Lyman-alpha MCRT

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Background Material

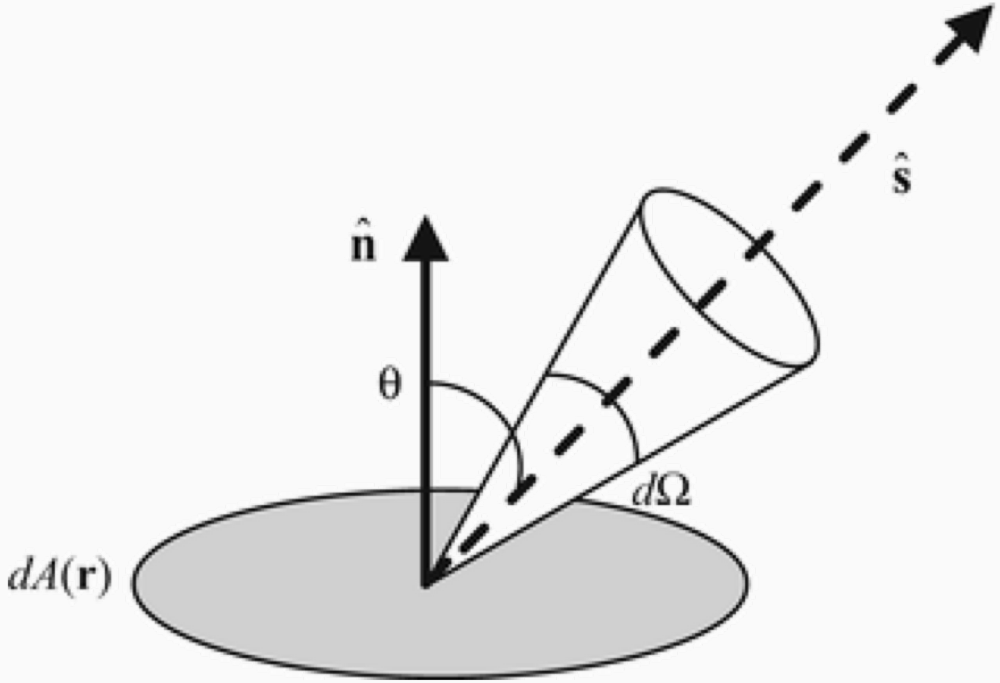
Review of radiative transfer concepts

- We describe radiation with equations in phase space.
- High dimensional problem: Position (3), momentum (3), frequency (1)
- But light travels at the same speed, so use direction and intensity.

$$I_\nu = \frac{\mathrm{d}E}{\mathrm{d}A\,\mathrm{d}t\,\mathrm{d}\Omega\,\mathrm{d}\nu}$$

$$[I_\nu] = \frac{\mathrm{erg}}{\mathrm{s\ cm^2\,arcsec^2\,Hz}}$$

$$f = \frac{\mathrm{d}N}{\mathrm{d}^3\mathbf{x}\,\mathrm{d}^3\mathbf{p}} = \frac{I_\nu}{h^4\nu^3/c^2}$$



RADIATIVE TRANFER EQUATION (RTE)

- Energy is conserved as a ray propagates in vacuum (collisionless):

$$I_\nu(t, \mathbf{x}) = I_\nu(t + \Delta t, \mathbf{x} + c\Delta t\hat{\mathbf{n}})$$

- Taylor expand in space and time to get a local transport equation:

$$\frac{\mathrm{d}I_\nu}{\mathrm{d}t} = \lim_{\Delta t \to 0} \frac{\Delta I_\nu}{\Delta t} = \ldots$$

$$\frac{1}{c}\frac{\partial I_\nu}{\partial t} + \hat{\mathbf{n}} \cdot \nabla I_\nu = (\text{sources}) - (\text{sinks})$$

- Absorption depends only on the traversed material optical depth:

$$\Delta I_\nu = -k_\nu \Delta \ell I_\nu$$

- Thus, pure absorption gives rise to Beer's law of attenuation:

$$\text{Transmitted radiant power} = \frac{I_\nu(\tau)}{I_\nu(0)} = e^{-\tau}$$

- The optical depth is the path-integrated absorption probability:

$$\tau = \int_0^\ell k(\ell')\mathrm{d}\ell' \qquad k = k(\mathbf{x}, \hat{\mathbf{n}}, t, \nu, \rho, T, \mathbf{v}, \ldots)$$

- The emissivity adds energy to beams independent of the intensity:

$$\Delta I_\nu = j_\nu \Delta\ell$$

- For example, in local thermal equilibrium (LTE) the intensity is equal to the blackbody distribution (steady-state solution).

$$I_\nu = B_\nu(T) = \frac{2h\nu^3}{c^2}\frac{1}{e^{h\nu/k_\mathrm{B}T} - 1}$$

- Therefore, balancing emission and absorption gives: $|\mathrm{d}T/\mathrm{d}\tau| \ll T$

$$\Delta I_{\nu,\mathrm{em}} + \Delta I_{\nu,\mathrm{abs}} = 0 \quad \Rightarrow \quad j_\nu = k_\nu B_\nu(T)$$

SCATTERING

- Scattering is absorption followed by re-emission.
- However, the direction and energy/frequency can change:

$$\iint \left(k_{\nu'} I_{\nu'} R_{\nu',\hat{\mathbf{n}}' \to \nu,\hat{\mathbf{n}}} - k_\nu I_\nu R_{\nu,\hat{\mathbf{n}} \to \nu',\hat{\mathbf{n}}'}\right) \mathrm{d}\Omega' \mathrm{d}\nu'$$

- If we assume isotropic elastic scattering then R ~ δ(v)/4π.

$$\frac{k_\nu}{4\pi} \int \left[I_\nu(\hat{\mathbf{n}}') - I_\nu(\hat{\mathbf{n}})\right] \mathrm{d}\Omega' = k_\nu (J_\nu - I_\nu)$$

- This is usually assumed, except when redistribution is needed.

- The general radiative transfer equation with source terms is:

$$\frac{1}{c}\frac{\partial I_\nu}{\partial t} + \hat{\mathbf{n}} \cdot \nabla I_\nu = j_\nu - k_\nu I_\nu$$

- If we assume LTE, isotropic elastic scattering, and grey opacity:

$$\frac{1}{c}\frac{\partial I}{\partial t} + \hat{\mathbf{n}} \cdot \nabla I = k_{\mathrm{a}}(B - I) + k_{\mathrm{s}}(J - I) + j_{\mathrm{ext}}$$

- The albedo defines purely scattering and absorbing components:

$$A = k_{\mathrm{s}}/(k_{\mathrm{s}} + k_{\mathrm{a}}) \qquad j_{\mathrm{ext}} = \text{external sources}$$

MONTE CARLO PHOTON PACKETS

- Radiation field is discretized by sampling photon packets with energy weight ε, position $\boldsymbol{r}$, direction $\boldsymbol{n}$, frequency ν, and time t.
- **Emission** can be calculated deterministically, e.g.

$$\Delta E_{\rm em} = c \Delta t V k_{\rm a} a_{\rm B} T^4 \qquad L_\alpha^{\rm rec} = h\nu_\alpha \int P_{\rm B}(T) \alpha_{\rm B}(T) n_e n_p {\rm d}V$$

- But then we have to draw random states (ε, $\boldsymbol{r}$, $\boldsymbol{n}$, ν, t).
- **Transport** is done stochastically too (exponential distribution).

$$P(\tau) \propto e^{-\tau} \quad \Rightarrow \quad \tau_{\bf scat} = -\ln \zeta \quad \text{where} \quad \zeta \in [0, 1]$$

- Move photon to the scattering location and change direction:

$$\Delta \mathbf{r} = \Delta \ell \hat{\mathbf{n}} \qquad \Delta t = c \Delta \ell \qquad \Delta \tau_{\bf scat} = -k_{\rm s} \Delta \ell$$

Lyman-α MCRT

Unique aspects of resonance lines

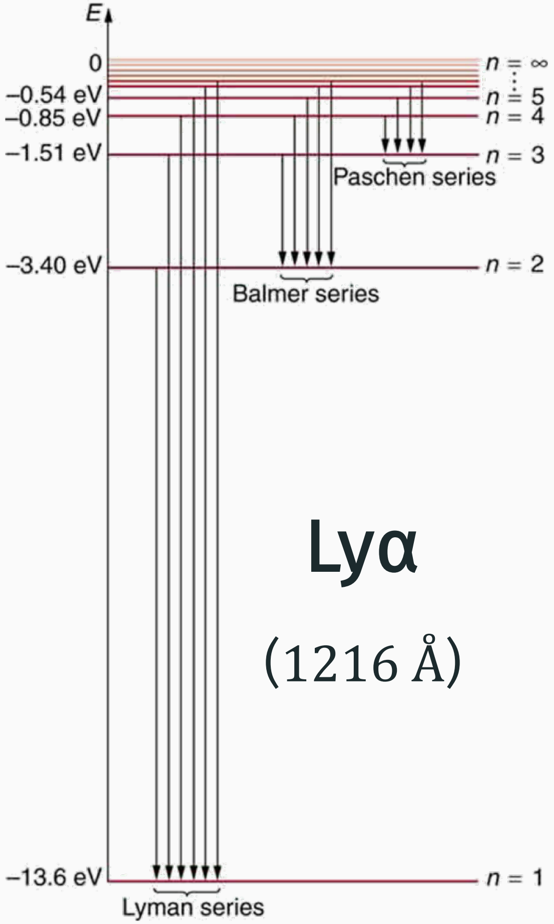
- Transform to dimensionless frequency and line profile.

$$x \equiv \frac{\nu - \nu_0}{\Delta\nu_{\rm D}} \qquad \Delta\nu_{\rm D} \equiv \frac{v_{\rm th}}{c}\nu_0$$

$$v_{\rm th} \equiv \sqrt{\frac{2k_{\rm B}T}{m_{\rm H}}} \qquad a \equiv \frac{\Delta\nu_{\rm L}}{2\Delta\nu_{\rm D}}$$

- Cross-section is given by the Hjerting–Voigt function:

$$H(a,x) = \frac{a}{\pi}\int_{-\infty}^{\infty}\frac{e^{-y^2}\,\mathrm{d}y}{a^2+(y-x)^2} \approx \begin{cases} e^{-x^2} & \text{‘core’} \\ a/\sqrt{\pi}x^2 & \text{‘wing’} \end{cases}$$



Lyα

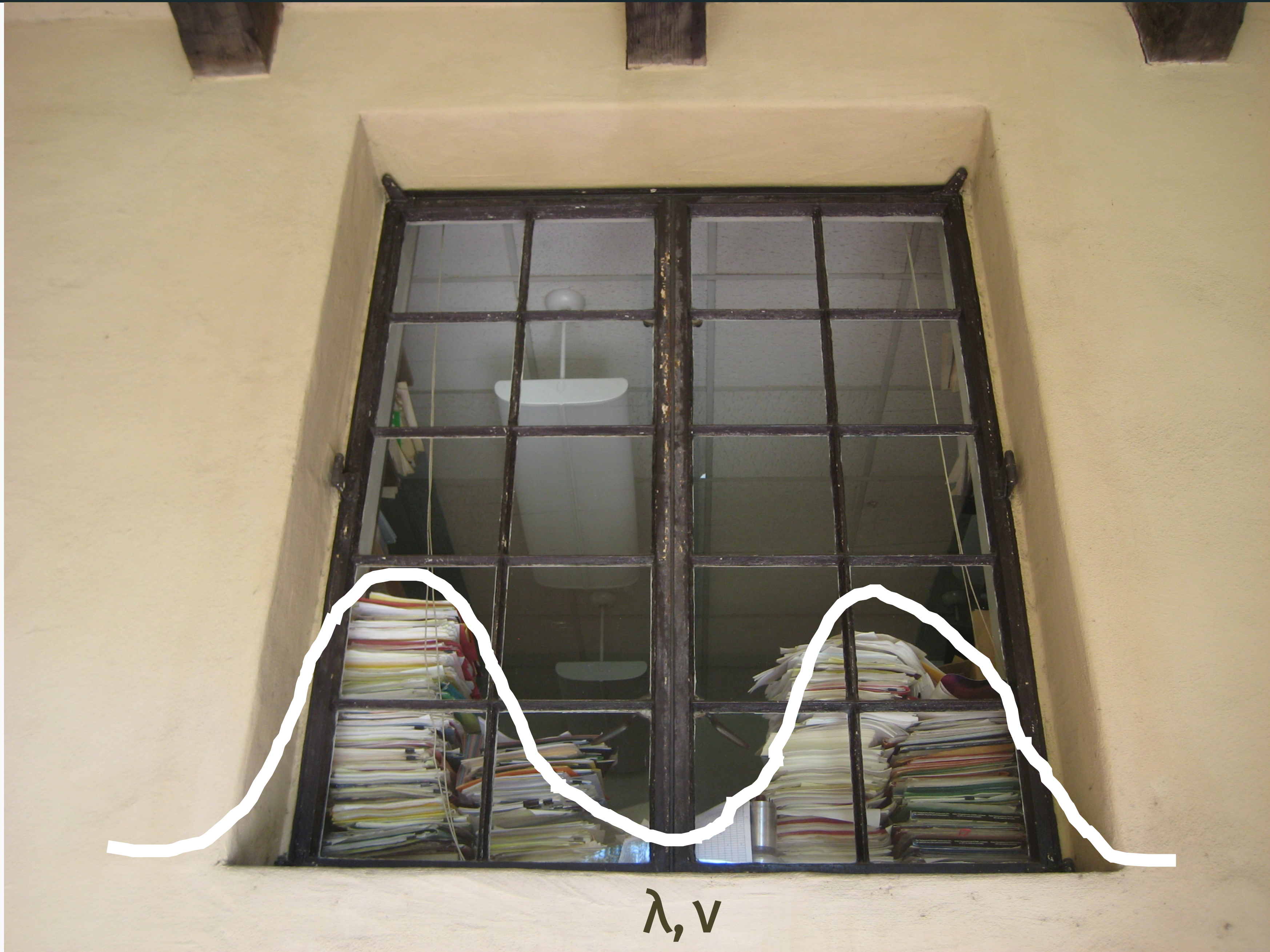
(1216 Å)

LYMAN-ALPHA PHOTONS UNDERGO RESONANT SCATTERING

Scattering Analogy:
Papers within reach cannot escape

Standard Picture:
Lyα photons escape in the wings ($\tau \ll 1$)
$\Rightarrow$ Double-peaked line profiles

Major Caveats:
Density & velocity gradients, dust, IGM transmission, 3D geometry, etc.



