The Lyman-α signature of the first galaxies

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ABSTRACT
We present the Cosmic Lyman-α Transfer code (COLT), a new massively parallel Monte-Carlo radiative transfer code, to simulate Lyman-α (Lyα) resonant scattering through neutral hydrogen (H I) as a probe of the first galaxies. We explore the interaction of centrally produced Lyα radiation with the host galactic environment. The Lyα photons emitted from the luminous starburst region escape with characteristic features in the line profile depending on the density distribution, ionization structure, and bulk velocity fields. For example, the presence of anisotropic ionized bubbles exhibits a tall peak close to line centre with a skewed tail that drops off gradually. Furthermore, moderate (~ 10 km s⁻¹) local outflow is capable of producing an amplified peak redward of line centre when compared with the blue peak. Idealized models of first galaxies explore the effect of mass, anisotropic H II regions, and radiation pressure driven winds on Lyα observables. We employ mesh refinement to resolve critical structures responsible for characteristic Lyα features. We also post-process an ab initio cosmological simulation and examine images from photons captured at various escape distances within the (1 Mpc)³ comoving volume. Finally, we discuss the emergent spectra and surface brightness profiles of these objects in the context of high-z observations. The first galaxies will likely be observed through the red damping wing of the Lyα line. Observations will be biased toward galaxies with an intrinsic red peak located far from line centre that reside in extensive H II super bubbles, which allows early Hubble flow to sufficiently redshift photons away from line centre and thereby facilitate transmission through the intergalactic medium (IGM). Even with gravitational lensing to boost the luminosity we predict that Lyα emission from stellar clusters within haloes of $M_{\text{vir}} < 10^9 M_\odot$ is generally too faint to be detected by the James Webb Space Telescope (JWST).

Key words: Lyman-α emission – radiative transfer – resonant scattering – line: profiles – cosmology: theory – galaxies: formation – galaxies: high-redshift

1 INTRODUCTION

Observations of Lyman-α (Lyα) sources are a powerful probe of the high-redshift Universe (e.g. Hu & McMahon 1996; Rhoads et al. 2000; Taniguchi et al. 2005; Finkelstein et al. 2009). In particular, the prominence of the Lyα line at $\lambda_{\text{Ly}\alpha} = 1216 \, \text{Å}$ ($1 + z$) allows for spectroscopic confirmation of redshift measurements of individual distant galaxies. Lyα sources are also a compelling probe of the cosmic dark ages leading up to reionization – see Dunlop (2013) for a perspective on high-z observations. Historically, Partridge & Peebles (1967a) determined that galaxies from the first billion years after the Big Bang would be powerful emitters of Lyα photons, though observations of these sources eluded us for longer than expected. However, robust detections are becoming more regular, especially if the stellar mass is comparable to the Milky Way or the star formation rate (SFR) is elevated (e.g. SFR $\gtrsim 100 M_\odot$ yr⁻¹; Pritchet 1994).

Within the earliest galaxies hard UV radiation from massive stars is reprocessed into Lyα photons; however, because neutral hydrogen (H I) is opaque to the Lyα line, many of these photons may be resonantly trapped, and consequently suffer significant dust absorption. Despite these effects, observations have determined that the Lyα escape fraction, $f_e$, actually increases at higher redshifts (Hayes et al. 2011; Curtis-Lake et al. 2012). At some point, although the photons are no longer destroyed by dust, they are scattered out of the line of sight and some fraction of the Lyα emission is lost to the background as their sources become spatially extended Lyα haloes (Loeb & Rybicki 1999). Various mechanisms have been explored to explain the unusually high $f_e$ of high-z galaxies. In all likelihood this is a result of the complicated resonant line trans-

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fer, galactic structure, and peculiar dust properties. For example, multiple scatterings that facilitate excursions to the wings of the frequency profile; large-scale flows that induce Doppler shifts; and the geometry of dense, dusty clouds within a clumpy interstellar medium that provide pathways for escape (e.g. Hansen & Oh 2006; Dijkstra & Loeb 2008; Zheng et al. 2010). In this work, we push these questions to the very first galaxies (for a review see Bromm & Yoshida 2011).

