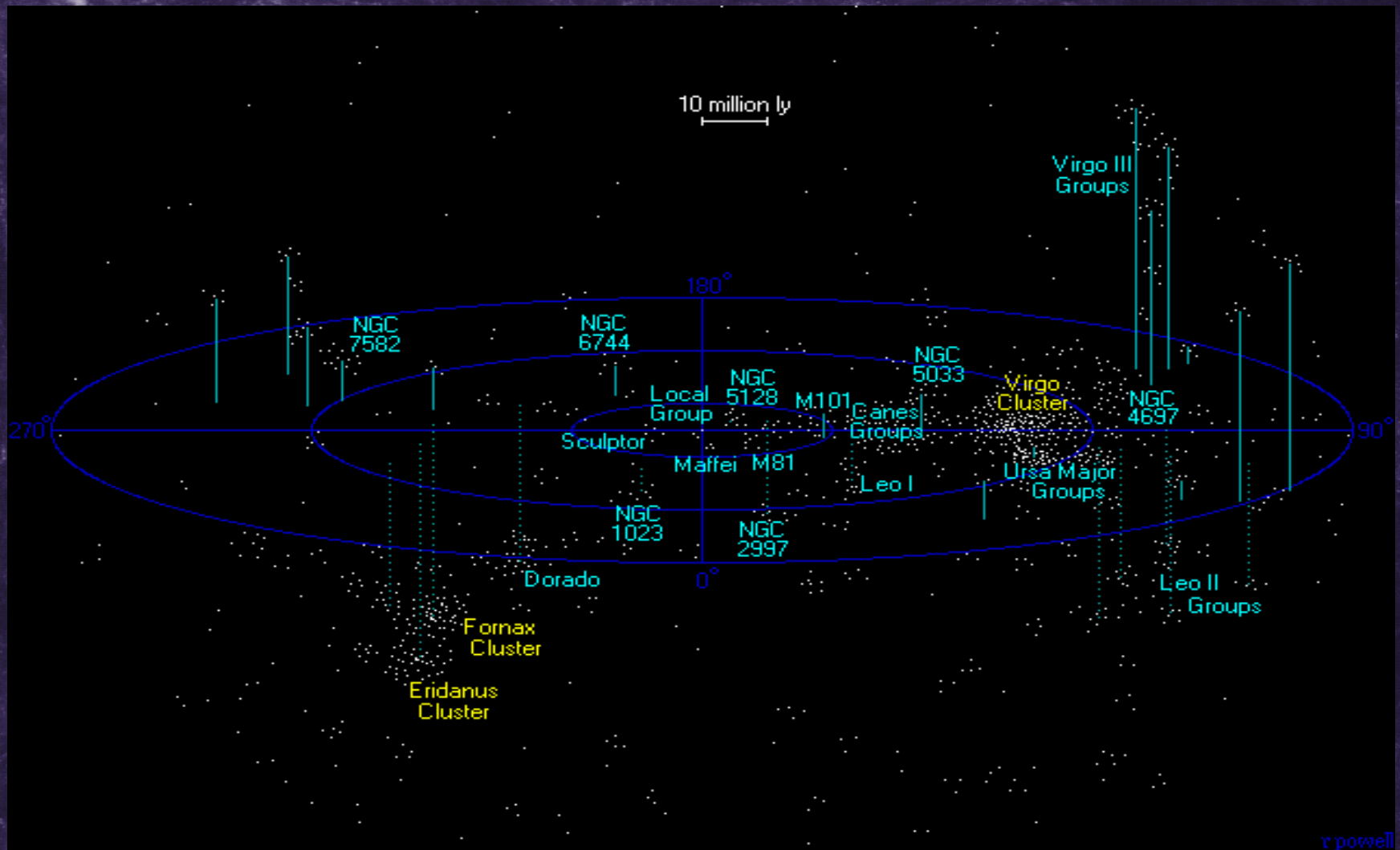
(Tilvi, Malhotra, Rhoads, Scannapieco, Thacker, Iliev & Mellema, 2009, ApJ, 704, 724)

- Source clustering agrees well with observed one.
- Model introduces a natural duty cycle





# Our neighbourhood

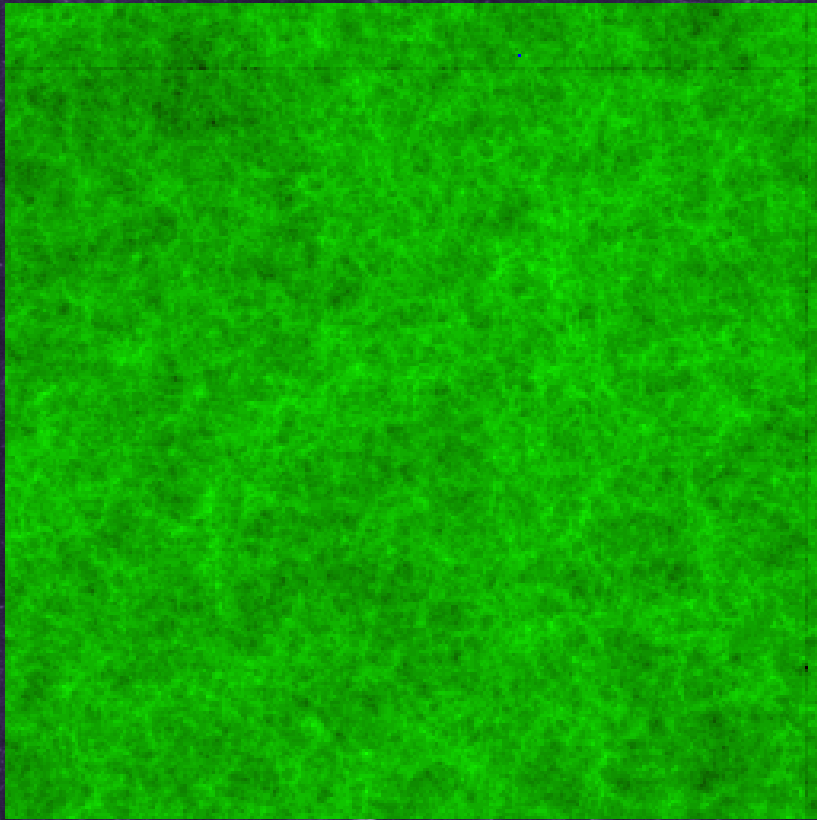




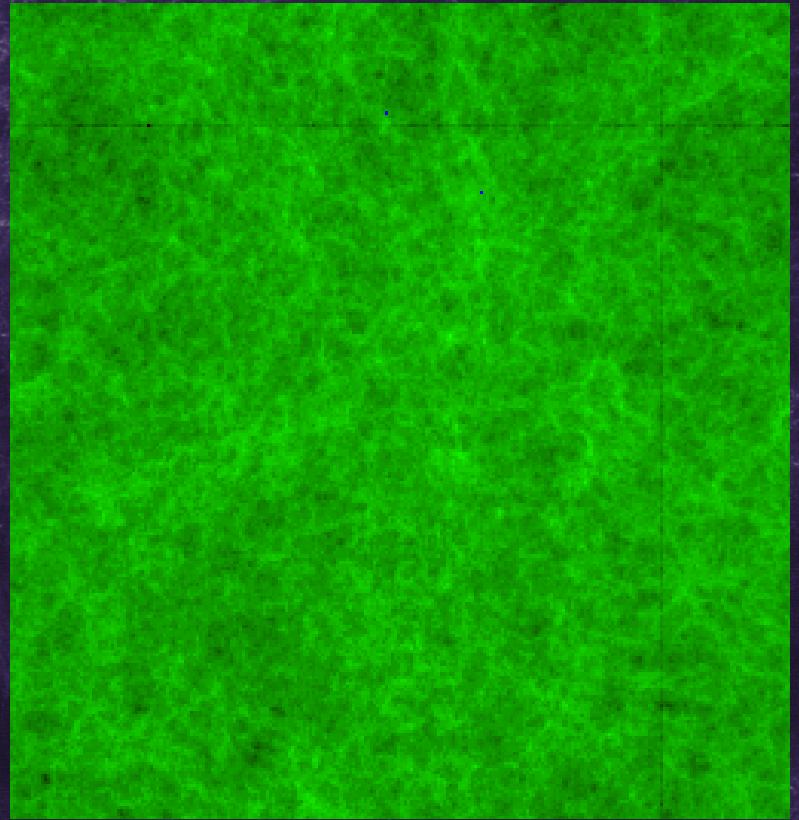
# Reionization of the Local Group

(w/B. Moore, G. Yepes, S Goetlobber, Y. Hoffman, G. Mellema;  
work in progress)

Constrained simulations of the formation of the LG and its  
neighbourhood (GADGET, 64/h Mpc box,  $1024^3$  particles) post-  
processed with radiative transfer (on  $256^3$  grid), same method.