- Scattering is coherent in the rest frame of the atom (not the fluid!) with the parallel velocity component affected by the resonance line

$$\Delta x = \Delta \mathbf{n} \cdot \mathbf{u}_{\text{atom}} + g(\mu - 1)$$
$$= (u_{||} - g)(\mu - 1) + u_{\perp}\sqrt{1-\mu^2}$$

- Note: $\Delta \boldsymbol{n}$ = difference between outgoing and ingoing propagation directions, μ = directional cosine, $\boldsymbol{u}_{\text{atom}}$ = atom's velocity in Doppler units, and g = $h\Delta\nu_{\text{D}}/2k_{\text{B}}T$ is the recoil parameter. The second line is given for a special reference frame aligned with the atom's motion.

$$P(u_{||}) \propto \frac{\exp(u_{||}^2)}{a^2 + (x - u_{||})^2} \qquad P(u_{\perp}) \propto \exp(u_{\perp}^2)$$

CALCULATING THE NUMBER OF CORE AND WING SCATTERINGS

$$\langle \Delta x | x \rangle \approx -1/x$$

$$\sqrt{\langle \Delta x^2 | x \rangle} \approx 1$$

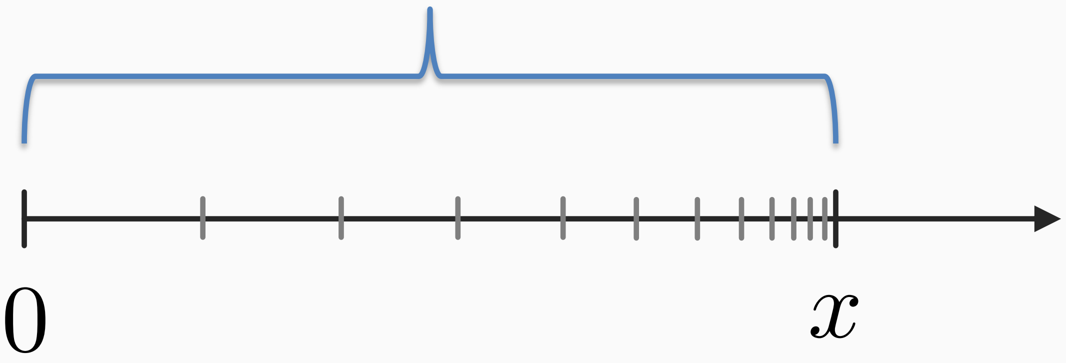
$$N_{\mathrm{scat,wing}} \approx x^2$$

$$N_{\mathrm{scat,wing}} \approx \tau^2$$

$$\tau(x) \approx \frac{a\tau_0}{\sqrt{\pi} x^2}$$

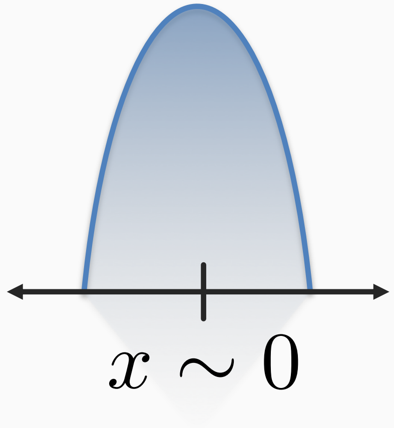
$$x_{\mathrm{esc}} \approx \left(\frac{a\tau_0}{\sqrt{\pi}} \right)^{1/3}$$

Returns to core after x^2 scatterings

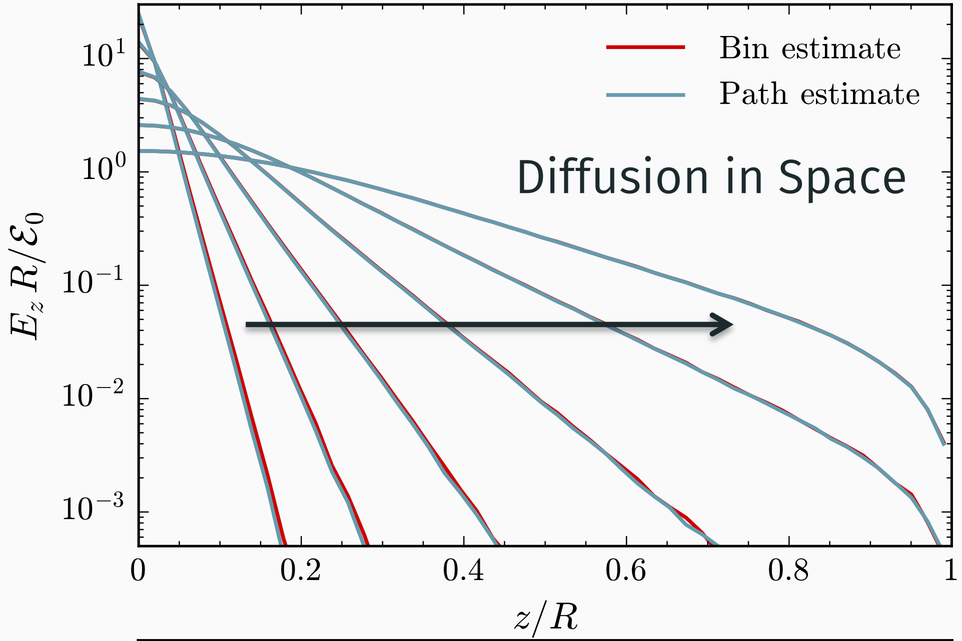


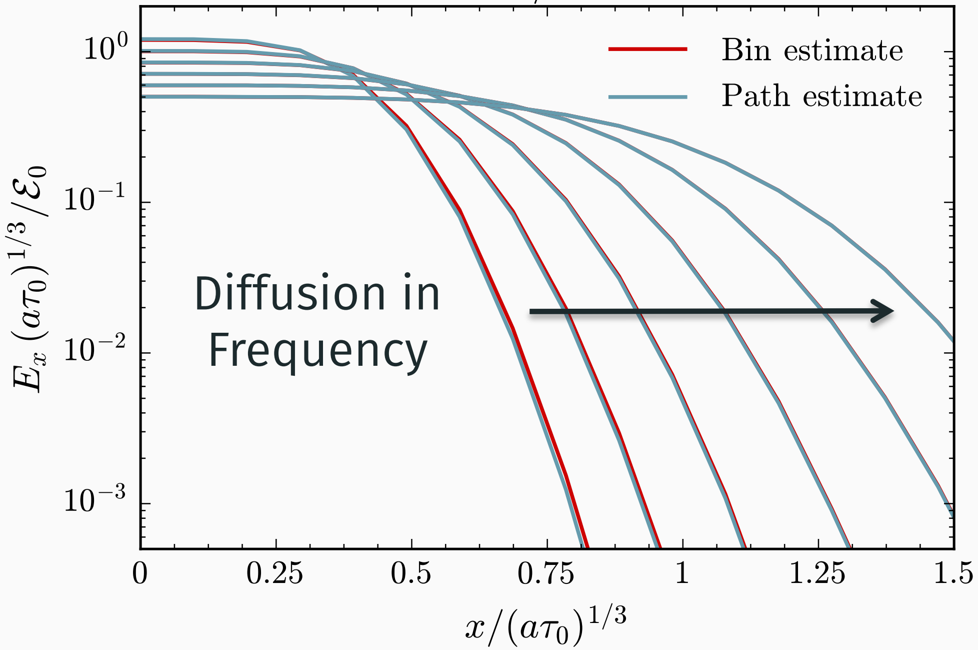
$$N_{\mathrm{scat,core}} \sim \tau_0$$

Extremely low probability of escaping the core (but $\lambda_{\mathrm{mfp}} \sim 0$)

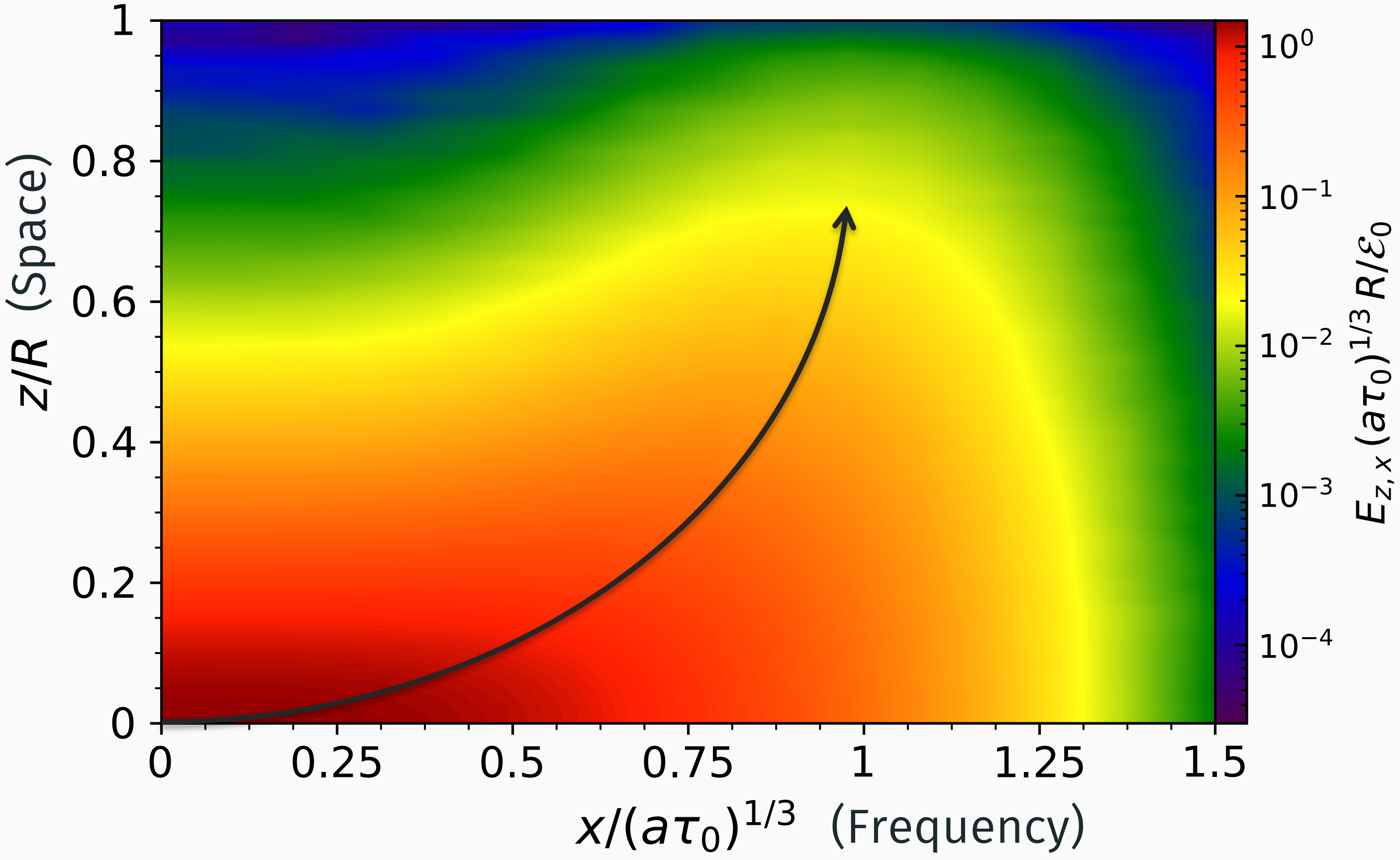


LYMAN-ALPHA ESCAPE AS A DOUBLE DIFFUSION PROCESS





Explicit time dependence of $E(z, x)$ shows the emergence of the double-peaked spectrum as photons diffuse in frequency and then space.



GALACTIC OUTFLOW MODELS

- Central source drives an outflow or “wind” & the Lyα line is redshifted.