Assessing the observability of such early Lyα sources is non-trivial. Indeed, going to higher redshifts introduces physical effects that compete in either strengthening or attenuating the Lyα signal (Latif et al. 2011a,b; Dunlop 2013). On one hand, the intergalactic medium (IGM) becomes increasingly neutral at higher z, resulting in a more difficult escape for Lyα photons (Ono et al. 2012). On the other hand, the same IGM also becomes increasingly devoid of dust (Pentericci et al. 2011). Furthermore, Population III (so-called Pop III) stellar sources are predicted to have been more efficient ionizers, boosting the Lyα luminosity (Bromm 2013; Glover 2013). The fact remains that high-redshift Lyα sources are being observed out to z ∼ 6.5. Still, many details regarding the epoch of reionization (EoR), or the inhomogeneous phase transition around z ∼ 6.5 − 15, are uncertain and may greatly affect interpretations of Lyα transfer through the IGM (Barkana & Loeb 2007; Meiksin 2009; Zaroubi 2013).

Some of the most effective methods for identifying high-redshift objects involve the Lyα line. In particular, Lyman-break galaxies (LBGs) are generally massive galaxies for which neutral hydrogen produces a sharp drop in the spectra due to absorption (Meier 1976a,b; Steidel & Hamilton 1992, 1993). Lyman-α emitters (LAEs) are young, less-massive galaxies with active star formation and strong Lyα emission (Charlot & Fall 1993). It is an important frontier to push Lyα selection methods towards the highest possible redshifts. For galaxies at z ≥ 6 the neutral fraction of the intervening IGM increases enough for their spectra to yield complete absorption of photons blueward of the Lyα line. This is the well-known “Gunn-Peterson trough” (Gunn & Peterson 1965) which is characteristic of LBGs. However, these massive, evolved galaxies become increasingly rare at high redshifts. The LAE luminosity function also declines as redshift increases, and the observed trend is robustly established for 4 ≤ z ≤ 7 (e.g. Bouwens et al. 2007; Oesch et al. 2012) and expected to continue beyond z ∼ 7 (Ellis et al. 2013). Because a strong detection of the highly-redshifted Lyα line requires the emitter to be young and relatively dust free – conditions which are naturally expected for the first galaxies – LAEs are likely their typical manifestation.

High-redshift Lyα candidates must be followed up by spectroscopy in order to guard against false positives from foreground contaminants. Fortunately, moderate- to high-z surveys are underway that will dramatically increase the sample size of Lyα galaxies and better characterize their statistical properties. For example, the Hobby-Eberly Telescope Dark Energy Experiment (HETDEX) is a large integral-field spectroscopic survey expected to detect a million LAEs (Adams et al. 2011; Finkelstein et al. 2011; Chonis et al. 2013). Currently, there are several candidates at z ≥ 7 (e.g. Ellis et al. 2013), with the highest spectroscopically-confirmed source announced at z = 7.51 by Finkelstein et al. (2013). Other records have been found using gamma-ray bursts (GRBs), active galactic nuclei (AGN), or (sub-)mm observations of redshifted thermal dust emission (Dunlop 2013). However, it is unclear how these other selection methods relate to Lyα predictions. Such connections may complement Lyα observations, even if the phenomena originate from the luminous deaths of individual massive stars (i.e. GRBs) or are not associated with a ‘normal’ activity of the first galaxies (e.g. AGN or high amounts of dust).