Milky Way



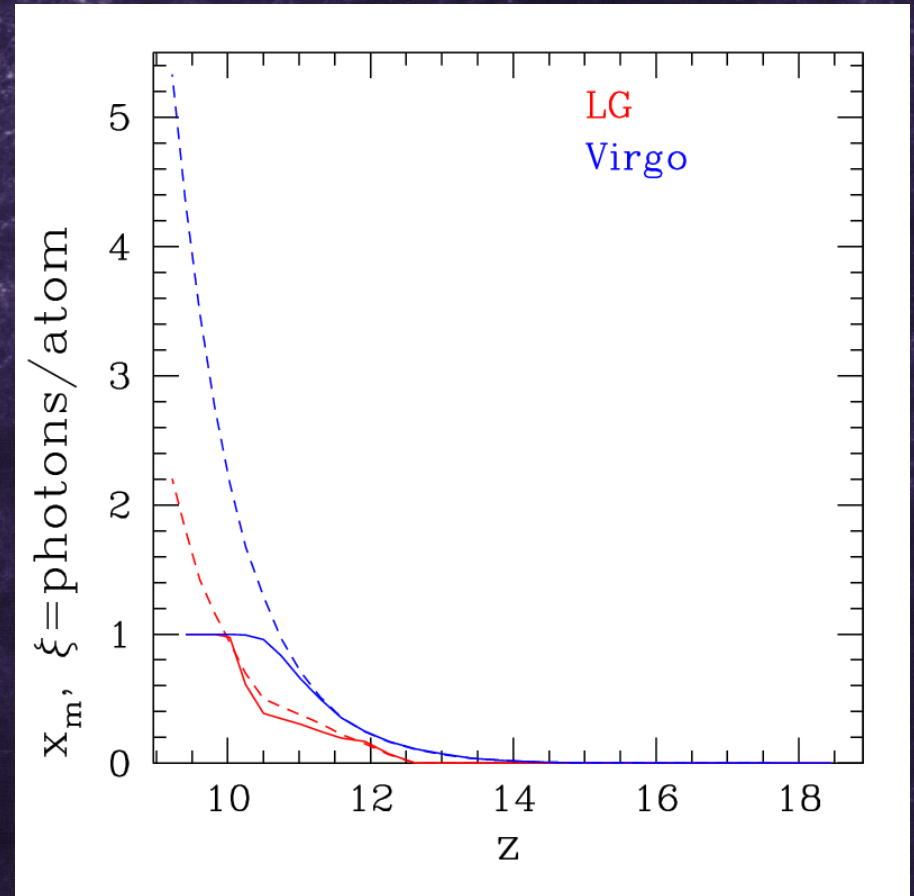
Virgo

WMAP3



# Reionization of the Local Group: the Photon Budget

- Both (proto-)LG and Virgo reionize around  $z \sim 10$ .
- At the time of LG reionization internal sources have barely produced less than 1 ionizing photons/atom  $\Rightarrow$  mostly **external** reionization
- By contrast, Virgo constituents have already produced multiple photons/atom by the time it is fully ionized ( $z \sim 10.5$ ), i.e. its reionization is **internal**.