- Spherical symmetry

  → 1D approx. for comp. feasibility & simplicity

- Reality:

  → 3D geometry

  → Multi-scale

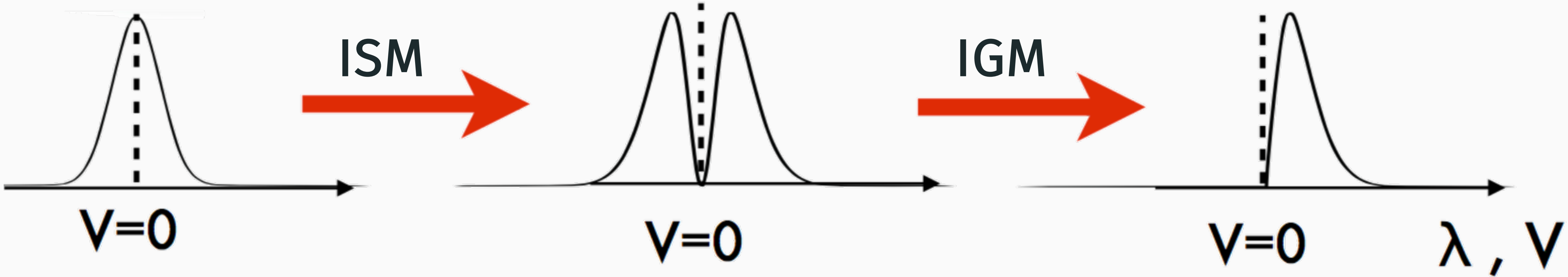
  → Multi-phase

  → Multi-physics

- A partially neutral IGM:

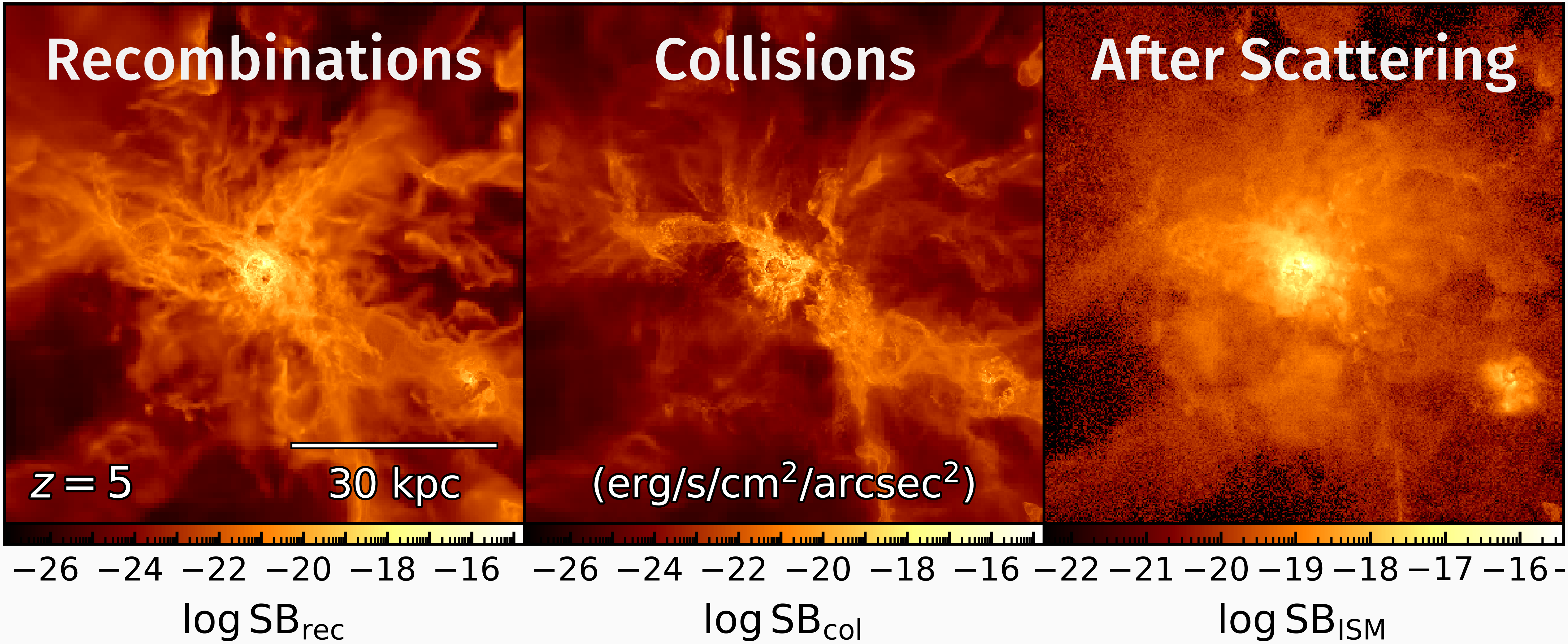
  → Reduces the visibility of LAEs

  → Boosts the clustering signal

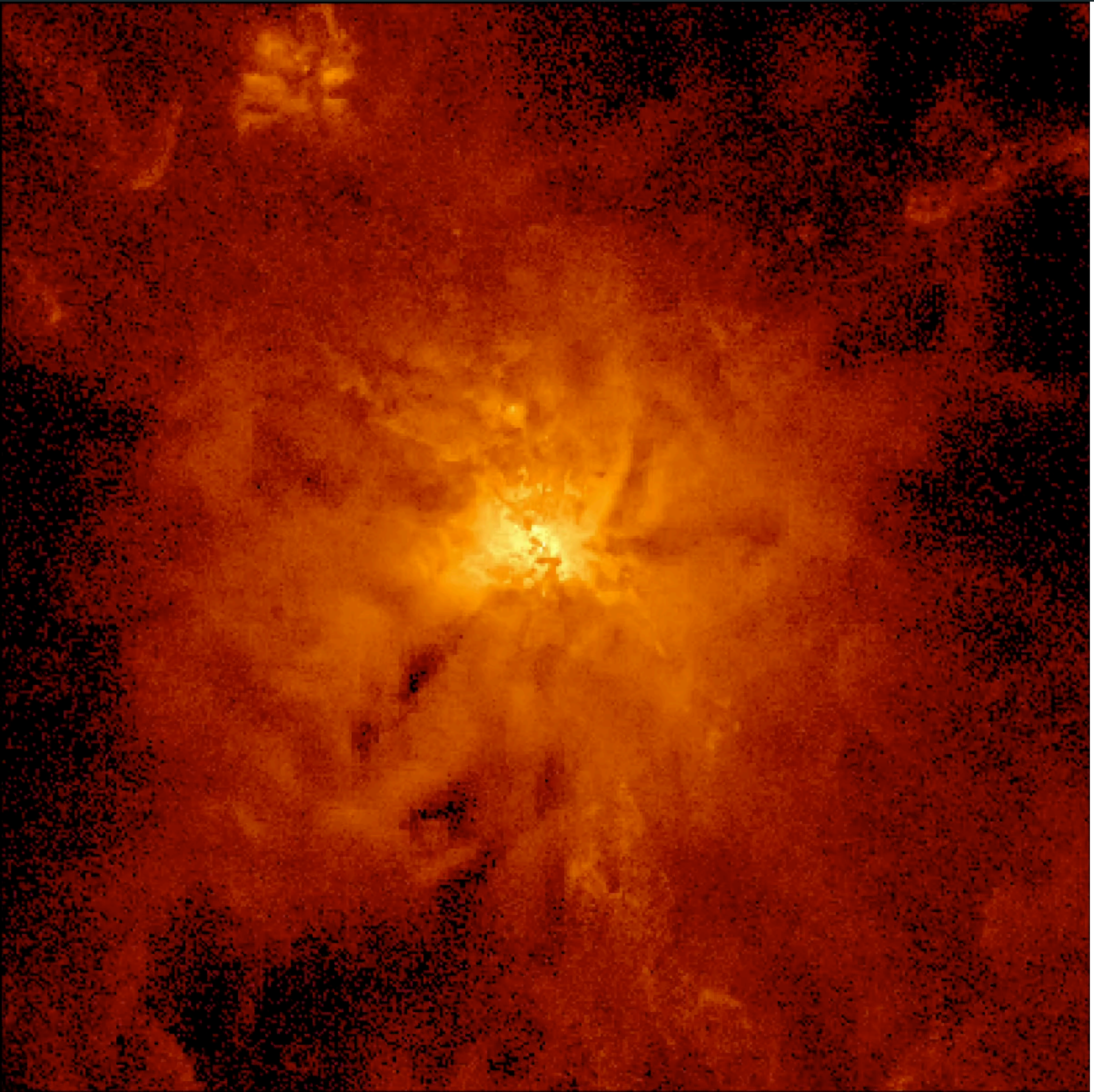


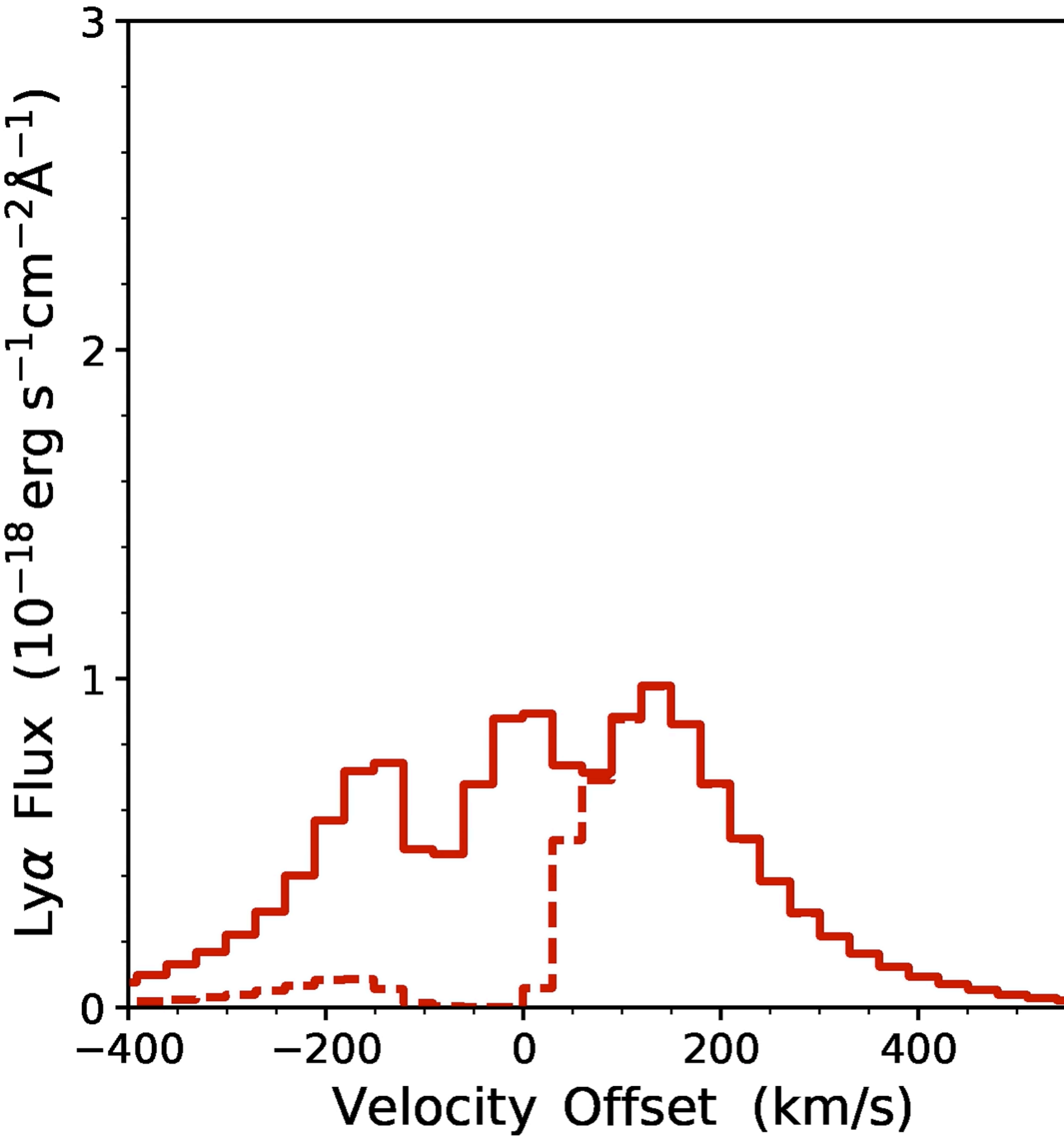
COSMOLOGICAL “ZOOM-IN” SIMULATION OF A REDSHIFT 5 GALAXY (GIZMO/FIRE, Ma et al. 2017)

Accurately model the ionizing radiation for the recombination/collisional emission.
Follow the resonant scattering in the ISM and transmission through the IGM.

