

# All HII Regions Great and Small

## An overview of C<sup>2</sup>-Ray

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# Contents

- Photo-ionization Gas Dynamics
- Method (C<sup>2</sup>-Ray)
- Some Results for Turbulent HII regions
- Some Results for Reionization

# Photo-Ionization Hydrodynamics

- The photo-ionization process is one of the important radiative feedback processes in astrophysics.
- The increase in pressure caused by it can trigger strong dynamic effects: photo-ionization hydrodynamics.
- The challenge in combining hydrodynamics with photo-ionization lies in the difference in time scales between the two process.

# Radiative Transfer

- Assuming that:
  - Speed of the ionization front is non-relativistic.
  - Recombinations to the ground level can be incorporated using a modified recombination rate (On The Spot approximation).
- The full radiative transfer equation

$$\frac{\partial I_\nu}{c \partial t} + \nabla \cdot (\Omega I_\nu) = j_\nu - \kappa_\nu I_\nu$$

- Simplifies to

$$\nabla \cdot (\Omega I_\nu) = -\kappa I_\nu$$

# Photo-Ionization Chemistry

$$\frac{\partial n(H^+)}{\partial t} = (r - n(H^+))\Gamma - n(H^+)n_e\alpha(T) + (r - n(H^+)n_e)C(T)$$

Photo-ionization

Recombinations

Collisional  
Ionization

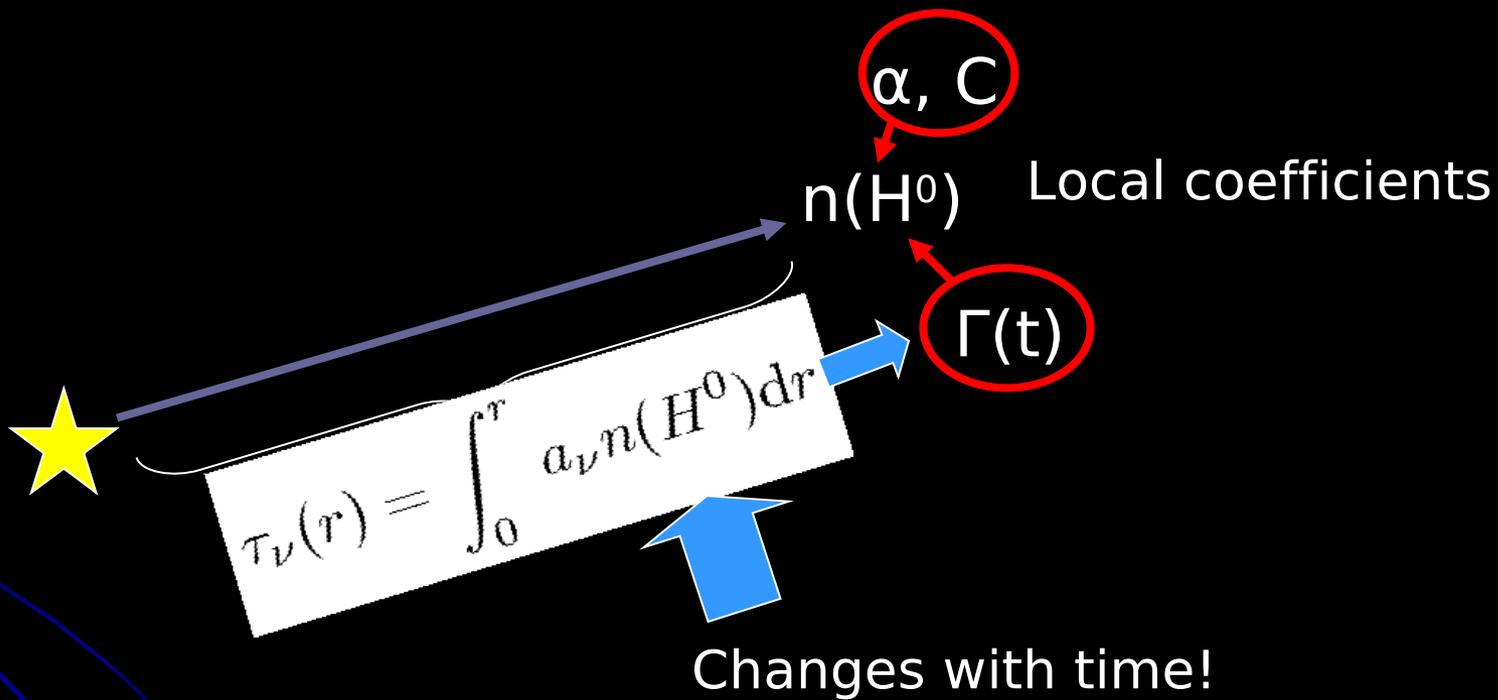
$$\Gamma = \frac{1}{4\pi r^2} \int_{\nu_0}^{\infty} \frac{L_{\nu}}{h\nu} a_{\nu} e^{-\tau_{\nu}(r)} d\nu$$

Photo-Ionization rate

Solution of the radiative transfer equation

$$\tau_{\nu}(r) = \int_0^r a_{\nu} n(H^0) dr$$

Optical depth between source and position  $r$



# Photo-Ionization Heating

$$\mathcal{H} = \frac{n(H^0)}{4\pi r^2} \int_{\nu_0}^{\infty} h(\nu - \nu_0) \frac{L_\nu}{h\nu} a_\nu e^{-\tau_\nu(r)} d\nu$$

Energy above  
the ionization  
energy

Note: the higher energy photons heat more, and have a lower optical depth

$$a_\nu = a_0 \left( \frac{\nu_0}{\nu} \right)^3$$

# Multi-Scale Problem: Time

- The ionization fraction evolves on a typical time scale  $t_i = 1 / (x[\text{H}^0] (\Gamma + C(T)) + x[\text{H}^+] n_e \alpha)$
- In addition  $\Gamma$  depends on non-local effects ( $\tau$ ), so there is also the time scale for **change in  $\tau$**  hence in  $\Gamma$ . This is related to speed of the ionization front.

$$\Gamma = \frac{1}{4\pi r^2} \int_{\nu_0}^{\infty} \frac{L_\nu}{h\nu} a_\nu e^{-\tau_\nu(r)} d\nu$$

- The gas evolves on a typical time scale  $t_{\text{hydro}} = \Delta x / (v + v_s)$
- These time scales are unrelated, and can be orders of magnitude different.
- In a gas dynamic simulation you prefer to use  $t_{\text{hydro}}$ !