Lyα radiative transfer within the first galaxies is a timely problem because next-generation facilities will provide high resolution data by the end of the decade. The James Webb Space Telescope (JWST; Gardner et al. 2006) and large-aperture ground-based observatories1 offer the prime avenue for observing Lyα emission at the high-z frontier and will significantly contribute to our understanding of the ionization history at the end of the dark ages (Stiavelli 2009). However, significant progress has also been made on a number of complementary probes of the high-z Universe. Several 21-cm line arrays are related through the Wouthuysen-Field mechanism for which Lyα scatterings pump electrons into the excited hyperfine state, thereby coupling the spin and kinetic temperatures (Wouthuysen 1952; Field 1958; Furlanetto, Oh & Briggs 2006). Finally, an ideal complementary Lyα probe is encoded in the cosmic infrared background (CIB) because the integrated radiation from all background stars and galaxies has been redshifted to IR wavelengths (Partridge & Peebles 1967b; Santos, Bromm & Kamionkowski 2002). The Lyα contribution is seen through the correlation of sources across characteristic length scales (for a review see Kashlinsky 2005).

A number of authors have studied Lyα radiative transfer within different contexts. We have greatly benefited from and hope to add to the body of work in this area. A partial list of references include: Ahn, Lee & Lee (2002); Zheng & Miralda-Escudé (2002); Dijkstra, Haiman & Spaans (2006); Tassis & Tremonti (2006); Verhamme, Schaerer & Maselli (2006); Semelin, Combes & Baek (2007); Laursen, Razoumov & Sommer-Larsen (2009); Yajima et al. (2012). The state of the art is to apply post-processing radiative transfer to realistic hydrodynamical simulations, which is justified for many large scale systems. We use this method in conjunction with semi-analytic models to ascertain the feedback of Lyα radiation on the galactic assembly process. Our focus on the very first galaxies, in their proper cosmological context, is different from previous research that has targeted more massive systems at redshifts close to, or after, reionization (e.g. Yajima et al. 2014). Such systems require a statistical description of Lyα transmission through the IGM as described by Dijkstra, Mesinger & Wyithe (2011) and Laursen, Sommer-Larsen & Razoumov (2011). Photons that scatter out of the line of sight due to the neutral fraction of the IGM are effectively lost to the background. Therefore, the observability of Lyα emitters will provide independent constraints on reionization (Fan, Carilli & Keating 2006; Jee & Daniel et al. 2012; Jensen et al. 2013, 2014; Dijkstra 2014).

Measurements of the Lyα flux from first galaxies depend

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1 Infrared telescopes with integral field spectrographs and adaptive optics imaging include the Giant Magellan Telescope (GMT; www.gmto.org), Thirty Meter Telescope (TMT; www.tmt.org), and the European Extremely Large Telescope (E-ELT; www.eso.org/sci/facilities/elt).

2 For example, the Low Frequency Array (LOFAR; www.lofar.org), the Murchison Wide-Field Array (MWA; www.mwatelescope.org), the Precision Array to Probe the Epoch of Reionization (PAPER; eor.berkeley.edu), and ultimately the Square Kilometer Array (SKA; www.skatelescope.org).

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heavily on the observed line of sight in addition to the properties of the host system and IGM. Therefore, rather than solving a potentially intractable transfer equation with complex angular dependence we take advantage of Monte-Carlo Radiative Transfer techniques to accurately build emergent spectral energy distributions (SEDs). In order to perform Lyα simulations we have developed a new massively parallel code called COLT – the Cosmic Lyman-α Transfer code. In Section 2, the basic physics of Lyα transport is presented. In Section 3.1, we discuss the general methodology behind COLT and provide further algorithmic details in Section 3.2. In Section 4, the code is tested against both static and dynamic setups. In Section 5.1, we construct idealized analytical models to explore how fundamental parameters, including halo mass, virialization redshift, bulk velocity, and ionization structure, affect Lyα transport in the first galaxies. These well-motivated models help test our methods and sensitivity. Section 5.2 describes our implementation of the \( \text{ab initio} \) cosmological simulation of Safranek-Shrader et al. (2012) as post-processing conditions for COLT. In Section 6 we analyze and discuss the emergent line of sight flux distributions and surface brightness profiles for both the idealized analytic cases and the cosmological simulation. Finally, in Section 7 we reflect on the implications of this study with regard to Lyα observations with the JWST.