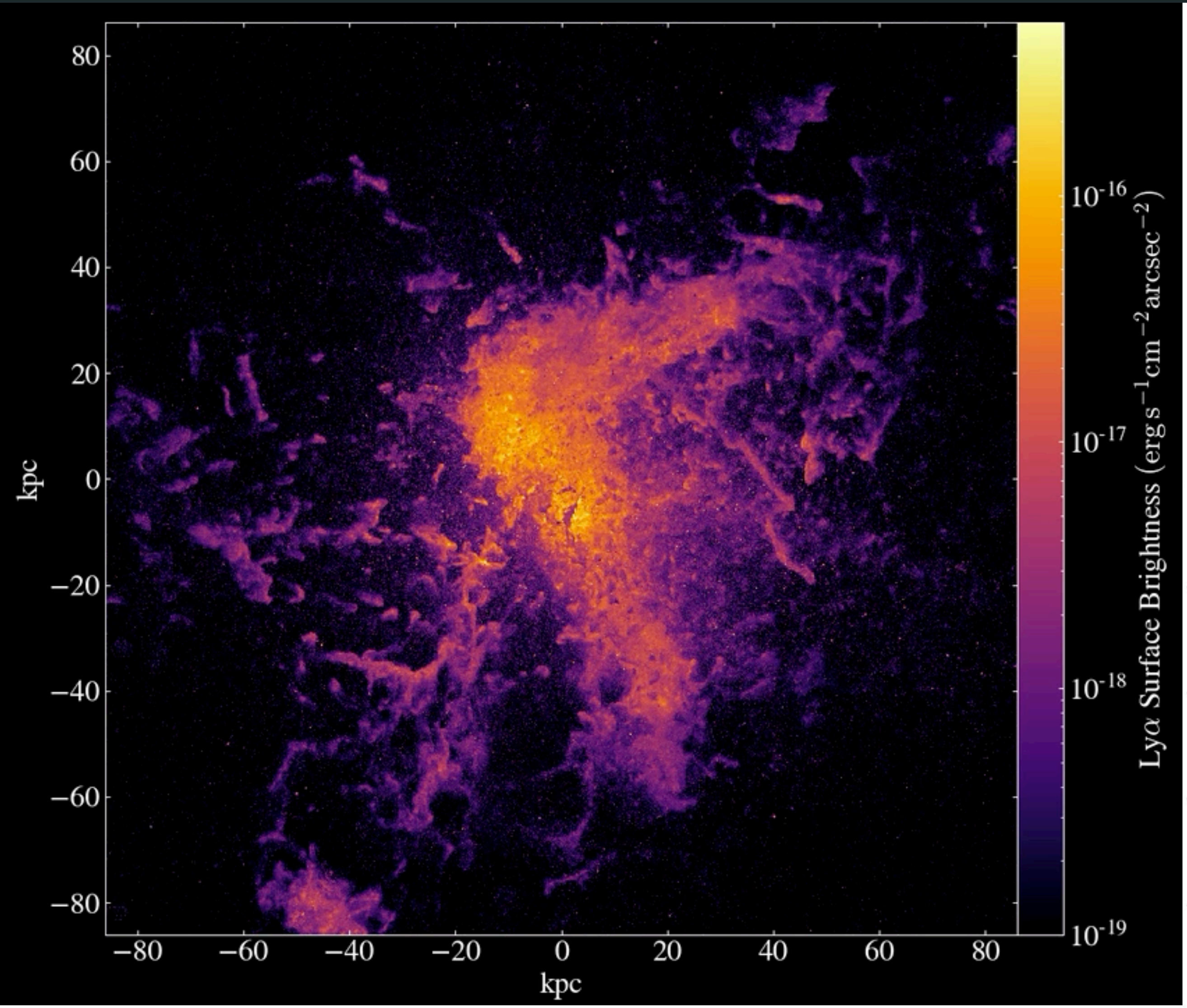


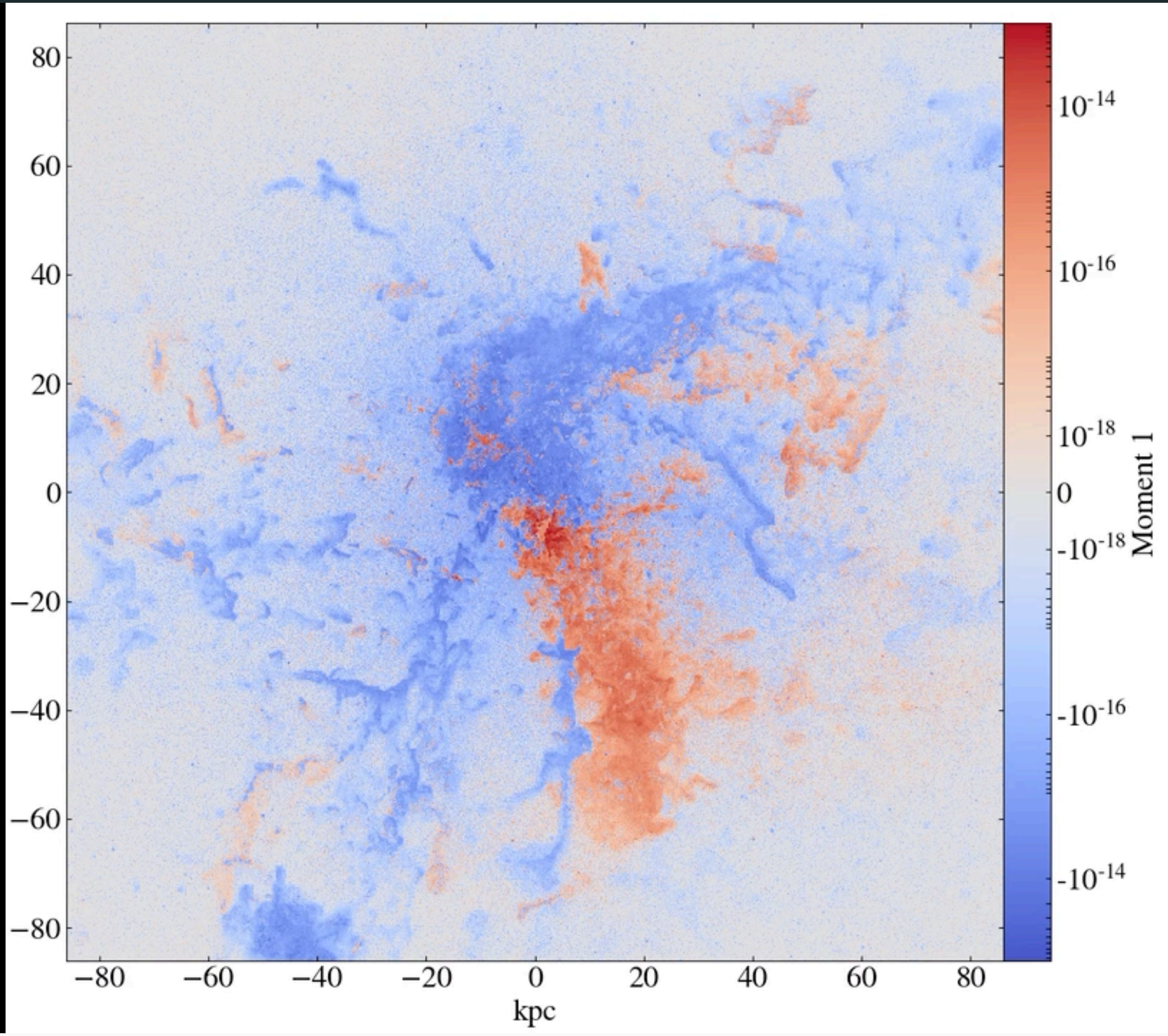
ROTATING CAMERA REVEALS NONTRIVIAL SIGHTLINE DEPENDENCE (CLOUDS, DOPPLER SHIFTS)





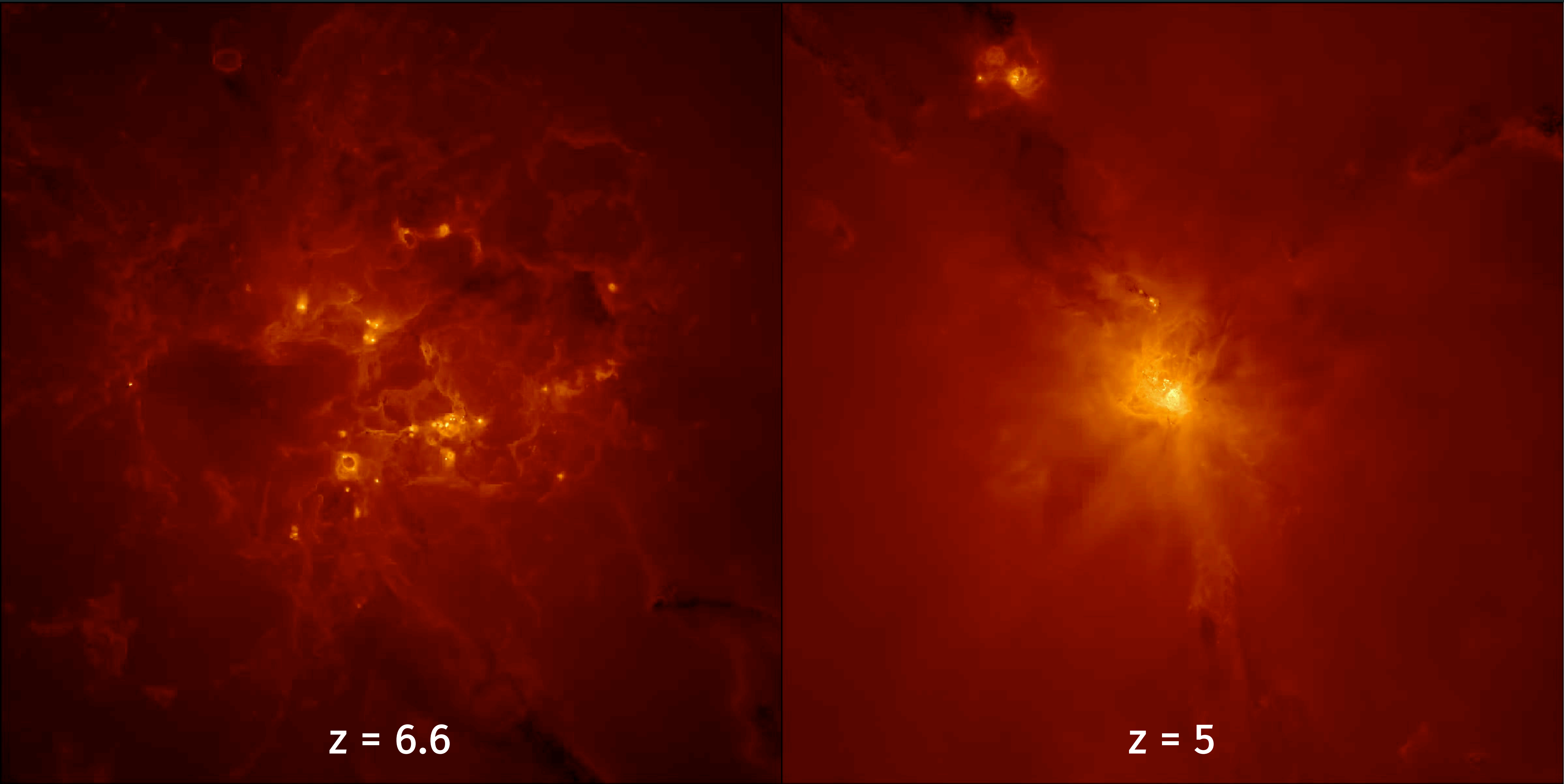
EXTENDED LYMAN-ALPHA HALOS (FREQUENCY MOMENT MAPS)



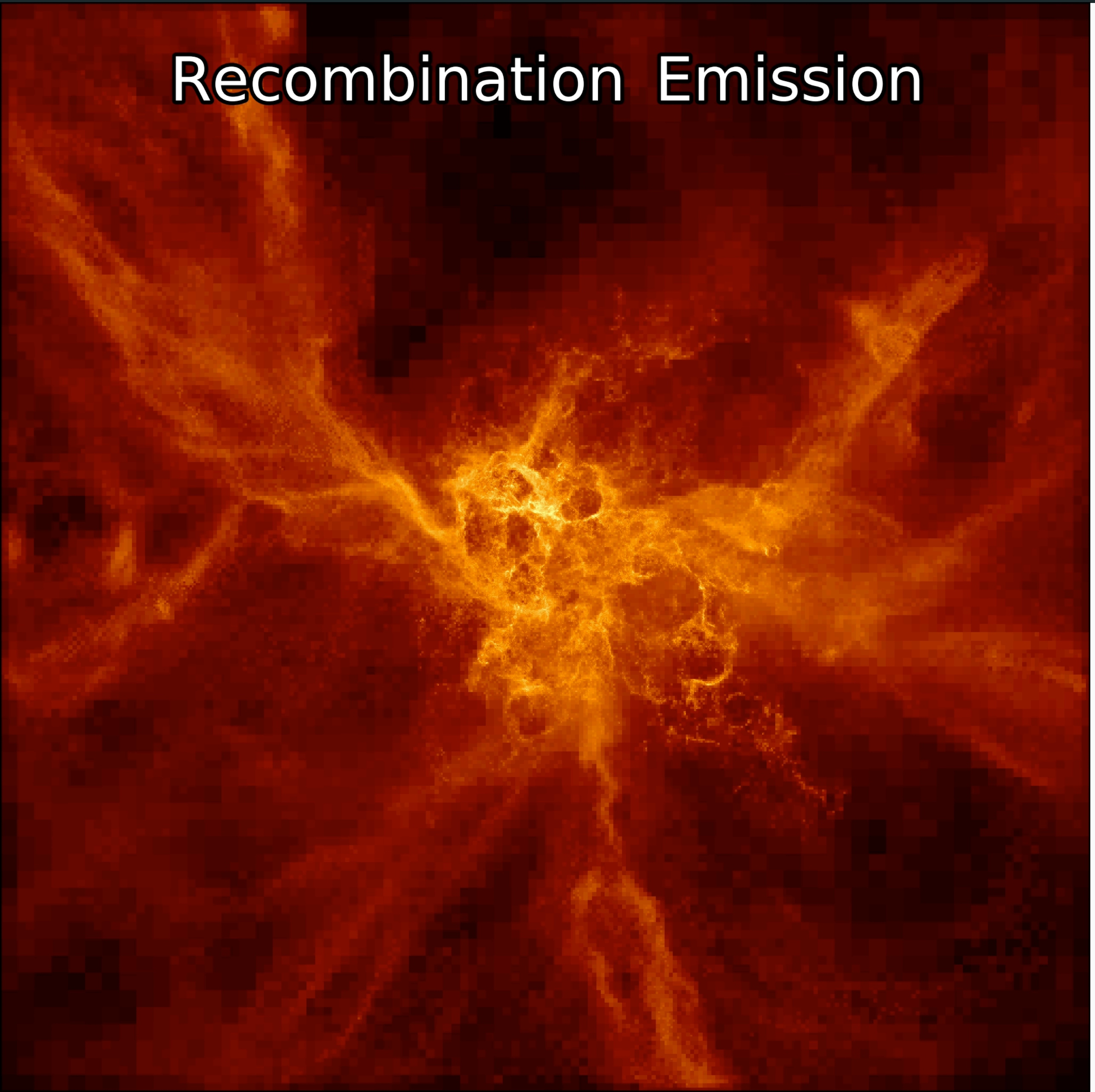


Lyman-alpha Blobs in Massive FIRE simulations. (Ben Kimock @ Univ. of Florida)