# Multi-Scale Problem: Length

- If our computational cells are rather large, it may happen that there is considerable optical depth over a cell:  $\Delta\tau_\nu = a_\nu n(\text{H}^0)\Delta r$ .
- If  $\Delta\tau_\nu \gg 1$  the photo-ionization rate  $\Gamma$  is *not* constant inside the cell.
- Using a value from a particular radius will either under- or overestimate the number of photo-ionizations.

$$\Gamma = \frac{1}{4\pi r^2} \int_{\nu_0}^{\infty} \frac{L_\nu}{h\nu} a_\nu e^{-\tau_\nu(r)} d\nu$$

# Diagnostic: Photon-Conservation

- There is a simple way to check whether you are solving the problem in the correct way: **photon-conservation**.
- The number of photons sent out by the source within a time step should either be used for ionizations (new, or balancing recombinations), or escape from the domain.
- So by comparing these numbers, the correctness of your solution can be checked.

# C<sup>2</sup>-Ray

- Conservative, Causal Ray Tracing (GM, Iliev, Alvarez, Shapiro, 2006).
- Uses time- and spatially averaged quantities to allow a photo-ionization calculation at  $\Delta t_{\text{hydro}}$  and  $\Delta x_{\text{hydro}}$ .
- The radiation transport is done using **short characteristics** ray tracing.
- With this method we can calculate three-dimensional photo-ionization on regular grids.
- We use a **modular approach** for developing the code:
  - Can be used as a stand-alone code (R-type fronts, reionization).
  - Can be coupled to hydrodynamics (HII regions).

# Photon-Conservation: Space & Time

- Dealing with **thick cells**: take it to be a volume in (Abel, Norman, Madau 1999).
- Dealing with **long time steps**: use the time-averaged optical depth

$$\Gamma = \int_{\nu_0}^{\infty} \frac{L_{\nu} e^{-\tau_{\nu}}}{h\nu} \frac{1 - e^{-\Delta\tau_{\nu}}}{(1-x)nV} d\nu$$

$$\langle \Delta\tau_{\nu} \rangle = a_{\nu} \Delta r \left( 1 - x_{\text{eq}} + (x_{\text{eq}} - x_0) (1 - e^{-\Delta t/t_i}) \frac{t_i}{\Delta t} \right)$$

- Derived from relaxation solution (Schmidt-Voigt & Köppen 1987; Mellema 1993, see Altay et al. 2008 for He version).

$$x(t) = x_{\text{eq}} + (x_0 - x_{\text{eq}}) e^{-\Delta t/t_i}$$

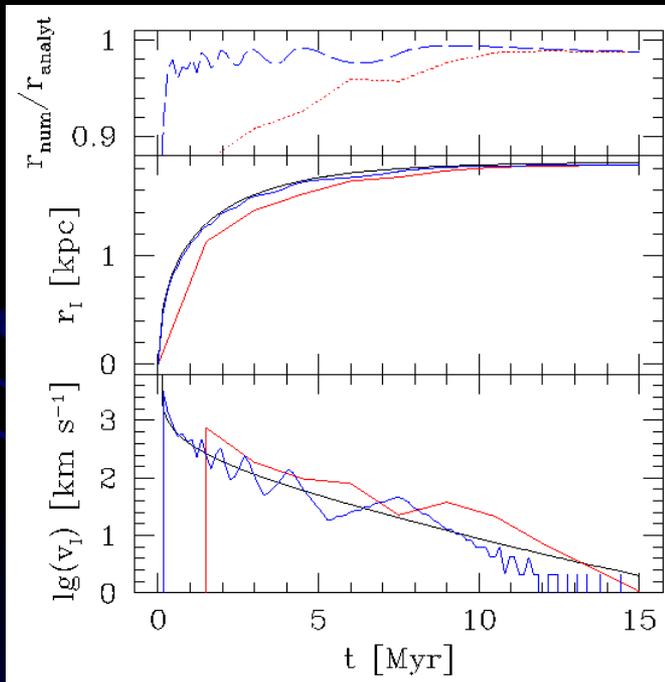
$$t_i = 1/(\Gamma + n_e \alpha)$$

$$x_{\text{eq}} = \frac{\Gamma}{\Gamma + n_e \alpha}$$

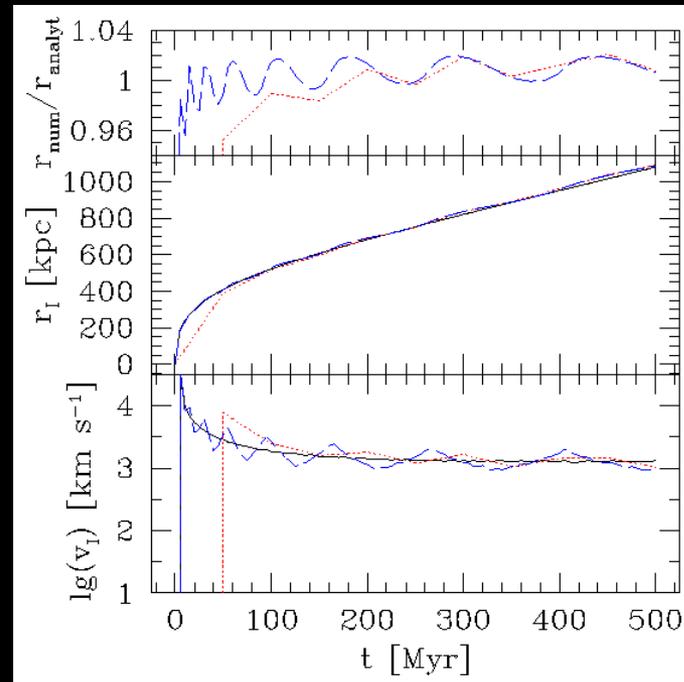
# Tests for Ionization

- Ionization fronts in different density environments.
- Worst case: 16 radial cells, 10 or 100 time steps.

1/r density



Expanding Universe



# Energy Conservation

- Photon-conservation automatically leads to energy conservation.
- Heating = (photon-energy<sub>in</sub> – photon-energy<sub>out</sub>) / Δt.
- Large time steps still give correct photo-ionization heating.

$$H = n_{\text{HI}} \int_{\nu_{\text{HI}}}^{\infty} h(\nu - \nu_{\text{HI}}) \frac{L_{\nu} a_{\nu} e^{-\tau_{\nu}}}{h\nu} d\nu,$$



$$H = \int_{\nu_{\text{HI}}}^{\infty} h(\nu - \nu_{\text{HI}}) \frac{L_{\nu} e^{-\langle\tau_{\nu}\rangle}}{h\nu} \frac{1 - e^{-\langle\Delta\tau_{\nu}\rangle}}{V_{\text{shell}}} d\nu,$$