## 2 BASIC PHYSICS OF LYMAN-\( \alpha \) TRANSPORT

Photons with frequencies close to the Lyα resonance line, corresponding to the transition from the first excited state (2p) to the ground state (1s), may be absorbed and quickly re-emitted by neutral hydrogen. Thus, in optically thick environments (\( \tau \gg 1 \)) spatial diffusion can only occur after a rare excitation to the wing of the spectral line, determined by the thermal state of the gas. The cross section \( \sigma_\nu \) and number density \( n_{\text{H}1} \) describe the optical depth \( \tau_\nu \) along a photon’s path:

\[
\tau_\nu = \int_{\text{path}} n_{\text{H}1} \sigma_\nu d\ell,
\]

where \( \nu \) specifies the frequency dependence.

Here the cross section is most conveniently described by the dimensionless ‘Doppler’ frequency

\[
x \equiv \frac{\nu - \nu_0}{\Delta \nu_D},
\]

where \( \nu_0 = 2.466 \times 10^{15} \) Hz is the frequency of Lyα and the thermal Doppler width of the profile is \( \Delta \nu_D \equiv (v_{\text{th}}/c) \nu_0 \). The thermal velocity in terms of \( T_s \equiv T/(10^4 \) K) is

\[
v_{\text{th}} = \sqrt{\frac{2k_B T}{m_{\text{H}}} = 12.85 T^{1/2}_s \text{ km s}^{-1}.}
\]

Furthermore, if the natural Lyα line width is \( \Delta \nu_L = 9.936 \times 10^7 \) Hz then the ‘damping parameter’ represents the relative broadening of the natural line width:

\[
a \equiv \frac{\Delta \nu_L}{2 \Delta \nu_D} = 4.702 \times 10^{-4} T^{-1/2}_4.\]

Therefore, the final cross section is

\[
\sigma_x = f_{12} \frac{\pi e^2}{m_e c} \phi_{\text{Voigt}} = f_{12} \sqrt{\pi e^2 \Delta \nu_D} H(a, x),
\]

where \( f_{12} = 0.4162 \) is the oscillator strength of the Lyα transition and the Hjerting-Voigt function \( H(a, x) \) is the dimensionless convolution of Lorentzian and Maxwellian distributions,

\[
H(a, x) = \sqrt{\pi \Delta \nu_D} \phi_{\text{Voigt}} = \frac{a}{\pi} \int_{-\infty}^{\infty} e^{-y^2} dy = \frac{\ell}{\sqrt{\pi x^2}} H_{\text{a,x}}(x).
\]

For reference, we define the cross section at line centre as \( \sigma_0 \equiv \sigma_x(H(a, x) = 5.898 \times 10^{-4} T^{-1/2}_4 \text{ cm}^2 \). For a region of constant density \( n_{\text{H}1} \) such as a cell in a computational domain – the integral in Equation (1) simplifies to

\[
\tau_x = n_{\text{H}1} \sigma_0 \ell H(a, x)
\]

\[
= 1.820 \times 10^3 \frac{H(a, x)}{T^{1/2}_4} \left( \frac{n_{\text{H}1}}{\text{cm}^{-3}} \right) \left( \frac{\ell}{\text{pc}} \right).
\]

Typically, the parameter \( a \) is much less than unity so the Hjerting-Voigt function is dominated in the centre by a resonant scattering Doppler core, \( \phi_a \), and the wings are dominated by the Lorentzian component, \( \phi_L \). If the approximate frequency marking the crossover from core to wing is denoted by \( x_{cw} \), i.e. where \( \phi_a(x_{cw}) \approx \phi_L(x_{cw}) \), then the Hjerting-Voigt function is roughly

\[
H(a, x) \approx \begin{cases} e^{-x^2} & |x| < x_{cw} \text{ ‘core’} \\ \frac{a}{\sqrt{\pi x^2}} & |x| > x_{cw} \text{ ‘wing’}. \end{cases}
\]