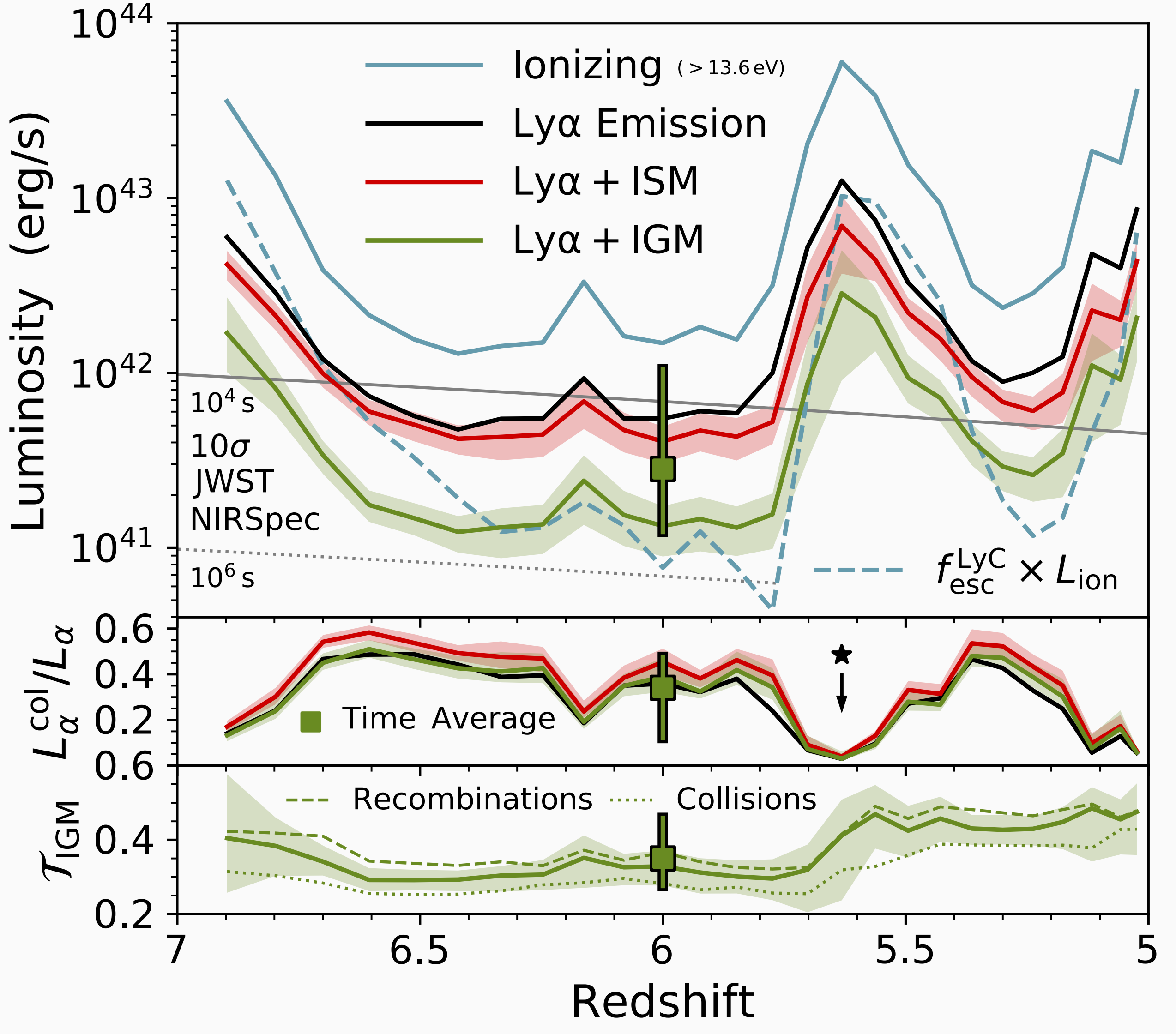
MORPHOLOGICAL DIFFERENCES IN THE LYMAN-ALPHA ENERGY DENSITY



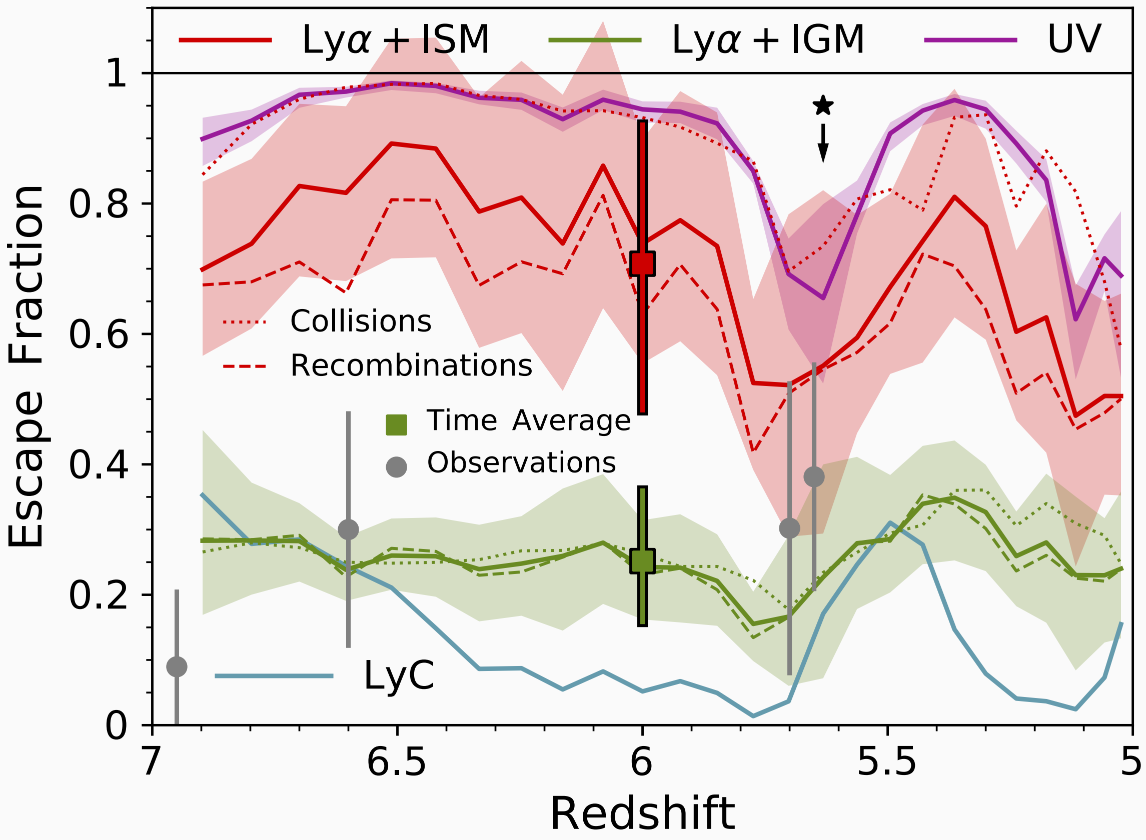
TIME-DEPENDENCE OF LYMAN-ALPHA PROPERTIES

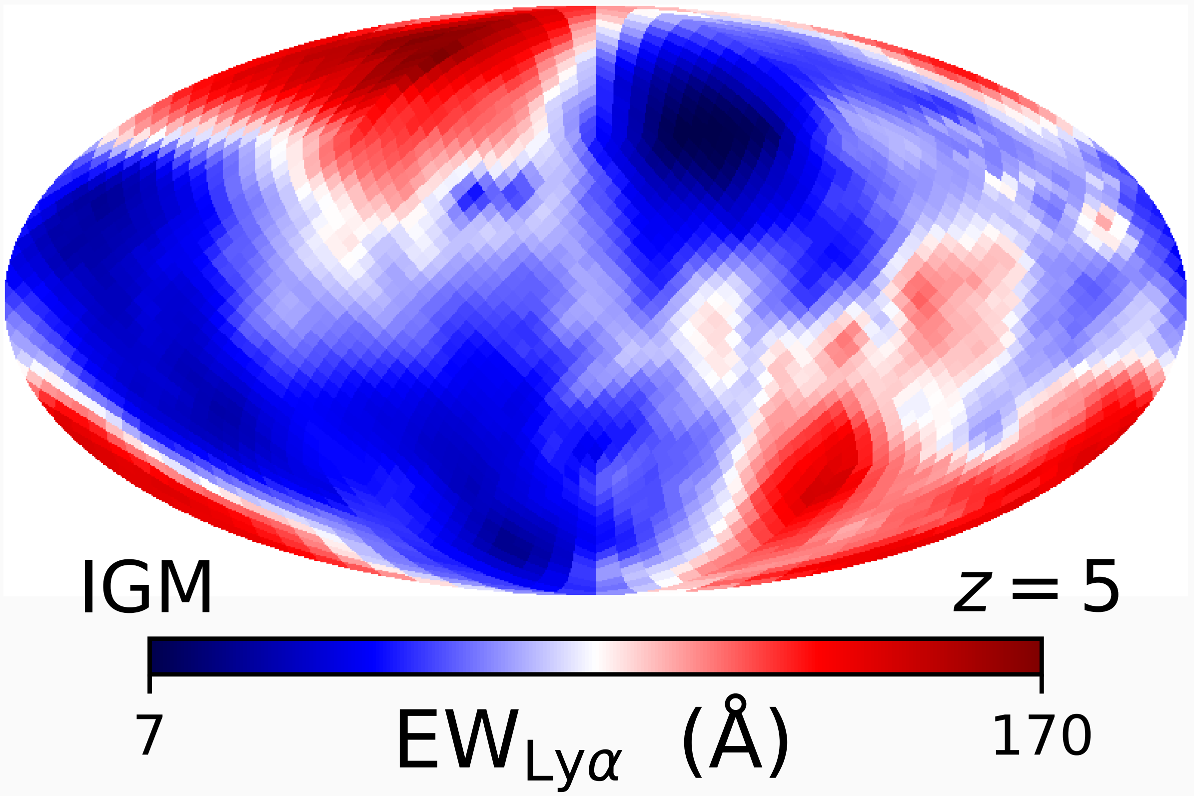


Properties fluctuate in response to the star formation activity.



OBSERVATIONAL PROPERTIES: ESCAPE FRACTIONS & EQUIVALENT WIDTHS





The Lyα escape fraction reacts to the star formation activity. Can be quite high lower mass galaxies with strong feedback.

High equivalent width ($F_{Ly\alpha}/f_{\lambda,UV}$) sightlines correspond to low density outflowing gas. This is a natural result of feedback processes.

Discrete Diffusion

What to do when scattering dominates

DISCRETE DIFFUSION MONTE CARLO (DDMC)

- We can discretize in space when the mean free path is unresolved.
- Apply Fick's law as a closure relation to the moment equation:

$$\mathbf{F} \approx -\frac{c\nabla E}{3k_\mathrm{s}} \qquad \Rightarrow \qquad \frac{1}{c}\frac{\partial J}{\partial t} = \nabla \cdot \left(\frac{\nabla J}{3k_\mathrm{s}}\right) \equiv \mathcal{L}J$$

- Finite volume codes approximate operators as volume-integrated:

$$\mathcal{L}J = \lim_{V\to 0}\frac{1}{V}\int \nabla \cdot \left(\frac{\nabla J}{3k_\mathrm{s}}\right)\mathrm{d}V = \lim_{V\to 0}\frac{1}{V}\oint \frac{\nabla J}{3k_\mathrm{s}} \cdot \mathrm{d}\mathbf{A}$$

- Discretization leads to a MCRT interpretation (conserved transport).

$$\mathcal{L}J_i = \sum_{\delta i}\frac{A_{\delta i}}{V_i}\frac{(J_{\delta i} - J_i)}{3\Delta\tau_{\mathrm{s},\delta i}} \equiv \sum_{\delta i} k_\mathrm{leak}^{\delta i}(J_{\delta i} - J_i)$$

Lyα LOCALIZED TRANSFER EQUATION

$$\frac{1}{c}\frac{\partial I_\nu}{\partial t} + \mathbf{n}\cdot\nabla I_\nu = j_\nu - k_\nu I_\nu + \iint k_{\nu'} I_{\nu'} R_{\nu',\mathbf{n}'\to\nu,\mathbf{n}} \mathrm{d}\Omega' \mathrm{d}\nu'$$

Angle average ⇒ Zeroth order moment equation

$$\frac{1}{c}\frac{\partial J_x}{\partial t} + \nabla\cdot\mathbf{H}_x = -k_x J_x + \int k_{x'} J_{x'} R_{x'\to x} \mathrm{d}x'$$

Diffusion approximation for space and frequency

$$\mathbf{H}_x = -\frac{\nabla J_x}{3k_x} \quad \& \quad \int k_{x'} J_{x'} R_{x'\to x} \mathrm{d}x' \approx k_x J_x + \frac{\partial}{\partial x}\left(\frac{k_x}{2}\frac{\partial J_x}{\partial x}\right)$$

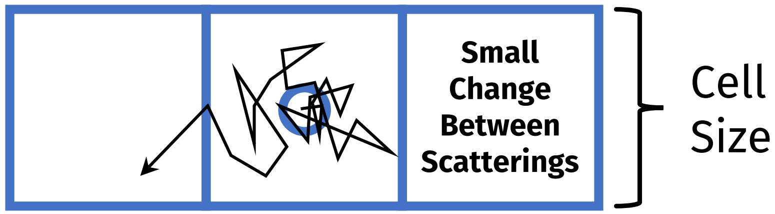
Put it all together for a Fokker-Planck equation

$$\frac{1}{c}\frac{\partial J_x}{\partial t} = \nabla\cdot\left(\frac{\nabla J_x}{3k_x}\right) + \frac{\partial}{\partial x}\left(\frac{k_x}{2}\frac{\partial J_x}{\partial x}\right)$$

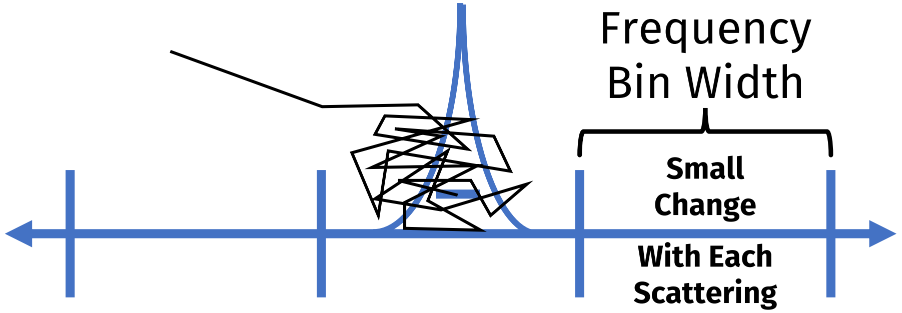
BREAKING THE EFFICIENCY BARRIER OF Lyα MCRT

Double Diffusion

$$\frac{1}{c}\frac{\partial J_{i,j}}{\partial t} = \sum_{\delta i} k^{\delta i}_{z\text{-leak}}\left(J_{\delta i,j} - J_{i,j}\right) + \sum_{\delta j} k^{\delta j}_{x\text{-leak}}\left(J_{i,\delta j} - J_{i,j}\right)$$



Unresolved Spatial Diffusion → **Condition:** $\ell_{\mathrm{mfp}} \ll \Delta z$ → **Runtime:** $\propto (\Delta z)^{-2}$