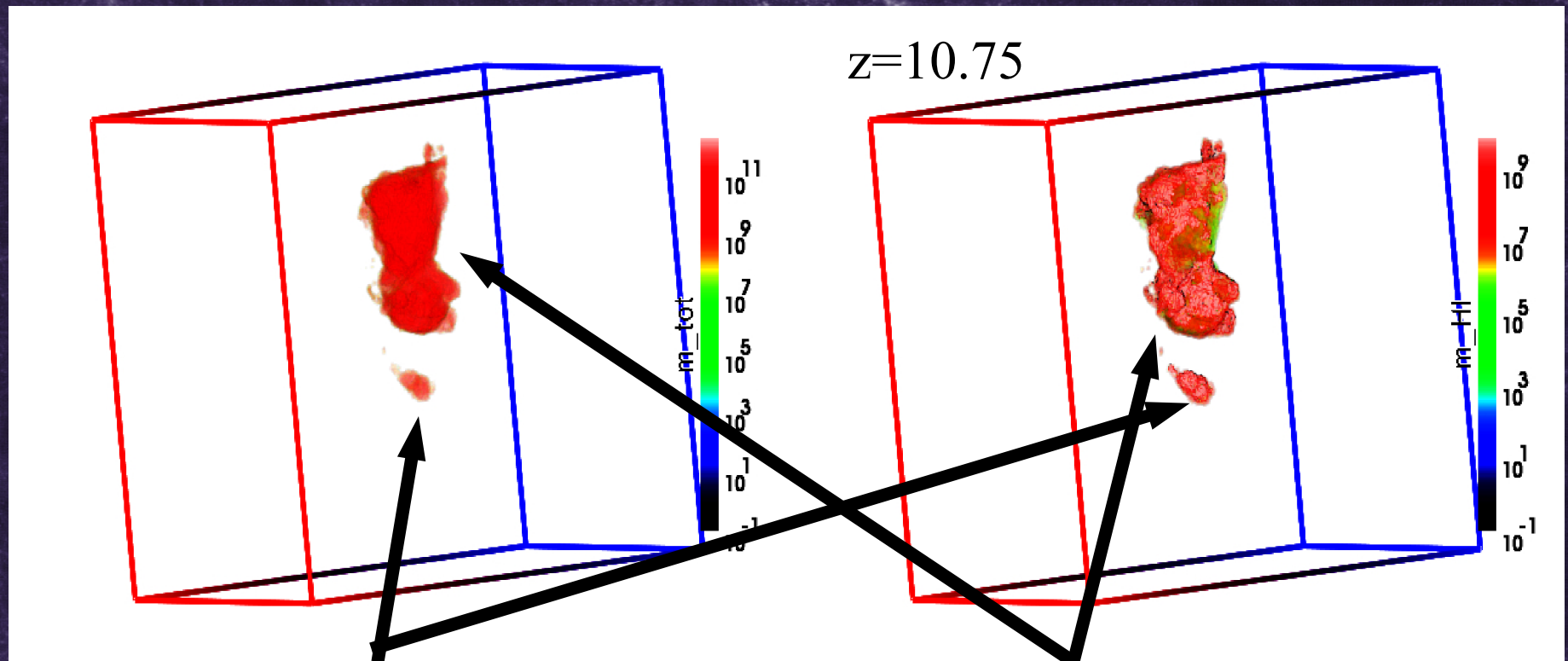


# Reionization of the Local Group: the evolution

**Total mass**

**Neutral mass**

$z=10.75$



(proto) Local Group

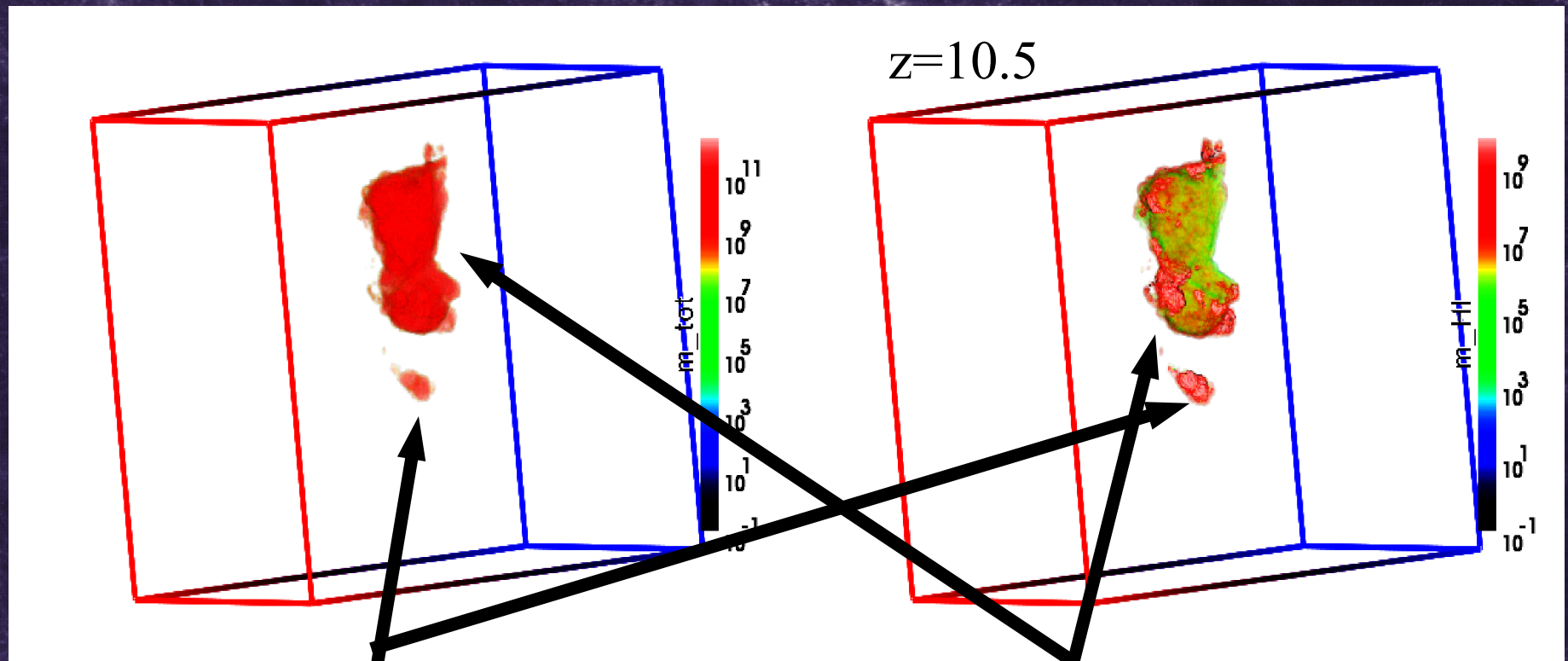
(proto) Virgo



# Reionization of the Local Group: the evolution

**Total mass**

**Neutral mass**



(proto) Local Group

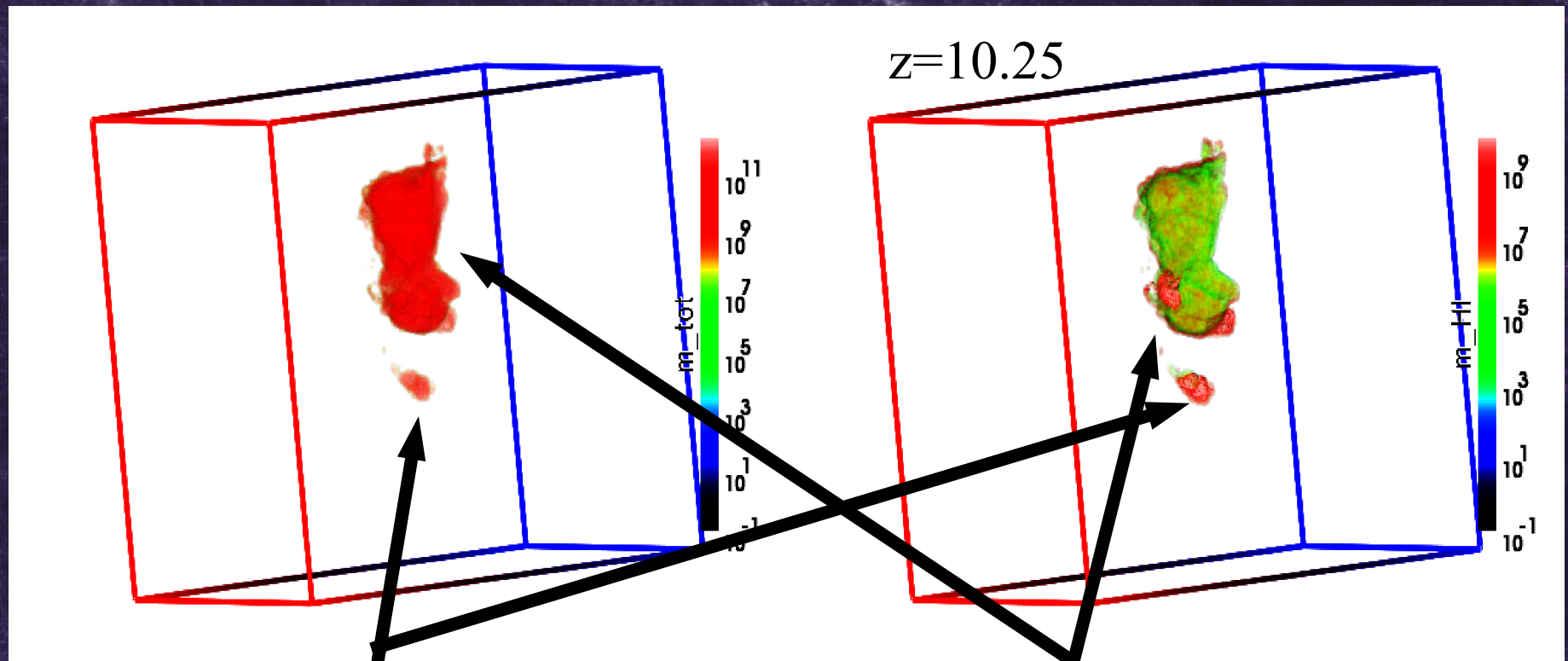
(proto) Virgo



# Reionization of the Local Group: the evolution

Total mass

Neutral mass



(proto) Local Group

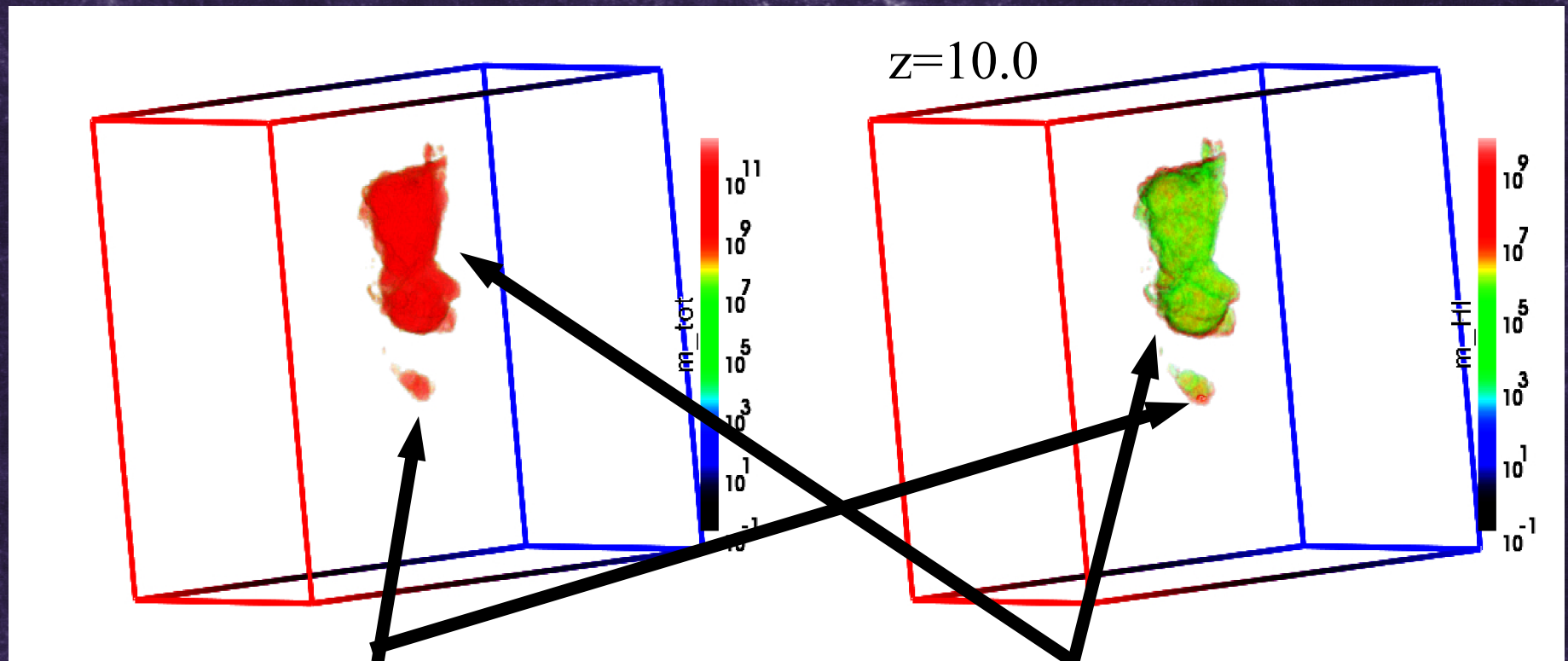
(proto) Virgo



# Reionization of the Local Group: the evolution

**Total mass**

**Neutral mass**



(proto) Local Group

(proto) Virgo

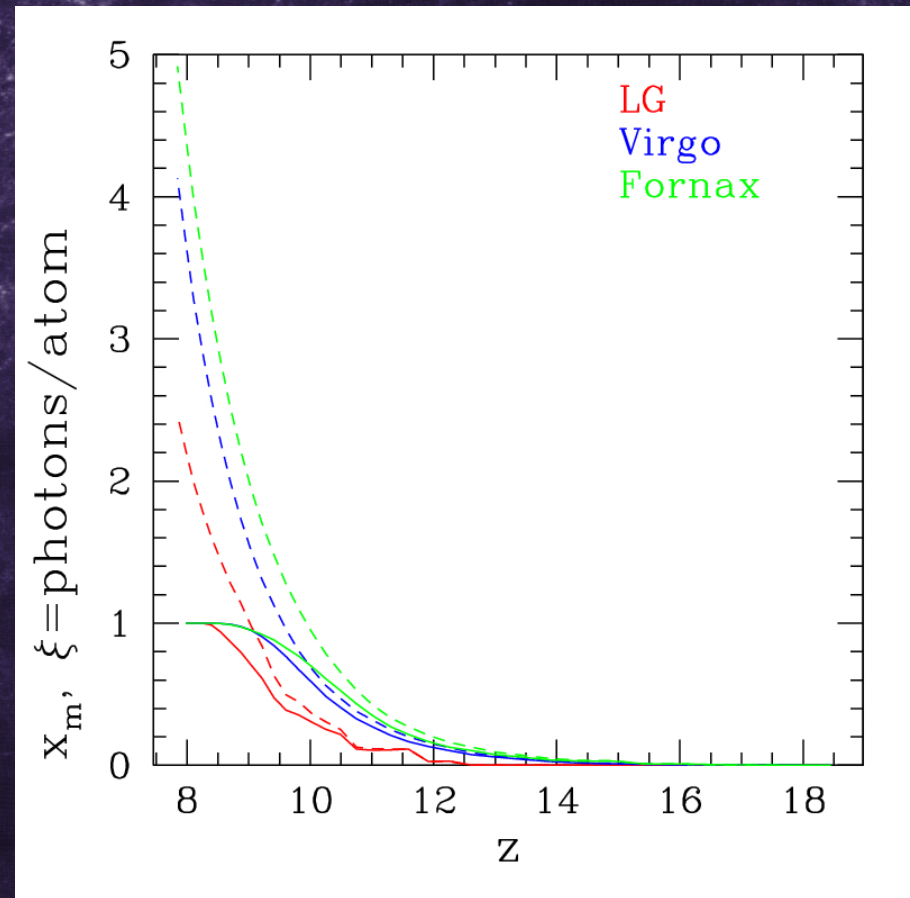


- How robust are the above conclusions? E.g. would they change for a different LG realization, constraints imposed, cosmology, ...?
- We address this by a new simulation, with different (and improved) representation of our neighbourhood. This now contains not only the LG and Virgo, but also the Fornax cluster.
- Cosmology is updated to WMAP5.



# Reionization of the Local Group, WMAP5: the Photon Budget

- Both (pre-)Fornax and Virgo reionize earlier, at  $z \sim 8.6$ .
- LG reionizes later, at  $z \sim 8.25$ .
- At the time of LG reionization internal sources have produced  $\sim 1.8$  ionizing photons/atom
- Virgo progenitors have produced  $\sim 2.2$  (2.9) photons/atom by  $z \sim 8.6$  (8.25), while Fornax ones have produced 2.8 (3.6) photons/atom by  $z = 8.6$  (8.25). Both are reionized predominantly **internally**, while also contributing to the LG reionization.