See Sections 3.2.1 and 3.2.2 for a more rigorous discussion as well as numerical approximations for \( H(a, x) \) and \( x_{cw} \). For most conditions with significant neutral hydrogen density the gas is optically thick to core photons. However, in the wing, \( H(a, x) \) can be quite small allowing a photon to escape with greater ease. The approximate optical depth for a wing photon is then

\[
\tau_{\text{wing}} \approx 48.28 \frac{x^2}{\ell^2} \left( \frac{n_{\text{H}1}}{\text{cm}^{-3}} \right) \left( \frac{\ell}{\text{pc}} \right).
\]

Regions of high column density, \( N_{\text{H}1} \gg 1 \) pc cm\(^{-3}\) \( \sim 10^{18} \) cm\(^{-2}\), and/or cooler gas \( T \ll 10^4 \) K may produce very high opacities. The trapped Lyα photons are therefore exposed to greater extinction from dust. This may be best measured by the optical depth at line centre, which can be read from Equation (7) as

\[
\tau_0 \equiv \tau_{|x=0} \approx 5.9 \times 10^6 \left[ N_{\text{H}1}/(10^{20} \text{ cm}^{-2}) \right] T^{-1/2}_4.
\]

## 3 NUMERICAL METHODOLOGY

The COLT code is based on previous Monte-Carlo radiative transfer (MCRT) algorithms (See e.g. Ahn et al. 2002; Zheng & Miralda-Escudé 2002; Dijkstra et al. 2006; Verhamme et al. 2006; Laurens et al. 2009). The code reads initial conditions of velocity, density, and temperature for each cell of a three-dimensional grid employing adaptive mesh refinement (AMR). Sampling the Lyα emission profile of high opacity systems is possible because acceleration schemes avoid unnecessary computations, e.g. frequent core scatterings. Additionally, COLT is massively parallel allowing a greater number of photon packets and therefore less statistical error. Section 3.1 outlines the general methodology for a Lyα transport code while Section 3.2 describes the specific implementations used in COLT.
3.1 Basic Methodology

3.1.1 Photon emission

The initial spatial distribution of Ly\(\alpha\) photons is based on the physical setup, i.e. initial conditions. The first mechanism for producing Ly\(\alpha\) line emission is interstellar recombination as a result of ionizing radiation from hot stars. The second mechanism is collisional excitation of neutral hydrogen, usually resulting from shocks caused by accretion or supernovae. An initialization criterion accounts for photoionizing sources and diffuse emission, both of which may be significant for atomic cooling haloes. However, throughout this work we choose to initialize photons from the central location \(r = 0\). The initial direction \(k_i\) of each photon is drawn from an isotropic distribution in the rest frame of the embedded source. For convenience, velocities are expressed in terms of the thermal velocity:

\[
u \equiv \frac{v}{v_{\text{th}}}.
\] (10)

The photon is emitted at the natural frequency of the Ly\(\alpha\) photon \(x_{\text{nat}}\) in the rest frame of the atom. To obtain the initial frequency \(x_i\) in the moving frame of ambient gas we apply a Doppler shift appropriate to the velocity of the atom \(v_{\text{atom}} = v_{\text{atom}}/v_{\text{th}}\) (Laursen et al. 2009)

\[x_i = x_{\text{nat}} + k_i \cdot v_{\text{atom}}.
\] (11)

To be explicit, \(x_{\text{nat}}\) is drawn from a Lorentzian distribution and the components of \(v_{\text{atom}}\) are each taken from a Maxwellian distribution describing the thermal motion of the ambient gas. Although we use the expression in Equation (11), the memory of \(x_i\) is quickly lost by multiple scattering events, so for optically thick environments one may simply inject the photon at line centre, or \(x_i = 0\).