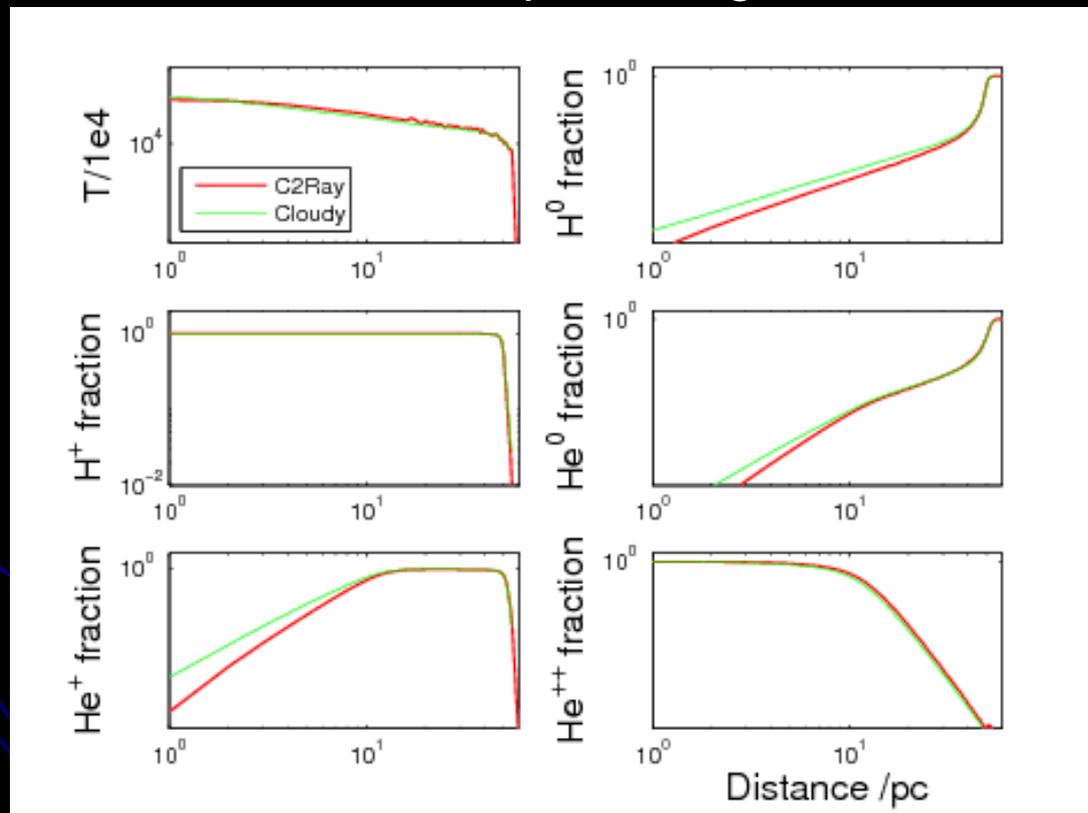
# Thermal Update

- Using the photon-conserving heating rate, we update the temperature by applying it together with a cooling rate.
- The **cooling rate** is determined from a **look-up tables**. These could be coronal cooling curve, or specified per ion. For the turbulent HII region simulations we used non-equilibrium  $H^0, H^+$  cooling plus approximate metal cooling.
- In order to deal with the stiff thermal equation (and the temperature dependent cooling rates) we **subcycle** the time step by limiting the change in thermal energy.

# In Progress: Adding Helium

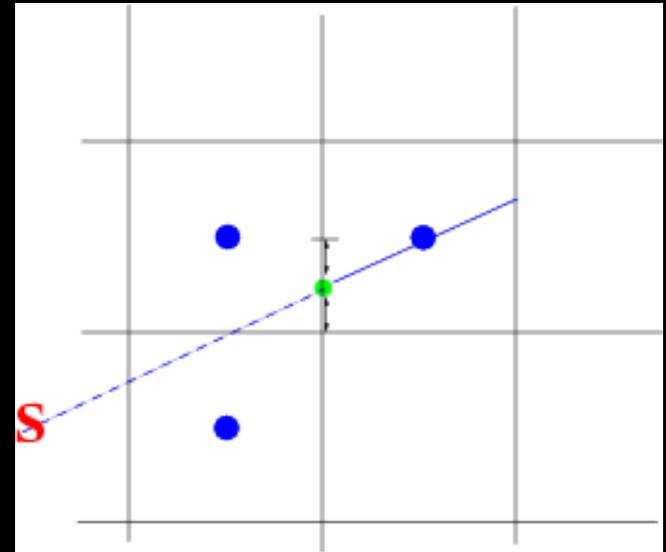
- Martina Friedrich (Stockholm) is working on putting back Helium to C<sup>2</sup>-Ray. First 1D test results look promising:

Equilibrium solution



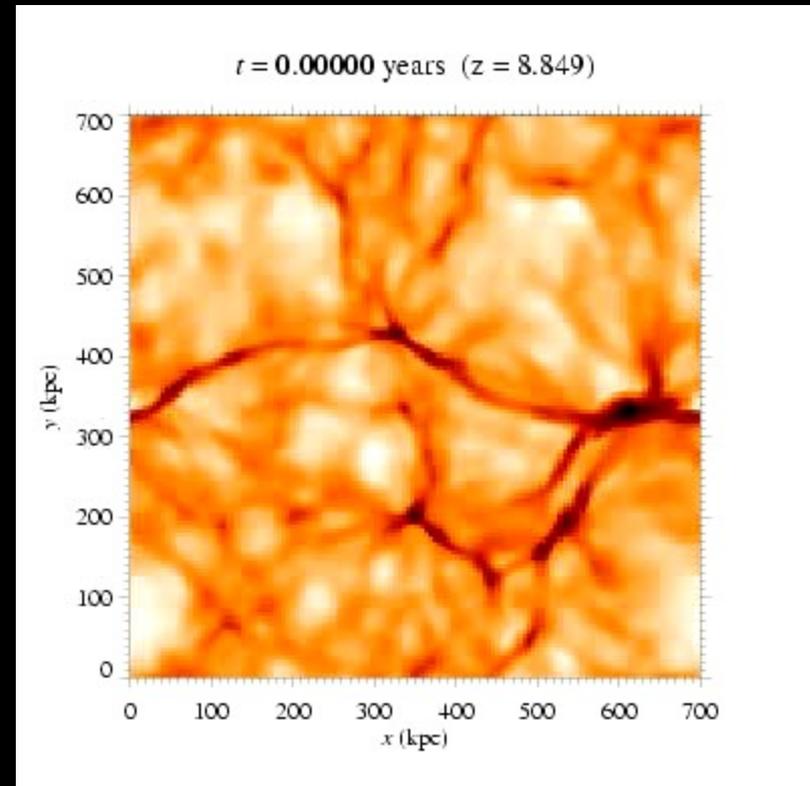
# Multi-dimensional Ray-tracing

- To calculate the transfer in 2 or 3 dimensions, one needs to do ray-tracing.
- We developed an efficient 3D ray-tracer for this, based on the technique of **short characteristics**.
- Optical depth is constructed from the solutions of cells closer to the source (**'causal'**).
- Note: short-characteristics does not guarantee photon-conservation (5% errors).



# Multiple Sources

- Handling multiple sources is possible.
- Each source has its own ray-tracing.
- Calculate and add the rates due to each source, but do not apply them.
- Apply the combined rates.
- Iteration needed to make sources 'feel' other sources.
- Sources can be processed in parallel (MPI).