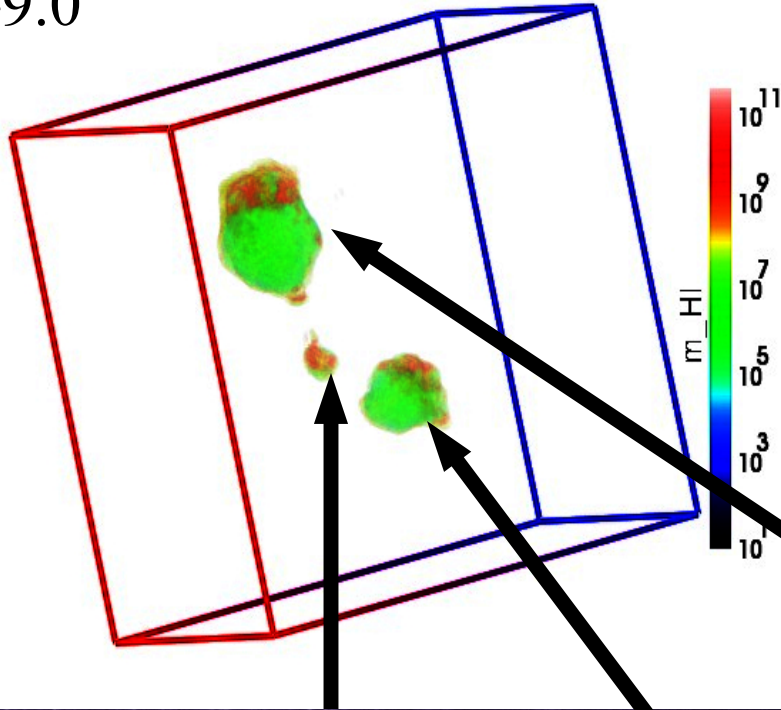




# Reionization of the Local Group, WMAP5: the evolution

Neutral mass

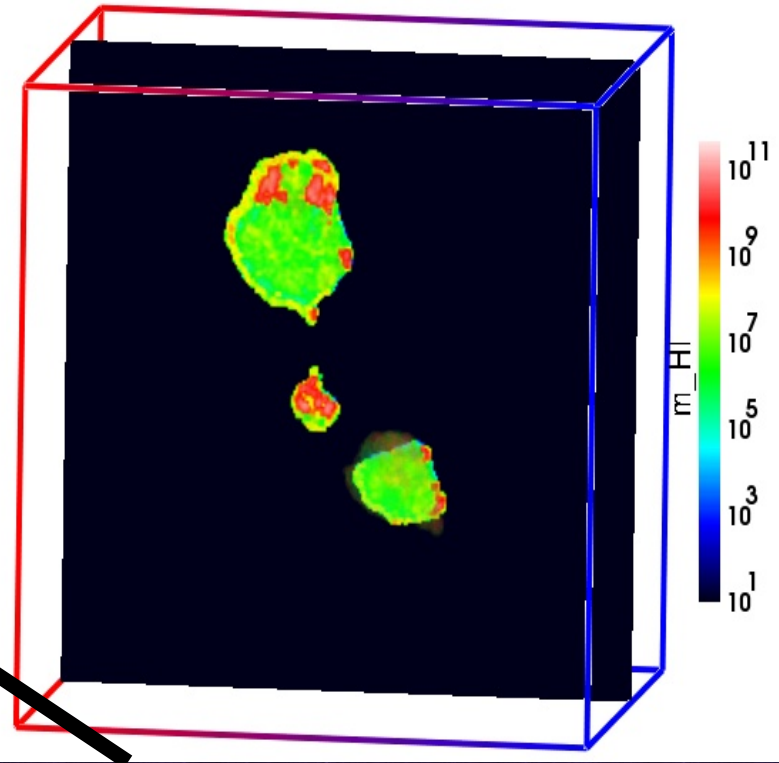
$z=9.0$



(proto) Local Group

(proto) Fornax

Neutral mass



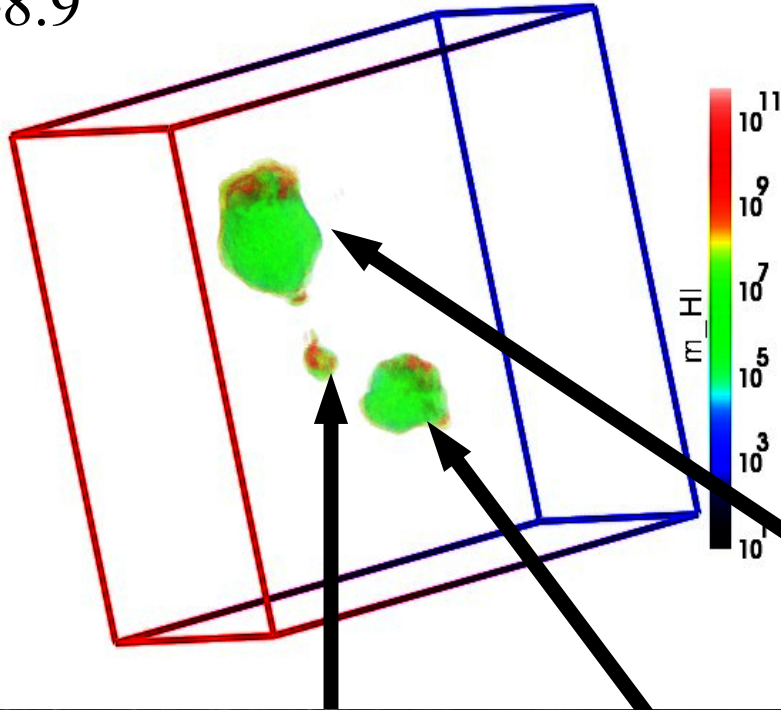
(proto) Virgo



# Reionization of the Local Group: the evolution

Neutral mass

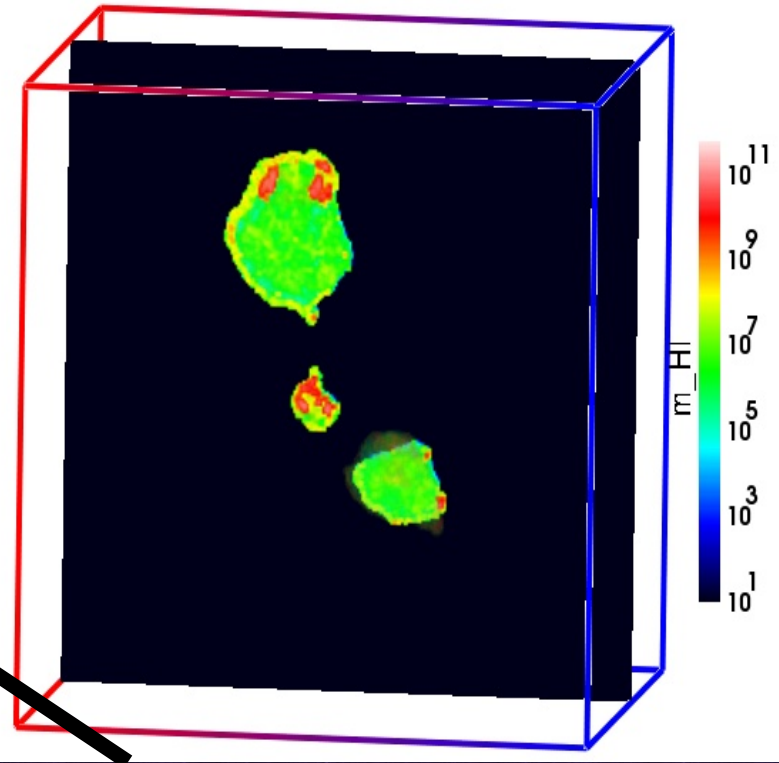
$z=8.9$



(proto) Local Group

(proto) Fornax

Neutral mass



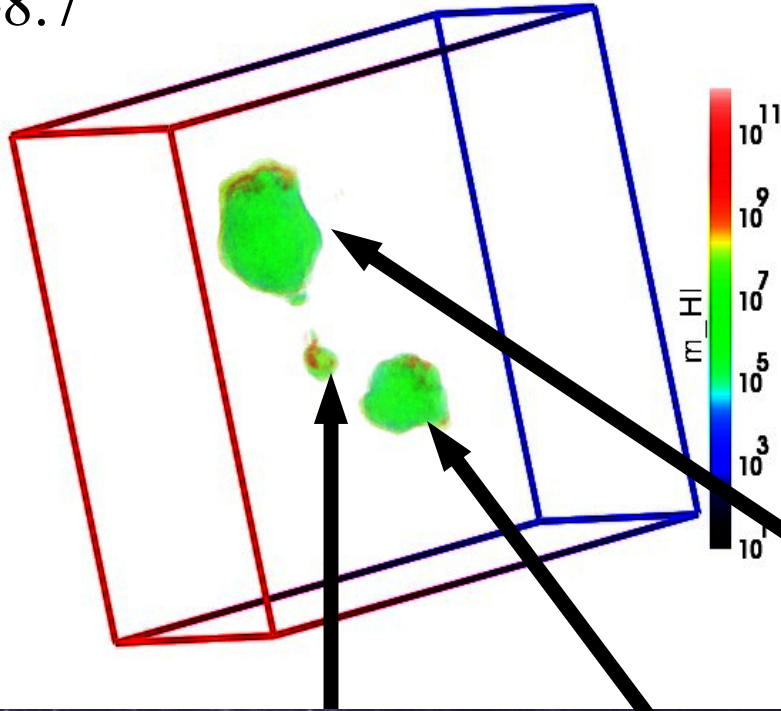
(proto) Virgo



# Reionization of the Local Group: the evolution

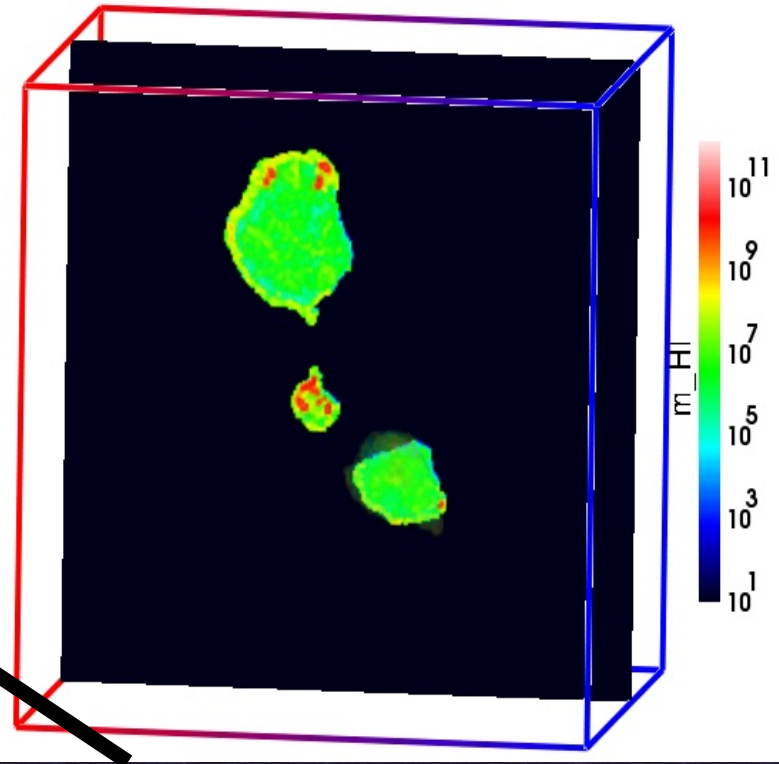
Neutral mass

$z=8.7$



(proto) Local Group

Neutral mass



(proto) Virgo

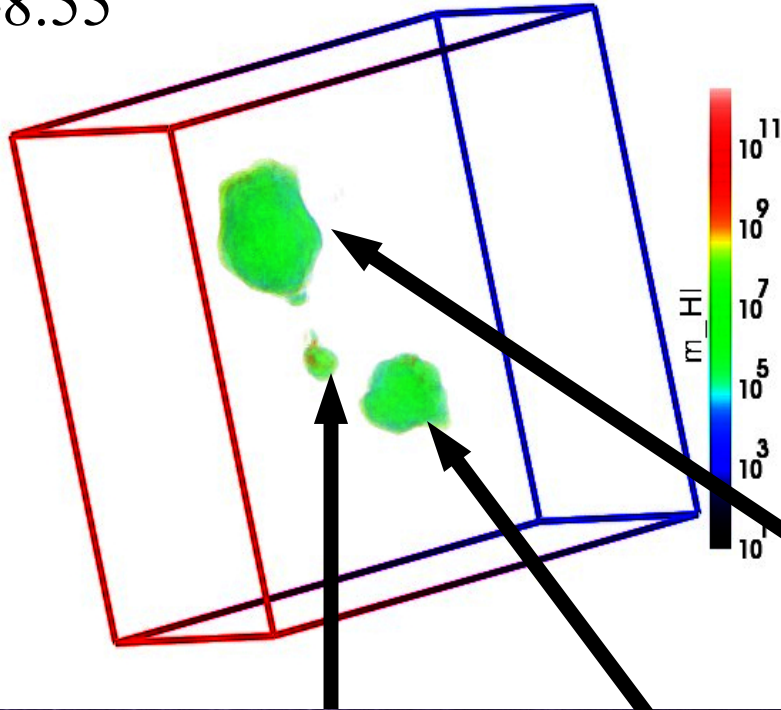
(proto) Fornax