3.1.2 Ray tracing

The propagation distance of any photon is determined by the optical depth \(\tau\) drawn from an exponential distribution. This is because the mean optical depth \(\langle \tau \rangle \equiv \int_0^\infty P(\tau) e^{-\tau} d\tau = 1\) defines the mean free path \(\lambda_{\text{mfp}}\), or the average distance a photon can travel without being absorbed (or scattered) by the intervening medium (Rybicki & Lightman 2004). Therefore, travel beyond each mean free path becomes less and less probable. Formally, the optical depth over the total path is the product

\[
P(\tau) = \lim_{N \to \infty} \left( 1 - \frac{\Delta \tau}{N} \right)^N e^{-\tau},
\] (12)

which has been normalized so that \(\int_0^\infty P(\tau) d\tau = 1\). The cumulative distribution function is the integrated distribution defined by \(F(\tau) \equiv P(\tau) = \int_0^{\tau} P(\tau') d\tau'\), which can be inverted to give the optical depth at which an interaction event occurs,

\[
\tau_{\text{event}} = -\ln R,
\] (13)

where \(R\) is drawn from a univariate distribution.

To perform Cartesian-like ray tracing, the Monte-Carlo method selects a photon with an optical depth \(\tau_{\text{event}}\) according to Equation (13). Because individual cells are regions of uniform density we may equate this with the calculated optical depth \(\tau_x\) from Equation (7) to find the propagation distance, i.e. \(\tau_x = \tau_{\text{event}}\) provides \(\ell(\tau_{\text{event}})\). However, this often leads to a scattering which is outside the original cell. Therefore, we first calculate the optical depth required to travel through the cell: \(\tau_{x,\text{cell}} = n_{\text{H}1,\text{cell}} \sigma_0 \ell_{\text{cell}} H(\nu_{\text{cell}}, x)\), where \(\ell_{\text{cell}}\) is the distance from the current position to the point where the photon exits the cell. If \(\tau_{\text{event}} > \tau_{x,\text{cell}}\) the ‘spent’ optical depth is subtracted from the current optical depth, i.e. \(\tau_{\text{event}} = \tau_{\text{event}} - \tau_{x,\text{cell}}\). Likewise, the current position is updated to \(r = r + \ell_{\text{cell}} k_i\) and ray tracing continues through the next cell.

As photons traverse from cell to cell the temperature \(T\) and ambient bulk velocity \(\mathbf{u}_{\text{bulk}}\) may change. Therefore, Doppler shifting induces terms of \(\pm k_i \cdot \mathbf{u}_{\text{bulk}}\) corresponding to a nonrelativistic Lorentz transformation, i.e. one where \(||\mathbf{u}_{\text{bulk}}|| \ll c\). Additionally, the frequency differs between cells due to the \(\propto T^{-1/2}\) scaling relation. The frequency in the new (primed) cell is then

\[\nu' = (x + k_i \cdot \mathbf{u}_{\text{bulk}}) \sqrt{T/T'} - k_i \cdot \mathbf{u}_{\text{bulk}}.\] (14)

If \(\tau_{\text{event}} \leq \tau_{x,\text{cell}}\) the optical depth is ‘exhausted’ in the current cell and the photon undergoes a scattering event. The propagation distance is recalculated according to the remaining optical depth, i.e. \(\ell_{\text{event}} = \tau_{\text{event}}/[n_{\text{H}1,\text{cell}} \sigma_0 H(\nu_{\text{cell}}, x)]\). The position is advanced by \(\ell_{\text{event}}\) in the \(k_i\) direction and the algorithm proceeds to update the frequency and direction as described in Section 3.1.3. The photon ray traces along a new direction with each subsequent scattering until it ultimately escapes the computational domain.

3.1.3 Scattering events

A scattering event changes the photon’s frequency according to the atom’s velocity \(v_{\text{atom}}\), the final \(k_f\) and initial \(k_i\) directions, and a small recoil effect to satisfy conservation of momentum

\[x_f = x_i + (k_f - k_i) \cdot v_{\text{atom}} + g (k_i \cdot k_f - 1).
\] (15)

The recoil parameter \(g\) is defined as (see e.g. Adams 1971)

\[g \equiv \frac{\hbar \Delta \nu_0}{2 k_B T} = 2.536 \times 10^{-4} T^{-1/2} \approx 0.54\alpha,
\] (16)

which is included but negligible for the applications of this paper.