Cut through cosmological density field, 16 sources (code comparison project, Test 4).

# Photo-Ionization Gas Dynamics

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

Continuity  
Equation

$$\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot (\rho \mathbf{v} \otimes \mathbf{v}) = -\nabla p$$

Momentum  
Equation

$$\frac{\partial e}{\partial t} + \nabla \cdot ((e + p) \mathbf{v}) = \mathcal{H} - \mathcal{C}$$

Energy  
Equation

A **multiscale** problem, in time and space

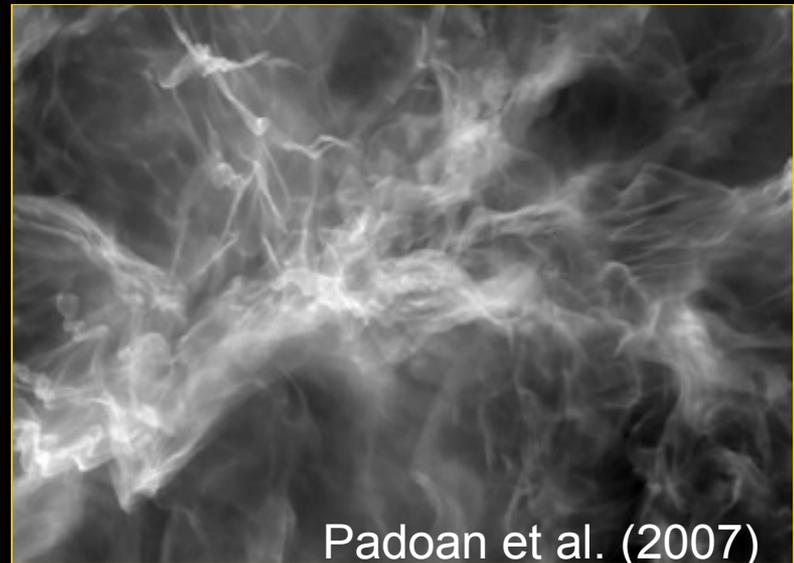
# Coupling to Hydrodynamics

- Coupling the photo-ionization radiative transfer and chemistry to hydrodynamics involves two points of contact:
  - **Advection** of the ionized fractions
  - Applying radiative **heating and cooling** rates to the thermal energy.
- Currently the 'chemistry' model is still very simplified: only H ionization fractions, H photo-heating, and H + approximate metal ion cooling. Working on: He, molecular cooling.
- C<sup>2</sup>-Ray has been coupled to a range of (M)HD codes: Capreole3D, Yguazú-a, Phab, and partly to CubeP<sup>3</sup>M.

# Application 1: Growing HII Regions in Turbulent Molecular Clouds

# Turbulent Molecular Clouds

- Observations show that Molecular Clouds have turbulent structures, with **supersonic** velocities.
- How this turbulence is maintained is one of the open questions of star formation theory.
- Several groups have been pursuing numerical simulations of driven turbulence (e.g. Padoan, Klessen, Burkert, Vazquez-Semadeni), both with and without magnetic fields.
- These models seem to mimic real MC structures, as well as the **Initial Mass Function** for stars.
- What does an HII region look like when growing into this? (Mellema et al. 2006)



Padoan et al. (2007)



N90

# High Resolution ( $512^3$ ) Simulations

- Henney, Arthur, Mellema, Vazquez-Semadeni, Iliev (2009)
- Single source
- Coupled with hydrodynamics (Capreole3D).

Initial conditions (Vázquez-Semadeni et al. 2005):

- $\langle n_0 \rangle = 1000 \text{ cm}^{-3}$ ;  $T_0 \sim 5 \text{ K}$
- $M_{\text{rms}} = 10$
- $L = 4 \text{ pc}$ ;  $L_j = 4 \text{ pc}$
- 1 collapsing object

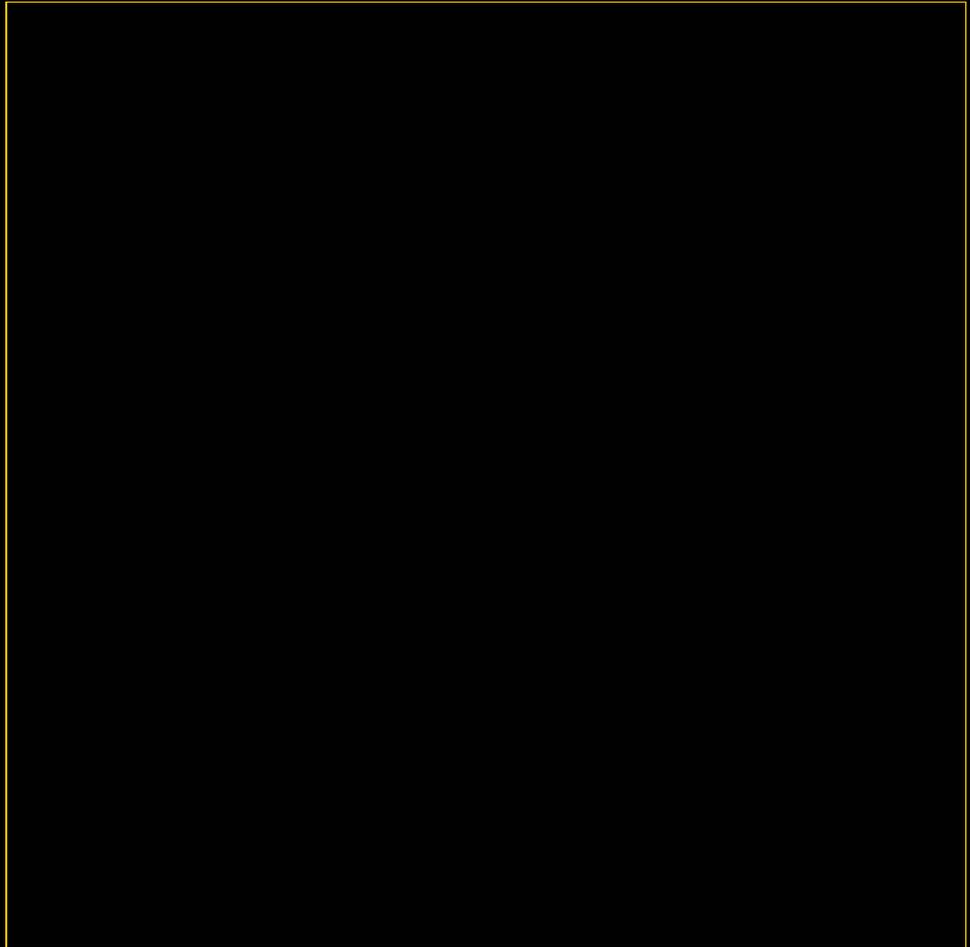
Ionizing source (O7.5,  $\sim 30 M_{\odot}$ ):

- $T_{\text{eff}} = 37000 \text{ K}$
- $Q_{\text{H}} = 10^{48.5} \text{ s}^{-1}$



# Evolution Movie

Soon at a Planetarium  
near you!  
(if you are in New York...)