# Reionization of the Local Group: the evolution

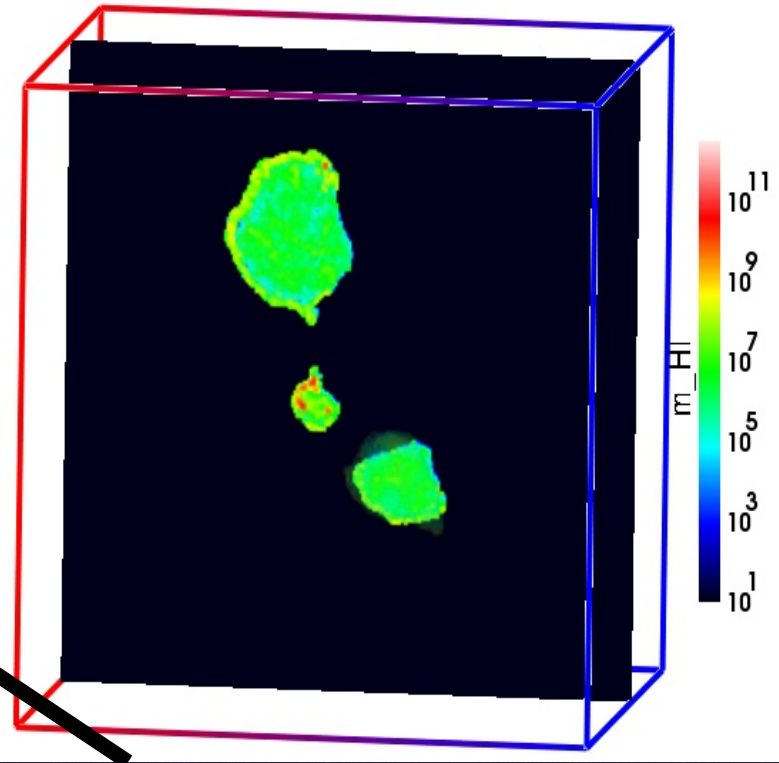
Neutral mass

$z=8.55$



(proto) Local Group

Neutral mass



(proto) Virgo

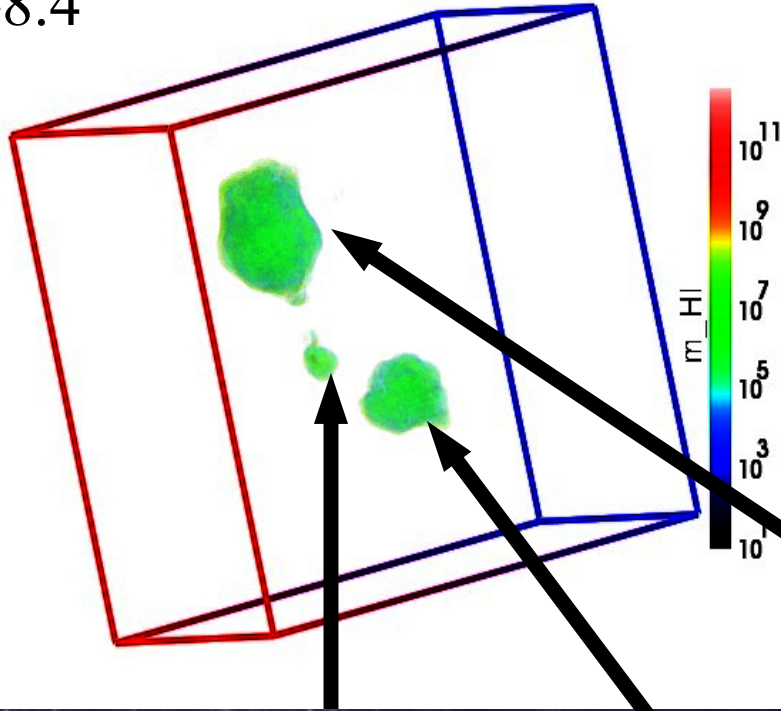
(proto) Fornax



# Reionization of the Local Group: the evolution

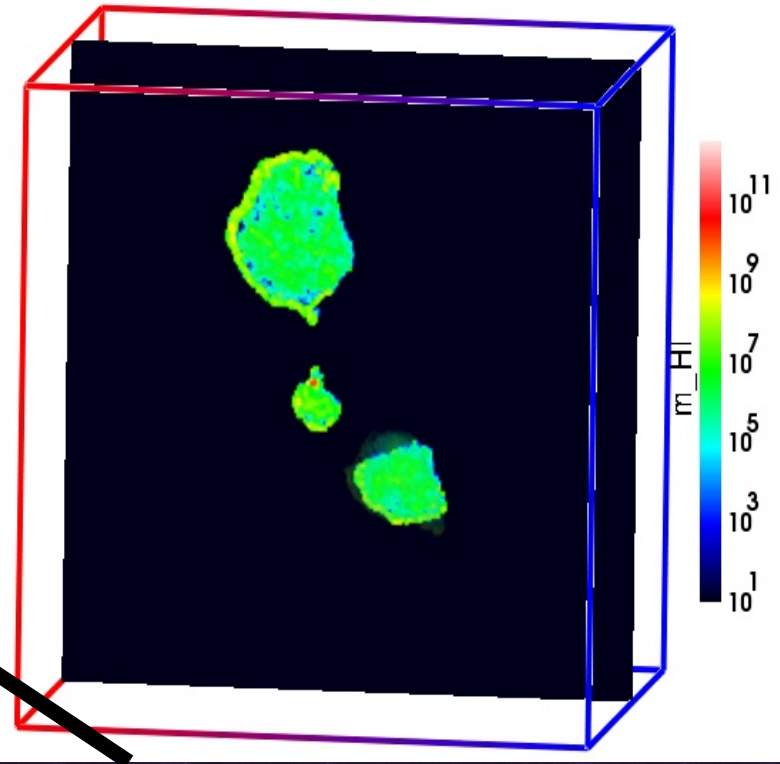
Neutral mass

$z=8.4$



(proto) Local Group

Neutral mass



(proto) Virgo

(proto) Fornax

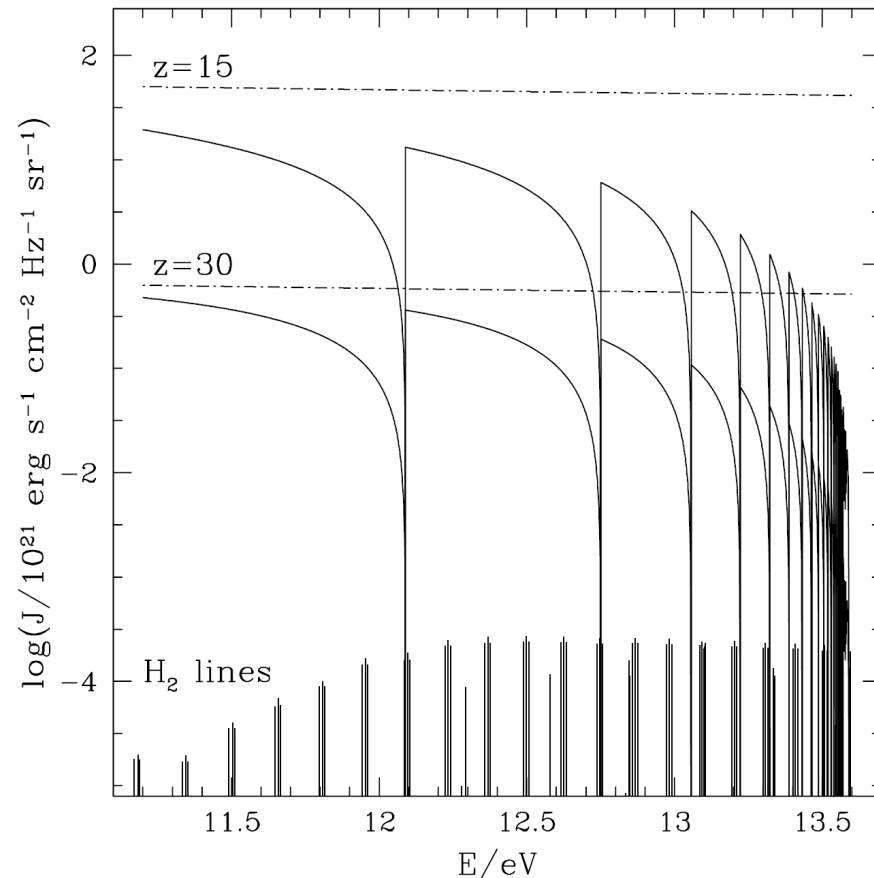


# Early H<sub>2</sub>-dissociating background (Lyman-Werner bands)

## Uniform source distribution case: Sawtooth Modulation

- LW band photons attenuated by H atom resonance lines
- Sawtooth-modulation (Haiman, Abel, Rees 2000)
  - ▣ Based upon uniformly distributed sources
  - ▣ Different horizon for different Lyman resonance lines