The velocity of the scattering atom is most conveniently expressed in terms of its parallel \(u_{||}\) and perpendicular \(u_{\perp}\) components. The perpendicular magnitudes are unbiased by the photon’s frequency and are therefore drawn from a Gaussian, i.e. \(\exp(-u_{\perp}^2)/\sqrt{\pi}\). However, the magnitude of the parallel velocity \(u_{||} = k_i \cdot v_{\text{atom}}\) is affected by the presence of the resonance line. The distribution function for \(u_{||}\) depends on frequency as the convolution of a Gaussian with a Doppler-shifted Lorentzian peak:

\[f(u_{||}) = \frac{\alpha}{\pi H(\alpha, x)} \frac{e^{-u_{||}^2}}{a^2 + (x - u_{||})^2},\] (17)

which highly favors velocities with \(u_{||} = x\) for core photons. For wing photons \(x \gg x_{\text{eq}}\), however, the probability that an atom has a high enough velocity to Doppler shift into resonance becomes vanishingly small, so \(f(u_{||})\) becomes increasingly Gaussian.

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The angle $\theta$ between the incident and outgoing scattering directions is governed by the phase (probability) function

$$W(\theta) \propto 1 + \frac{R}{Q} \cos^2 \theta,$$

where $R/Q$ is the degree of polarization for $90^\circ$ scattering. Due to the physical symmetry the phase function is independent of the azimuthal angle $\phi$. For core photons with $x < x_{cw}$ the electron transition to the $2p_{1/2}$ state results in isotropic scattering, i.e. $R/Q = 0$, while the $2p_{3/2}$ transition results in polarization with $R/Q = 3/7$ (Hamilton 1940). Since a quantum state with angular momentum $j$ has a spin multiplicity of $2j+1$, Ly$\alpha$ photons in the core are excited to the $2p_{1/2}$ state with $1/3$ probability and the $2p_{3/2}$ state with $2/3$ probability. Nonresonant wing photons on the other hand are dominated by Rayleigh scattering because their wavelength is much larger than the Bohr radius, $\lambda_{\text{Ly}\alpha} \gg a_0$, therefore the resultant polarization is maximal, i.e. $R/Q = 1$ (Stenflo 1980). Anisotropic scattering is used throughout COLT.

### 3.2 Computational optimization schemes

The previous section was written with little regard to computational efficiency, something we now seek to remedy. The details are presented in order of introduction, rather than importance.

#### 3.2.1 Approximation for $H(a,x)$

An approximation for the Voigt profile is important because $H(a,x)$ is evaluated after every scattering. A substantial effort has gone into studying this profile and implementing efficient algorithms with double precision accuracy – see e.g. Schreier (2011) and references therein. However, the Ly$\alpha$ resonance line is a unique application with a specific parameter range, so the approximations used in this work are entirely our own. We require our algorithm to provide better than one per cent accuracy for all frequencies and all realistic temperatures. To do this we first evaluate the integral $H(a,x)$ with special functions and expand to second order in $a$:

$$H(a,x) = \frac{a}{\pi} \int_{-\infty}^{\infty} \frac{e^{-y^2}}{a^2 + (y-x)^2} dy = \text{Re}\left( e^{a(1-ix)} \text{erfc}(a-ix) \right)$$

$$= e^{-x^2} + \frac{2a}{\sqrt{\pi}} (2x F(x) - 1)$$

$$+ a^2 e^{-x^2} (1 - 2x^2) + O(a^3),$$

where the (complex) complementary error function is related to the area under a Gaussian by $\text{erfc}(z) \equiv 1 - 2 \int_0^z e^{-y^2} dy / \sqrt{\pi}$ and the associated Dawson integral is $F(x) \equiv \int_0^x e^{y^2} y^2 dy$.