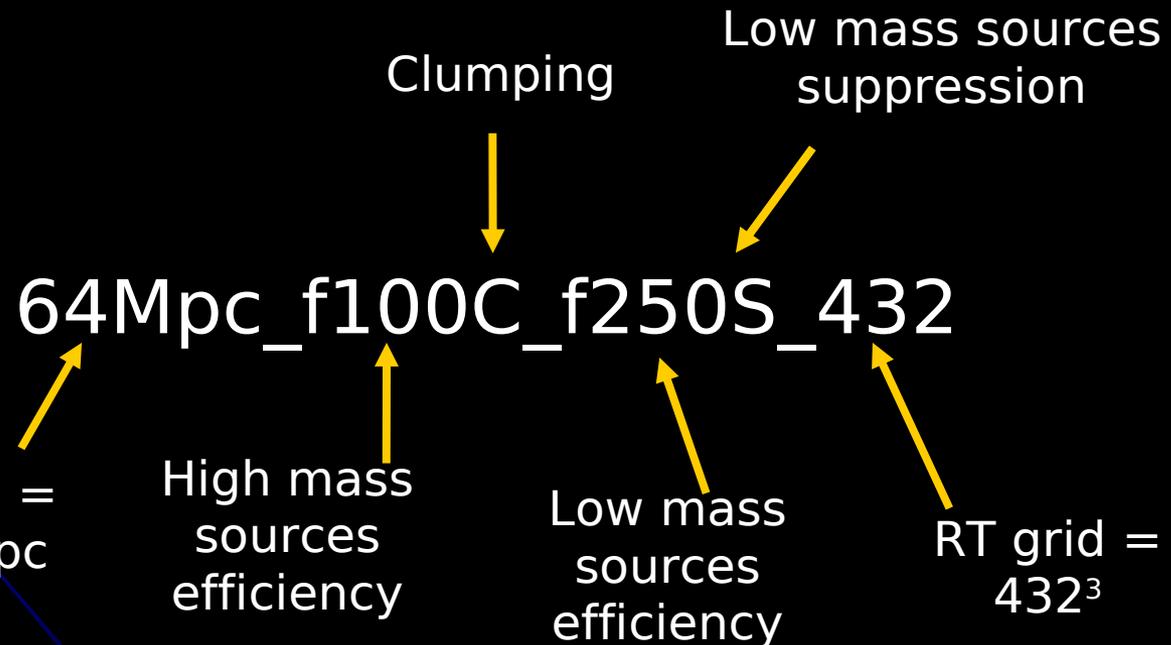
# Simulating Reionization

- The coming decade should bring us the first observations of the redshifted 21cm signal from reionization
- To better understand the properties of the signal we are studying it with **detailed large scale cosmological simulations**.
- Three steps:
  - Evolution of IGM density ( $\delta$ ) & (proto-)galaxies from a **cosmological simulation**.
  - **Assign EUV luminosity** to (proto-)galaxies.
  - **Transfer EUV radiation** through the IGM ( $x_{\text{HI}}$ ).
- For large scale simulations galaxy formation is unresolved and baryons and dark matter have the same distribution:
  - Cosmological N-body simulation (for DM).
  - Transfer of EUV radiation can be done in postprocessing mode.

# Application 2: Large Scale Simulations of Reionization

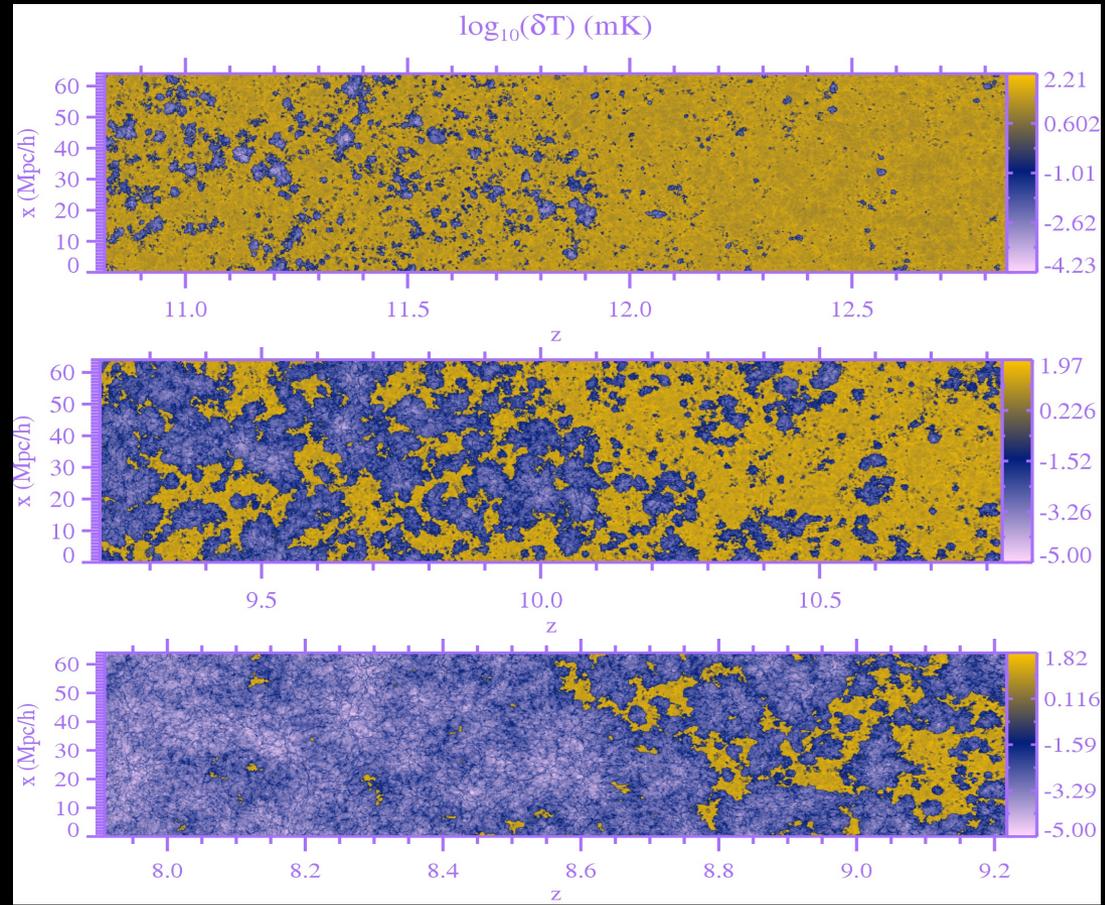
# Notation

- Our simulations are characterized by



# 21cm LOS Reionization History

- From the calculated evolution of the ionized densities we can construct **reionization histories** along the **line of sight**.
- Frequency/redshift direction contains **evolutionary**, **geometrical** and **velocity** information.
- Simulation shown: 64Mpc\_f100\_f250S\_432 (64/h Mpc,  $M_{\text{halo}} > 10^8 M_{\odot}$ ), with feedback on low mass sources.