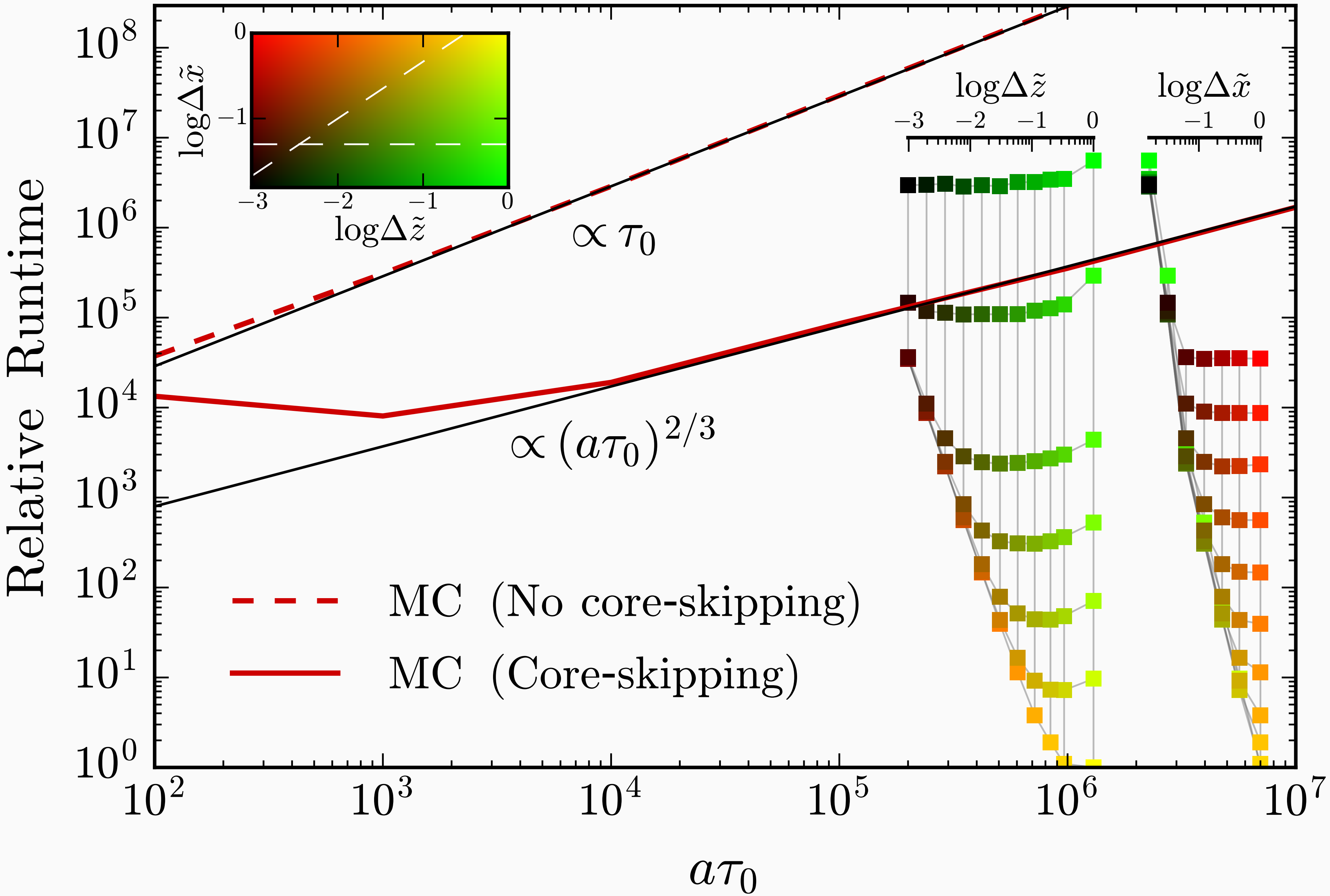


Unresolved Frequency Diffusion → **Condition:** $\Delta x \gg 1$ → **Runtime:** $\propto (\Delta x)^{-3}$

Frequency Redistribution

Spatial Transport		Continuous	Discrete
	Continuous	Optically Thin Core Photons	Optically Thin Wing Photons
	Discrete	Optically Thick Core Photons	Optically Thick Wing Photons

Lyα RESONANT DDMC – COMPARISON WITH TRADITIONAL MONTE CARLO

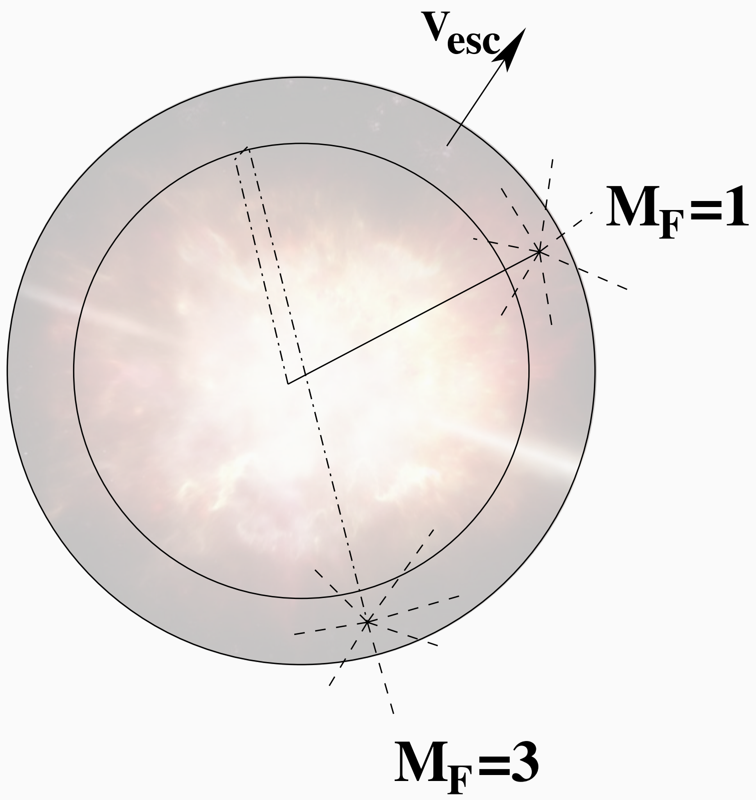


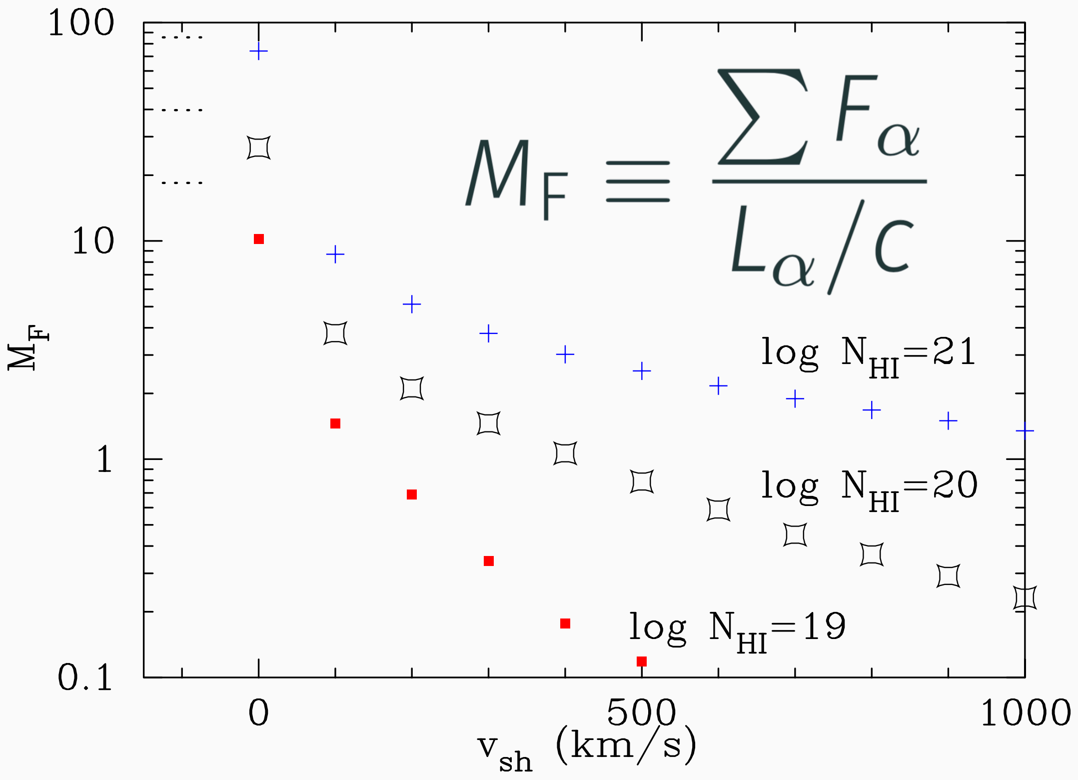
Lyα Radiation Pressure

Coupling to the hydrodynamics

Lyα RESONANT SCATTERING ACTS AS A FORCE MULTIPLIER

Example: Lyα trapping in the expanding shell model based on MCRT calculations (Dijkstra & Loeb 2008,2009).