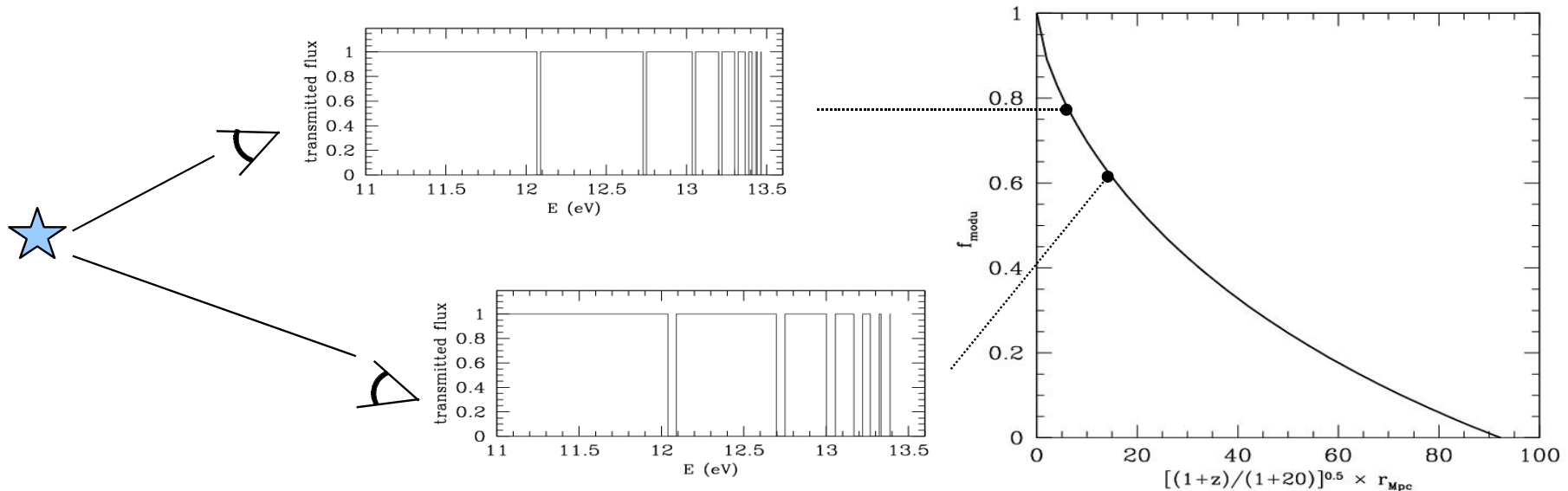
Ahn, Shapiro, Iliev,  
Mellema, Pen, ApJ,  
2009, 393, 1449





# Non-uniform source distribution: Picket-Fence Modulation

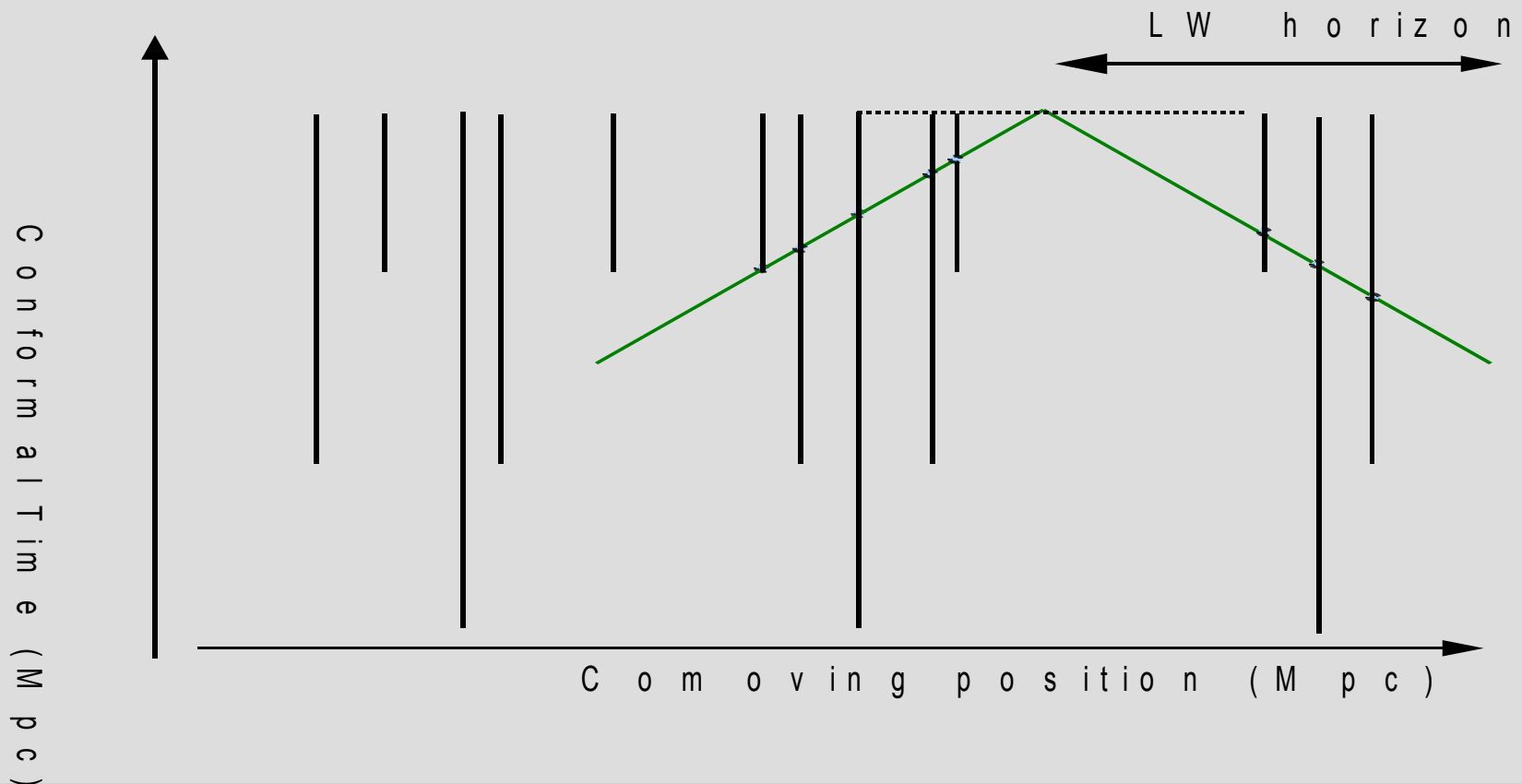
- Sources distributed inhomogeneously: Need to sum individual contribution
- One single source is observed as a picket-fence in spectrum: Can effectively follow attenuation by multi-frequency phenomenon by pre-calculated modulation factor -> Computations become hugely cheaper.