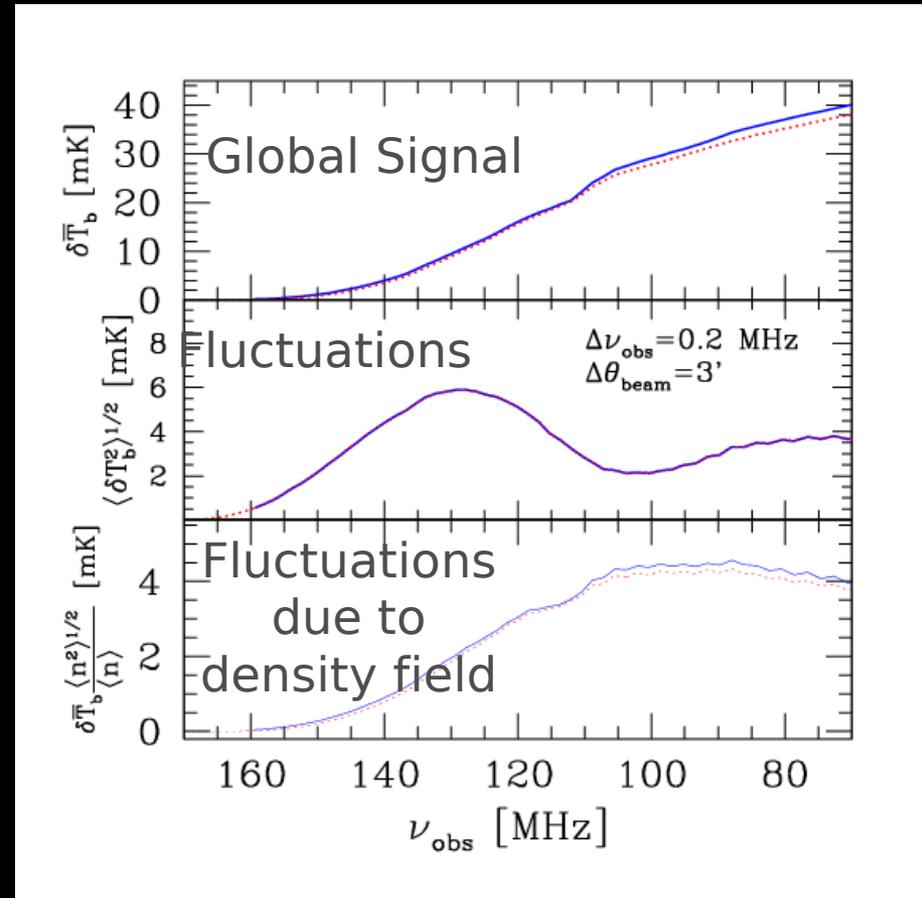
redshift

# Statistical Measurements

- The **sensitivity** of the upcoming EoR experiments will be **too low** to **image** 21cm from reionization pixel by pixel: Statistical measurements needed.
  - **First goal**: to reliably **detect** signatures from reionization (and separate them from foreground and instrumental effects).
  - **Second goal**: to **interpret** them in terms of astrophysics (source population and properties).
- Luckily, the 21cm line signal is rich in **properties**:
  - Global signals: mean signal, fluctuations.
  - Angular properties: power spectra
  - Frequency properties: Kaiser effect, correlation length.
  - Non-Gaussianity: skewness

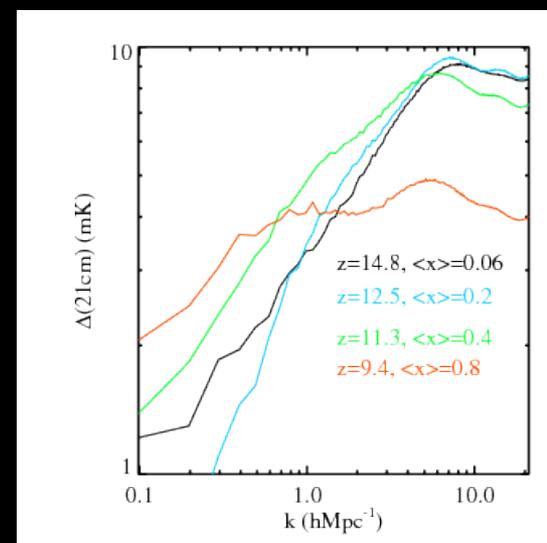
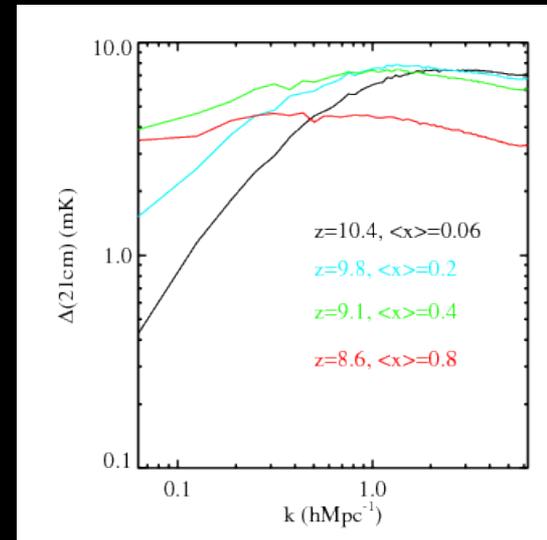
# Global Signals

- A **single dish telescope** could measure the change of the **global signal** with frequency: simulations do not show a sharp transition.
- The corresponding measurement by an **interferometer** would be the change of the 21cm (rms) **fluctuations**. Peak of these falls around 60-70% ionized.
- Simulations shown:  
64Mpc\_f100\_f250S\_432 and  
64Mpc\_f100\_f250S\_216



# Power Spectra

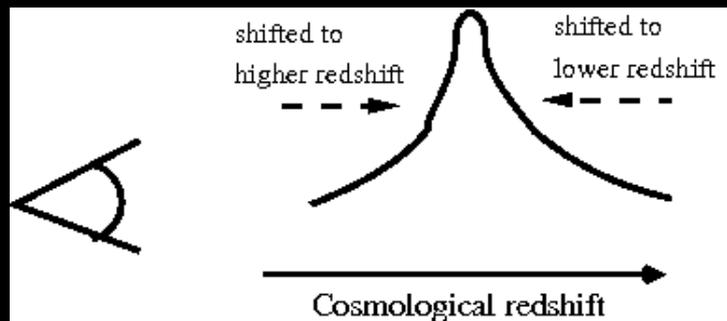
- Information about the **length scales** can be obtained from the power spectra.
- Simulations show clear trends of shifting power to larger scales as reionization progresses, and a **flattening** of the power spectra.
- Note that the angular power spectrum is measured directly by an interferometer, the multipole  $l$  is equivalent to  $\sqrt{u^2+v^2}$  in a visibility map.