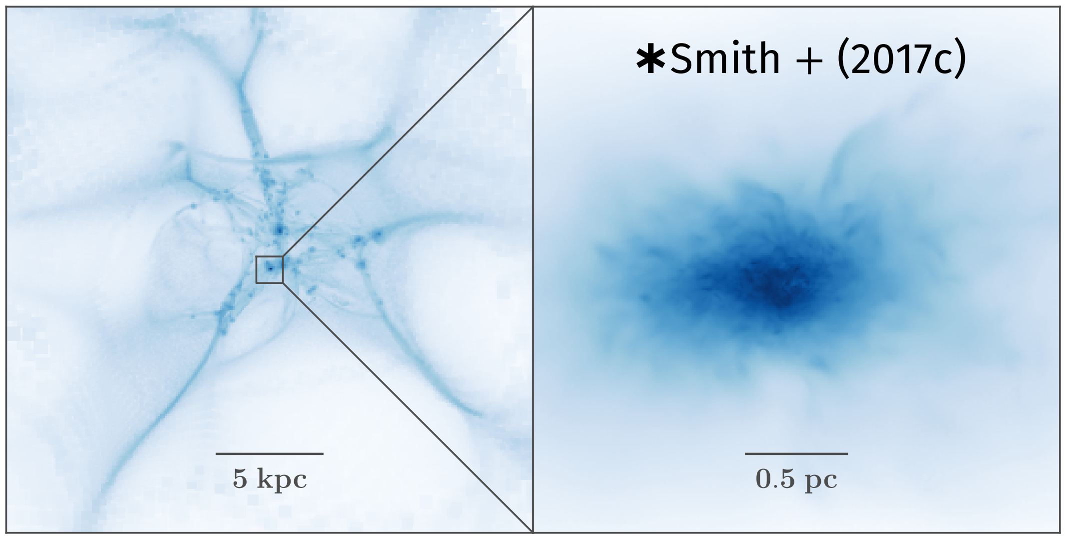


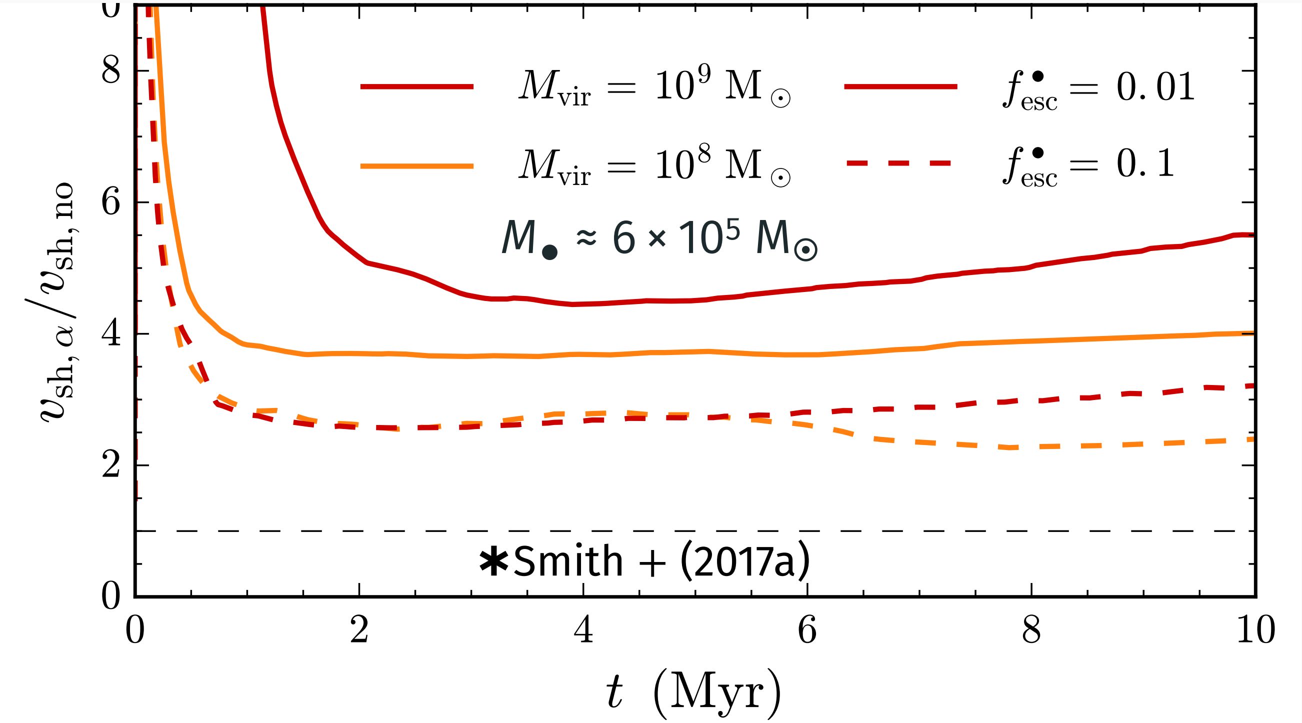


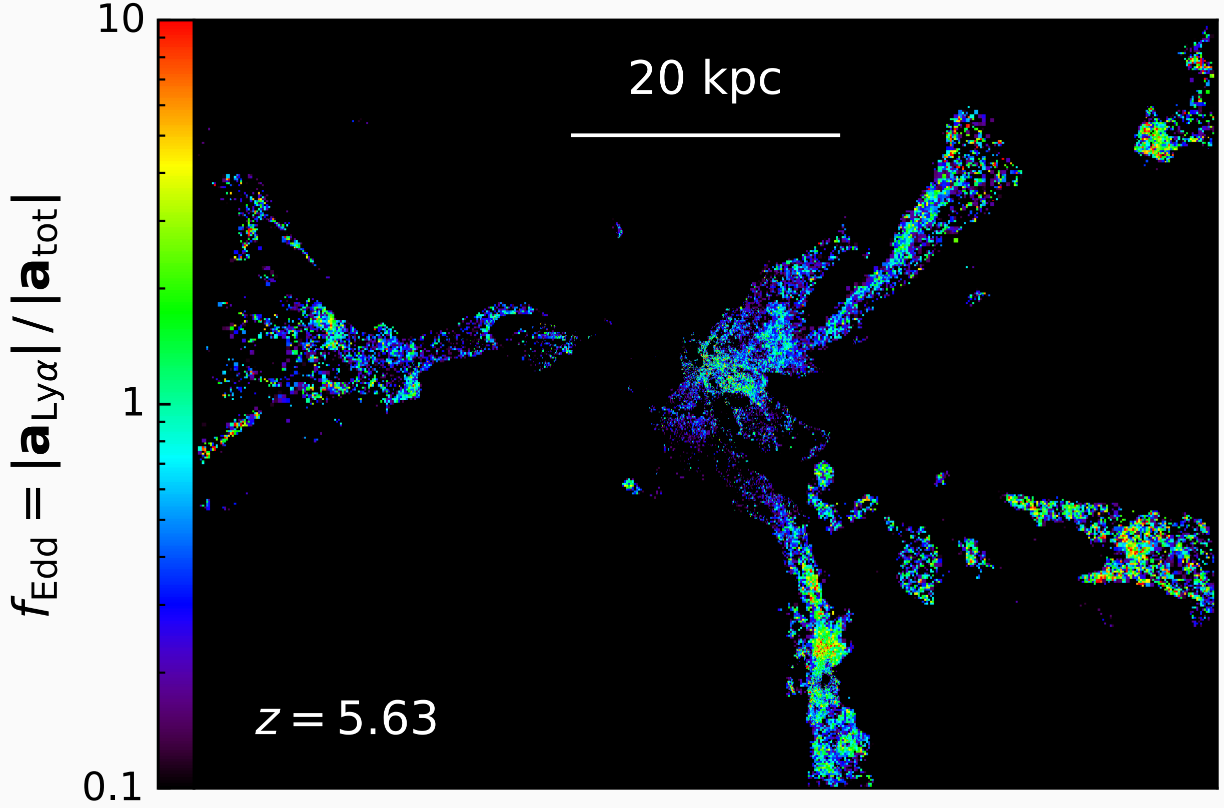
- Other works use order of magnitude estimates based on idealized Lyα RT:
  Cox (1985), Bithell (1990), Haehnelt (1995), Henney & Arthur (1998), Oh & Haiman (2002), McKee & Tan (2008), Milosavljević et al. (2009), Wise et al. (2012)

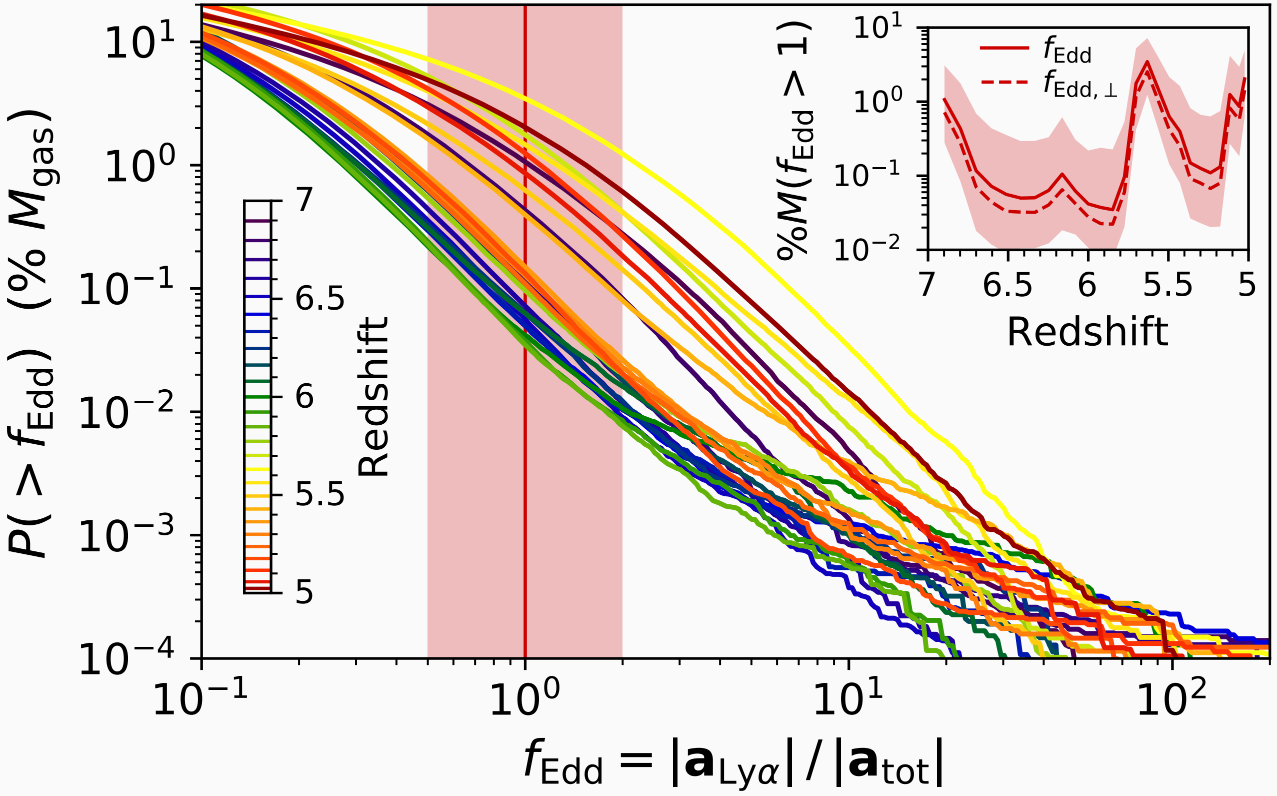
Lyα RADIATION PRESSURE CAN BE DYNAMICALLY IMPORTANT

- 1D radiation hydrodynamics simulations with Lyα pressure
- Radiation-driven winds can be accelerated by Lyα trapping
- 3D post-processing analysis of a Direct Collapse Black Hole
- Thermal and chemical feedback can be important too.
  (Ge & Wise 2017, Johnson & Dijkstra 2016)



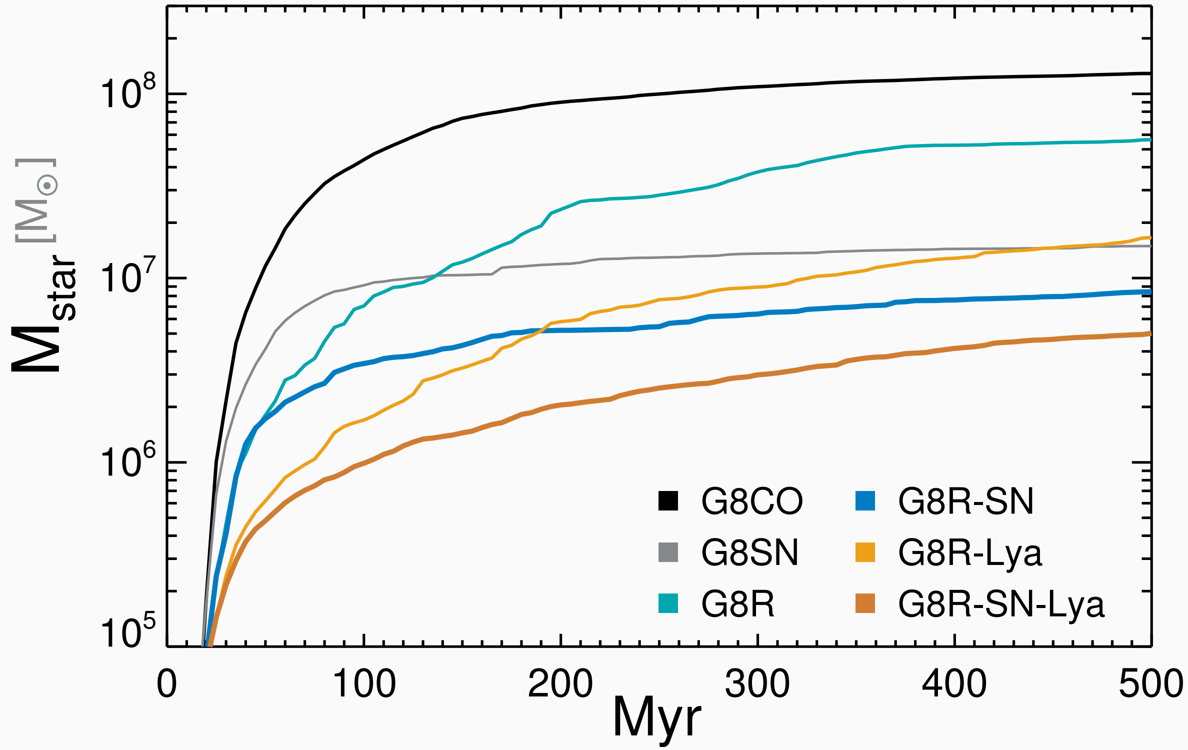


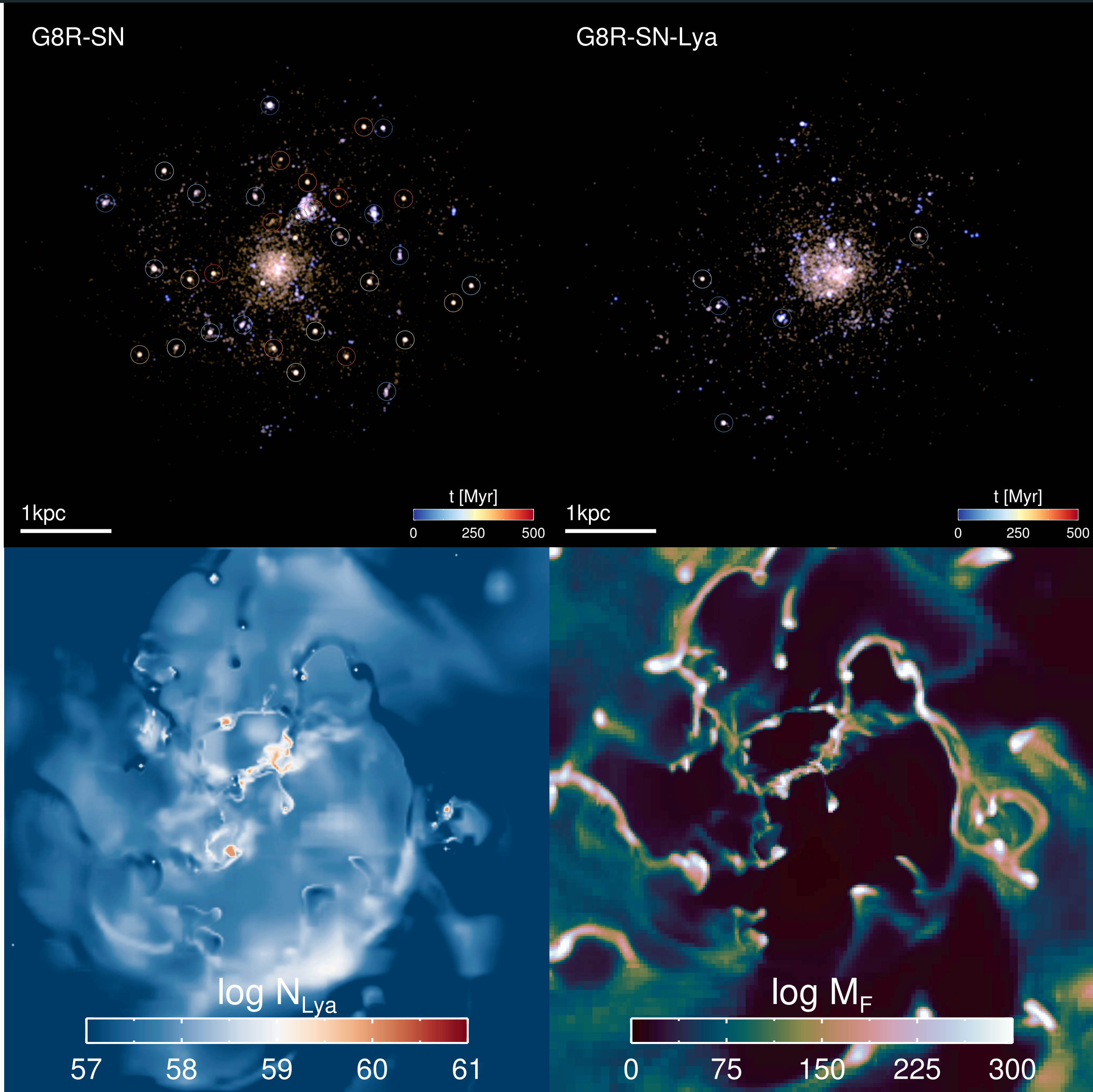




- Lyα pressure is likely to play only a minor role in the overall galactic dynamics.
- However, we find high Eddington factors in the neutral, low-metallicity filaments.
- $M_{\mathrm{gas}}(>f_{\mathrm{Edd}})$ fluctuates with redshift in the range of 0.01–10% of the total gas mass.