## Retarded time emissivity

- Sources form in hierarchy. Evolution is fast (exponential rise in source population).
- Horizon for LW background is very large ( $\sim 100$  comoving Mpc)
- Construct spacetime diagram and draw past line cone at a given space-time to account for LW



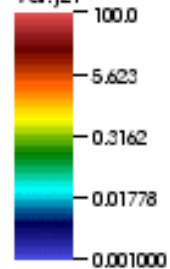


# H<sub>2</sub> Dissociating Background during EOR

DB: 19.175-slide.vtk  
Cycle: 175

Pseudocolor

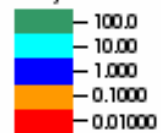
Var: j21



Max: 0.07659  
Min: 0.0003371

Contour

Var: j21

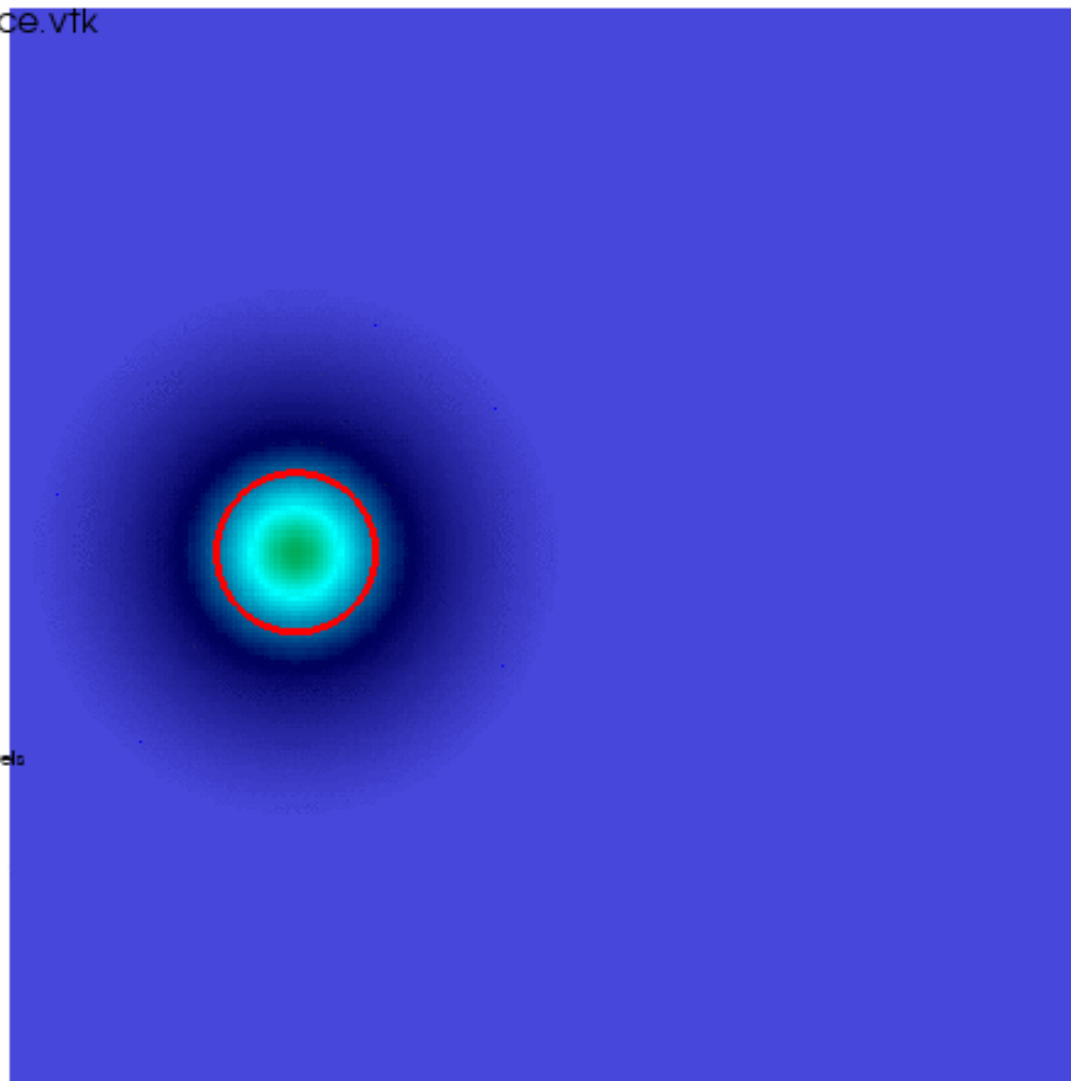


Max: 0.07659  
Min: 0.0003371

Contour

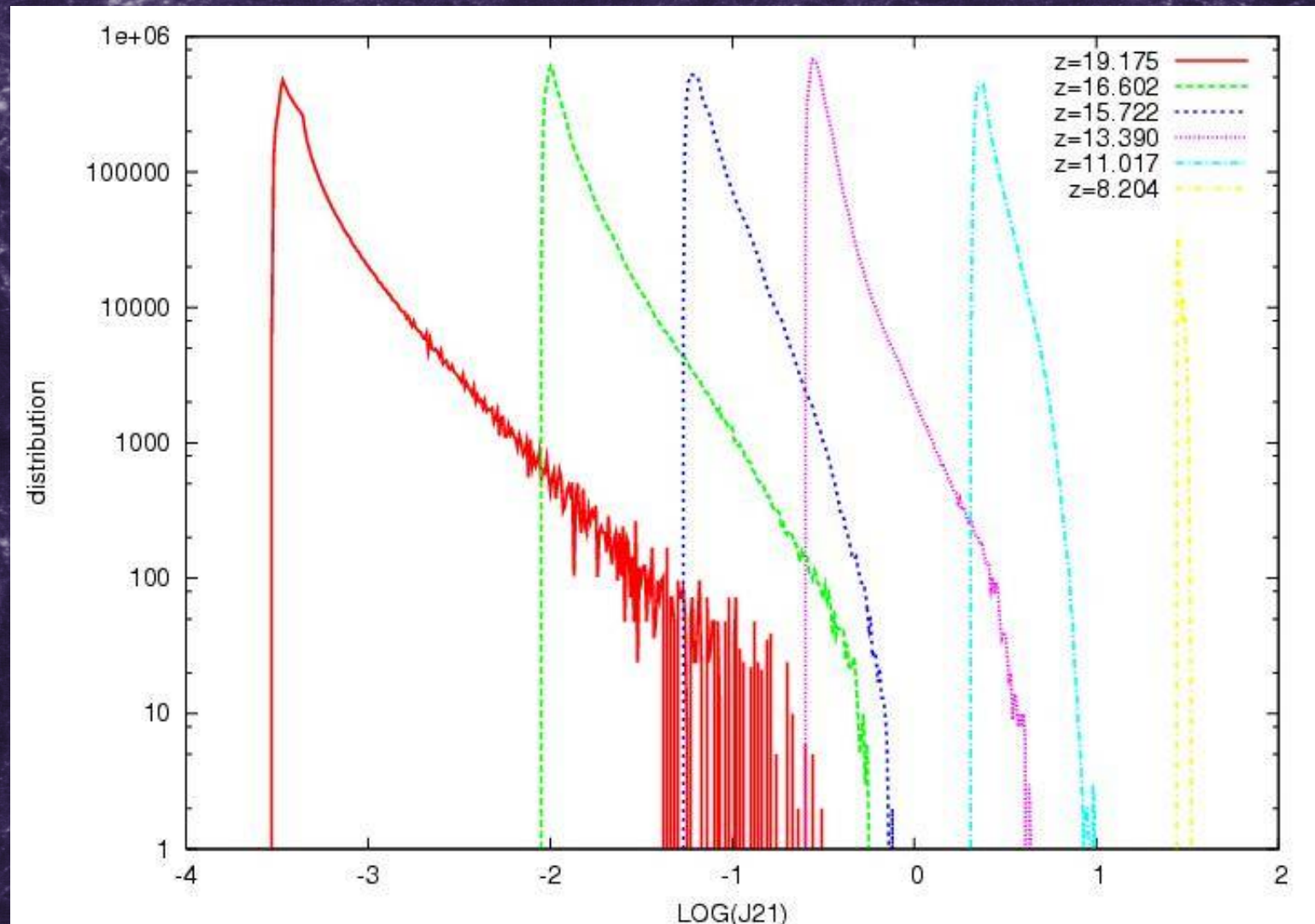
Var: x

Unable to compute levels





# Degree of Fluctuation in LW Background





# Summary

- Large-scale, accurate EoR simulations at the large scales relevant to observations are now possible.
- High- $z$  structure formation differs from low- $z$  one in many important features — mass function, halo bias ...
- Patch reionization creates strong CMB fluctuations at small scales due to kSZ effect. The derived sky power spectra peak strongly to  $> 10 (\mu\text{K})^2$  at  $l \sim \text{few thousand}$  (dependent on details of reionization). Large-scale bulk velocities are important.
- The first constrained simulations of the reionization of our neighbourhood show that our Local Group was mostly reionized from outside, by Virgo and Fornax.
- LW H<sub>2</sub>-molecule destroying background at large scales can now be modelled numerically in a self-consistent way. It is highly spatially inhomogeneous and time-dependent. Minihaloes could be important sources.



Thank you for your attention!

Time for questions...