100Mpc\_f250C\_f0\_203 64Mpc\_f100\_f250S\_432

# Velocity Distortions

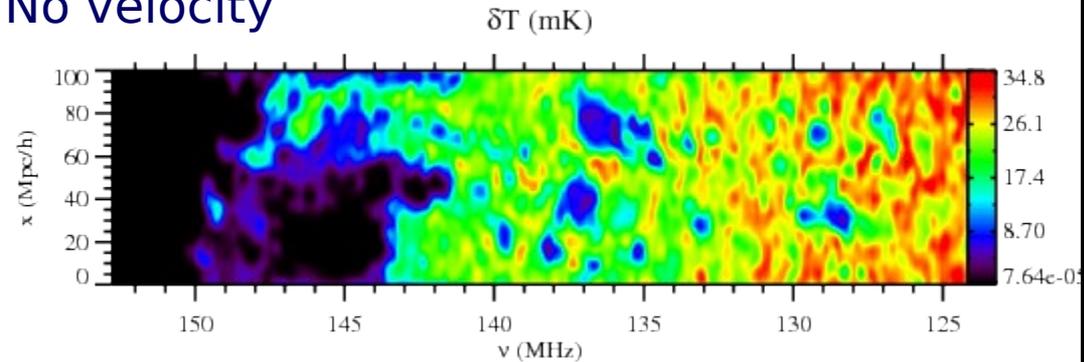
- Due to the peculiar velocity field, the signal can be displaced from its cosmological redshift.
- `Kaiser effect` or `velocity compression`: due to **infall**, signal concentrates at the high density peaks.
- This is clearly seen in the simulations and gives ~30% **increase in fluctuations** (and up to a factor of 2).
- This shows that fluctuations calculated from density and ionization fractions alone miss some power → better to use image cubes.



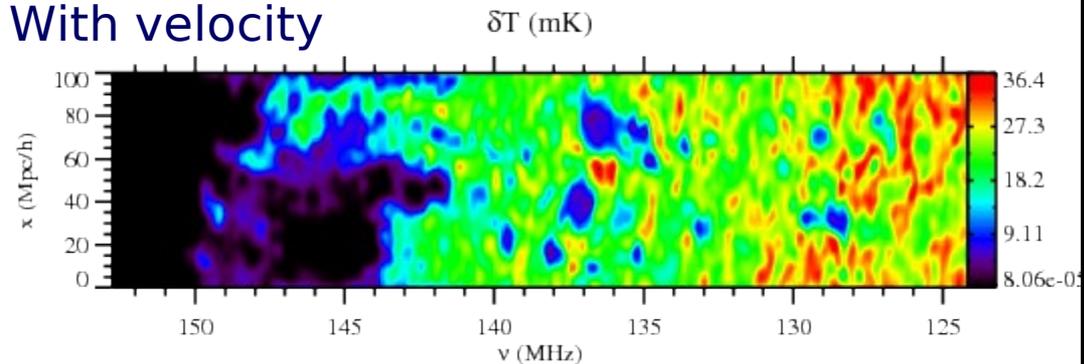
# Effect of the Velocity Field

- Adding the velocity distortions visibly **increases the fluctuations** in the neutral medium.
- Maximum value also larger.
- The effect remains noticeable even at LOFAR-like resolution (3', 200 kHz).
- Simulation shown: 100Mpc\_f250C\_f0\_203.

No velocity



With velocity



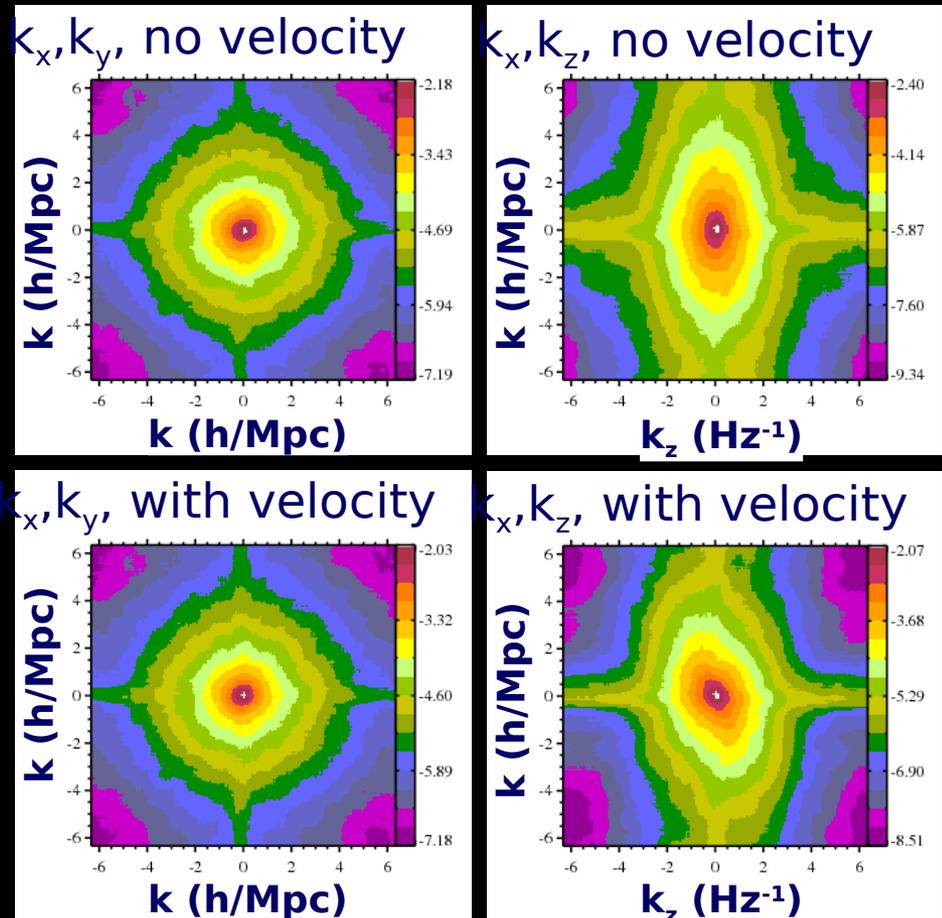
# And in Fourier Space...

- Since the velocity gradients responsible for the distortions are related to the density field, one can write the total (3D) power  $P(\mathbf{k})$  in terms of a polynomial in  $\mu = \cos(\theta_{\mathbf{k}})$ , the angle between the LOS and the  $\mathbf{k}$  vectors (see Barkana & Loeb 2005).
- $P(\mathbf{k}) = (P_{\delta\delta} - 2P_{x\delta} + P_{xx}) + 2(P_{\delta\delta} - P_{x\delta})\mu^2 + P_{\delta\delta}\mu^4$
- Since  $P_{\delta\delta}$  goes with  $\mu^4$ , it should be possible to separate it from the dependence on the ionized fraction  $x$ , and thus to directly find the **density power spectrum**.