IMACT OF Lyα PRESSURE ON METAL-POOR DWARF GALAXIES



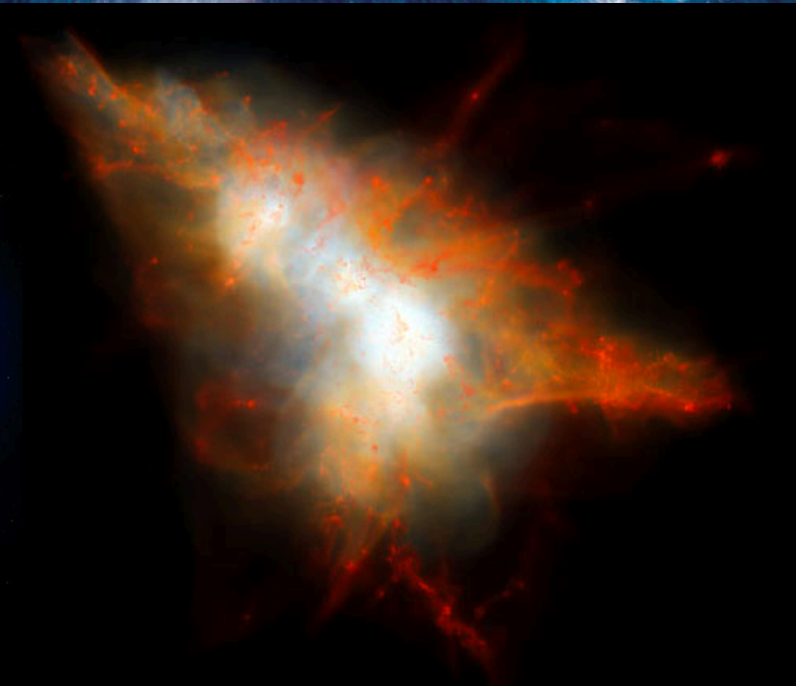


Kimm et al. (2018) showed that Lyα feedback can shape galaxy evolution.

- Suppresses star formation early on
- Significantly fewer star clusters form
- Weaker galactic outflows (less bursty)

APPLYING RADIATION HYDRODYNAMICS TO RESONANCE LINES

- On the fly 3D Lyα radiation hydrodynamics is feasible with the new resonant discrete diffusion Monte Carlo method.
- Initial collapse of massive seed black holes, e.g. DCBHs.
- Study line driven winds, e.g. massive stellar systems and lanthanide-rich kilonova from binary neutron-star mergers.
- Scenarios where optically-thin approximations break down.



Monte Carlo RHD

More on code accuracy and efficiency

- **Absorption** is treated deterministically by reducing photon weights.

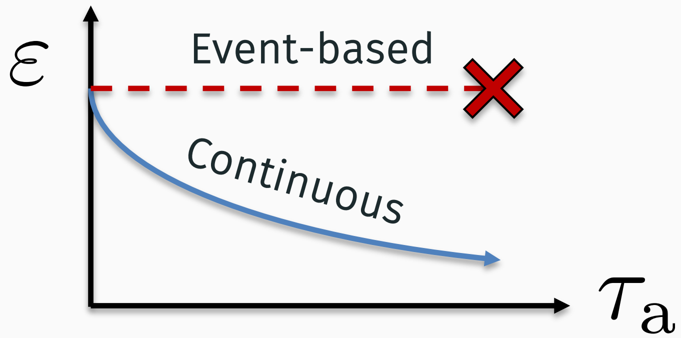
$$\Delta E_{\mathrm{abs}} = \varepsilon \left(1 - e^{-\tau_{\mathrm{a}}}\right) \qquad \text{where} \qquad \tau_{\mathrm{a}} \equiv k_{\mathrm{a}} \Delta \ell$$

- **Momentum deposition** is also path-based (add kinetic energy too).

$$\Delta \mathbf{p} = \frac{\tau \varepsilon}{c} \left(\frac{1 - e^{-\tau_{\mathrm{a}}}}{\tau_{\mathrm{a}}} \right) \hat{\mathbf{n}} \qquad \Delta E_{\mathrm{kin}} = \mathbf{v} \cdot \Delta \mathbf{p}$$

- The momentum correction factor accounts for the decreasing photon energy contribution due to absorption along the path:

$$\frac{\int_0^{\tau_{\mathrm{a}}} e^{-\tau_{\mathrm{a}}'} \mathrm{d}\tau_{\mathrm{a}}'}{\int_0^{\tau_{\mathrm{a}}} \mathrm{d}\tau_{\mathrm{a}}'} = \frac{1 - e^{\tau_{\mathrm{a}}}}{\tau_{\mathrm{a}}}$$



ADAPTIVE CONVERGENCE

- Monte Carlo noise can compromise the accuracy of radiation hydrodynamics simulations if convergence is not reached.
- Fortunately, we can quantify the relative signal to noise ratio:

$$\mathrm{SNR} \propto \sqrt{N_{\mathrm{ph}}}$$

- In our case, we have a weighted Poisson process with relative error:

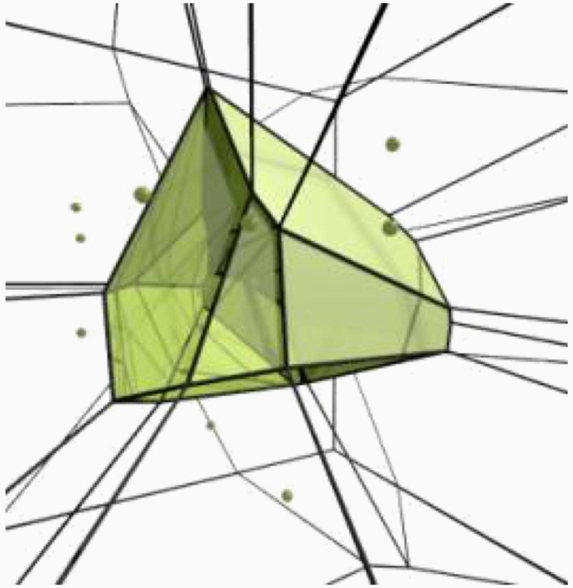
$$\delta_i \equiv \frac{\sqrt{\sum \Delta E^2}}{\sum \Delta E} \qquad \delta_{\mathrm{goal}} \approx 1\%$$

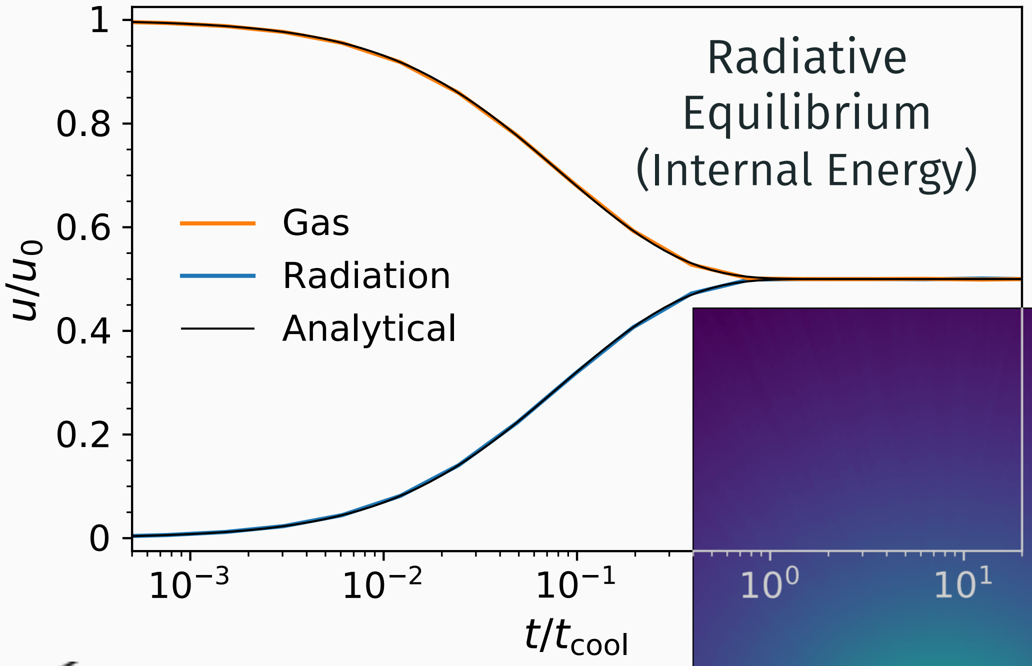
- Continue adding photon packets until the convergence is reached.

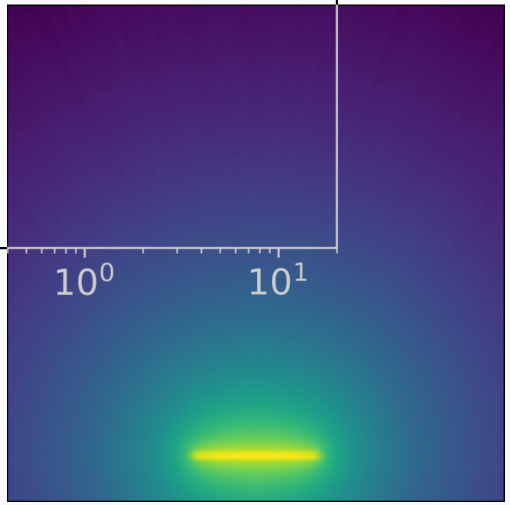
$$f \equiv \sum_{\delta_i > \delta_{\mathrm{goal}}} w_i \qquad f_{\mathrm{goal}} \approx 1\%$$

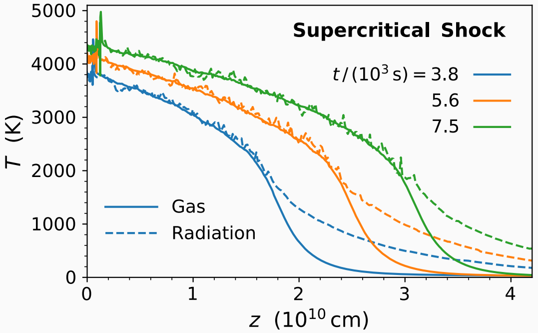
Advantages of MCRT:

- Accurate in optically thin/thick limits
- Multiple scattering RHD coupling
  e.g. dust and line radiation pressure
- Maintains high resolution by running natively on unstructured mesh data
- Efficiency improvements:
  - Implicit transport (IMC)
  - Discrete diffusion (DDMC)
  - Continuous absorption
  - Adaptive convergence
  - Luminosity boosting









- **Status:** Optimizing the code for production simulations

Other Options for RT

Comments about numerical methods

- The radiation energy density, flux, and pressure can be given in terms of directional moments of the intensity over solid angle.

$$J_\nu = \frac{1}{4\pi}\int I_\nu \mathrm{d}\Omega \qquad E_\nu = \frac{4\pi}{c} J_\nu$$

$$\mathbf{H}_\nu = \frac{1}{4\pi}\int \mathbf{n}\, I_\nu \mathrm{d}\Omega \qquad \mathbf{F}_\nu = 4\pi \mathbf{H}_\nu$$

$$\mathsf{K}_\nu = \frac{1}{4\pi}\int \mathbf{n}\otimes\mathbf{n}\, I_\nu \mathrm{d}\Omega \qquad \mathsf{P}_\nu = \frac{4\pi}{c}\mathsf{K}_\nu$$

- Zeroth moment equation (RTE integrated over all directions)

$$\frac{\partial E}{\partial t} + \nabla \cdot \mathbf{F} = ck_{\mathrm{a}}(a_{\mathrm{B}}T^4 - u)$$

- First moment equation ($\mathbf{n} \times$ RTE integrated over all directions)

$$\frac{1}{c^2}\frac{\partial \mathbf{F}}{\partial t} + \nabla \cdot \mathsf{P} = -\frac{k\mathbf{F}}{c}$$

- Conservation equations continue to higher order moments.
- Note: N-1 equations with N unknowns. We need a closure relation.
- Several numerical methods to solve the RTE, each with pros/cons.

- Flux-limited diffusion (FLD) uses the Eddington closure relation:

$$\mathbf{F}_\nu = \frac{\lambda_{\mathrm{L}}\tilde{c}}{k_\nu}\nabla\cdot\mathsf{P}_\nu \quad \text{where} \quad \mathsf{P}_\nu = \frac{1}{3}E_\nu\mathsf{I}$$

- With the 'flux-limiter' given by the gradient of the radiation field:

$$\lambda_{\mathrm{L}} = \frac{6+3\mathcal{F}}{6+3\mathcal{F}+\mathcal{F}^2} \quad \text{and} \quad \mathcal{F} = \frac{|\nabla E_\nu|}{k_\nu E_\nu}$$

- The 'moment-one' (M1) method relates the pressure P to the flux F for improved accuracy. The advantage of fluid methods is that they do not scale with the number of sources (good for hydro codes).

RAY TRACING METHODS

- **Long characteristics** methods solve the 1D RTE along rays.
- **Monte Carlo** methods sample random photon trajectories.
- These particle-based (collisionless) schemes can converge to give the "exact" solution, even below the simulation resolution.
- Approximations for computational efficiency:
  - Limited numbers of rays (N_{rays}) or photon packets (N_{ph})
  - Infinite/reduced speed of light approximations (e.g. equilibrium)
  - Spatial/frequency discretization schemes (adaptive resolution)
  - Short characteristics with less accurate non-local treatment
  - Implicit transport – absorption and re-emission → scattering
- Main drawback is computational expense:
  - Ray tracing scales as $\propto N_s^2$ not good for numerous sources
  - Monte Carlo has brute force convergence of $\propto \text{sqrt}(N_{\text{ph}})$

- **What about other methods?** Tailor method to your problem.
    - How accurately do I need to treat [*insert physics*]?
    - What is the geometry and dimensionality? Symmetry?
- Look out for new/hybrid schemes: e.g., Ryan & Dolence (2019) Method of Characteristics Moment Closure (MOCMC)
    - RTE closed with a swarm of "transport samples"
    - Local adaptivity with convergence as $\propto N_{samples}$
- It is good to be aware of the following:
    - Discrete Ordinates and S_N etc. methods
    - Diffusion solvers (many variations!)
    - Flux-limited Diffusion (FLD), Moment 1 (M1)
    - Variable Eddington Tensor (VET)
    - Tree methods (scaling as $\propto N\,logN$)