# And in Fourier Space...

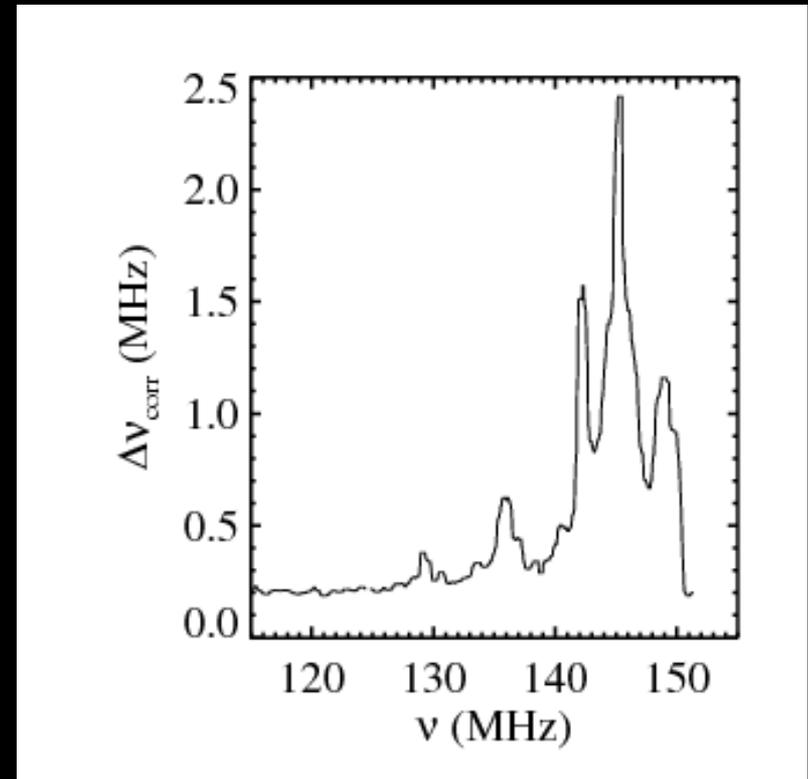
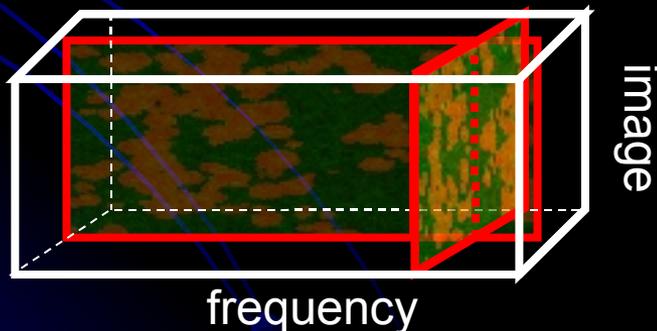
Spatial plane      Frequency-spatial plane

- **3D Fourier transform** of (part) of the **image cube** shows the effect of velocities.
- Without velocity distortions contours are spherical in the **spatial plane** and (here) elliptical in the **frequency-spatial plane** (due to transformation from spatial coordinate to frequency).
- With velocity distortions the 1<sup>st</sup> is still spherical, but the 2<sup>nd</sup> shows **tilted contours**.



# Correlation Length

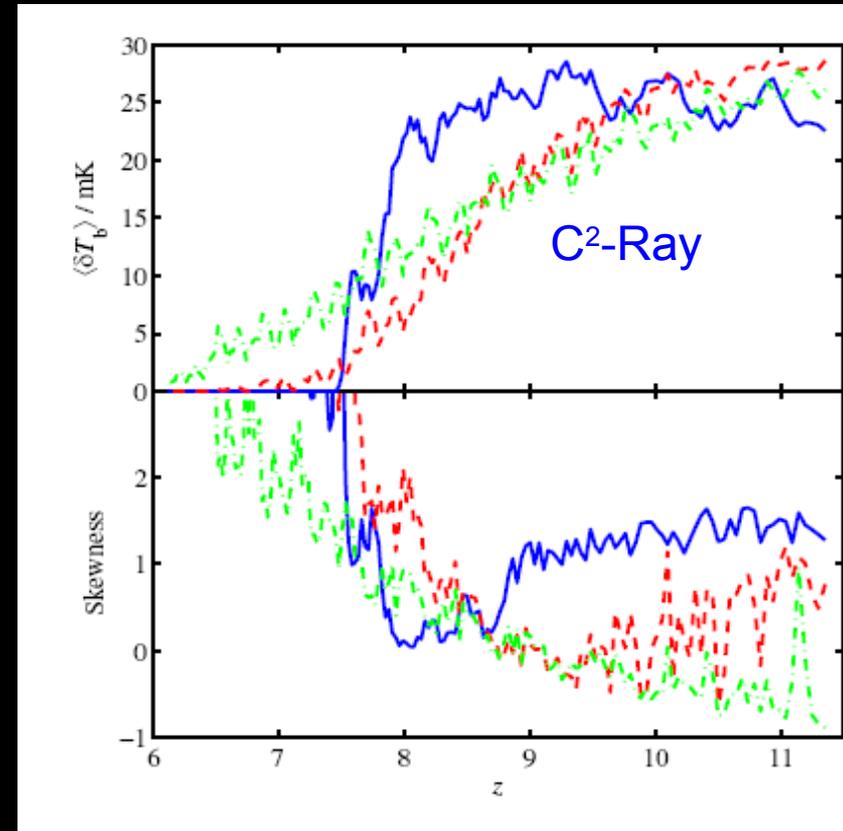
- Reionization changes the **correlation length along the frequency axis** in a characteristic way: formation of large HII regions increases correlation length from  $\sim 200$  kHz to  $\sim 1$  MHz.
- Still substantially shorter than for the continuum foregrounds, so this can be used as a test for proper **foreground subtraction**.



Simulation  
100Mpc\_f250C\_f0\_203

# Skewness

- The 21cm signal is strongly **non-Gaussian**.
- This suggests that measuring the **skewness** could be an interesting diagnostic.
- The simulations show a characteristic evolution of skewness with increasing ionization: constant  $\rightarrow$  decreasing  $\rightarrow$  increasing.
- Skewness may offer a good way to detect/confirm the signal, if remnants of foreground subtractions and other effects are dominantly Gaussian (cf. Harker et al. 2008).



# Conclusions

- The C<sup>2</sup>-Ray methodology (finite volume/time-averaged optical depth) allows for efficient calculation of photo-ionization inside or outside a hydrodynamic calculation
- HII regions growing in the density field of a turbulent molecular cloud resemble observed HII regions.
- The 21cm signal from reionization is characterized by a range of statistical properties which should help in (confirming) its detection.