COLT takes advantage of the fact that $H(a,x)$ is symmetric by first evaluating $z = x^2$. Then because the behavior of the profile differs for small and large $z$ the domain is decomposed into three regions. The ‘core’ region is derived by expanding around $z = 0$, while the ‘wing’ region is an asymptotic expansion. An intermediate region acts as a smooth transition between the two. The approximations utilize continued fractions in order to maximize the efficiency of a small number of operations, e.g. 8 additions and 4 divisions. See Appendix A1 for the implementation of $H_{\text{approx}}$.

Second and higher order terms in $a$ are required to achieve one per cent accuracy for sub-Kelvin temperatures. However, since the CMB temperature floor prevents gas from reaching such low temperatures only first order terms are used in COLT. Figure 1 demonstrates the relative error, i.e. $100 \left[ 1 - H_{\text{approx}}(a,x)/H(a,x) \right]$ where $H_{\text{approx}}(a,x)$ is given by Equ. (A1). The yellow, blue, green, and red curves correspond to temperatures of 1 K, 10 K, 500 K and $10^4$ K, respectively. The overlying dashed lines represent the best case scenario when only keeping first order terms in $a$, i.e. using the exact Dawson integral.

#### 3.2.2 Approximation for $x_{cw}$

The crossover from core to wing $x_{cw}$ determines when $H(a,x)$ changes from a Gaussian to a Lorentzian. This is important because $x_{cw}$ marks the point where difficulties arise in generating $u_{ij}$ and also identify whether core skipping is necessary (see Sections 3.2.3 and 3.2.4). Our calculation assumes that the core and wing limits of $H(a,x)$ compete in their contribution to the profile:

$$e^{-x^2_{cw}} \approx \frac{a}{\sqrt{\pi x_{cw}}}. \quad (20)$$

Equation (20) provides a conservative approximation for $x_{cw}$, providing a sharp boundary with the core (see Fig. 1). The exact solu-
tion can be written in terms of the lower branch of the Lambert $W$ function, which in turn may be approximated by a low-order rational function with a relative accuracy of less than 0.1 per cent for the same parameter range as $H_{\text{approx}}(a, x)$. In summary, our optimal calculation of the core-to-wing crossover frequency is

$$x_{\text{cw}} = \sqrt{-W_{-1} \left( -\frac{a}{\sqrt{\pi}} \right)}$$

$$\approx \sqrt{L_1 - L_2 + \frac{L_2}{L_1} + O(L_1^{-2})}$$

$$\approx 6.9184721 + \frac{81.766279}{\log a - 14.651253} \; \text{ (21)}$$

where $L_1 = \log(a/\sqrt{\pi})$ and $L_2 = \log[- \log(a/\sqrt{\pi})]$. The relative per cent error is shown in Fig. 2.

3.2.3 Generating the scattering velocity $u_{||}$

As described in Section 3.1.3 (cf. Equation 17) the distribution for the parallel velocity $u_{||}$ with respect to the incoming photon is

$$f(u_{||}) \propto e^{-u_{||}^2 / a^2} \; \text{ (22)}$$

To good approximation this profile resembles a Gaussian with a sharp peak around the point $u_{||} = x$ (see Fig. 3).

Unfortunately, $f(u_{||})$ is not integrable so we instead use the inverted cumulative distribution function method on a related distribution and employ the rejection method to accept each draw. In this case the comparison function is chosen to be

$$g(u_{||}) \propto \frac{1}{a^2 + (x - u_{||})^2} \; \text{ (23)}$$

and draws are accepted with a probability of $f/g = \exp(-u_{||}^2)$. However, we only employ this algorithm for small frequencies, i.e. $x \ll 1$, because as $x$ increases the method becomes quite inefficient.

We learn more about $f(u_{||})$ by examining its behavior when $x \rightarrow \infty$. Here the peak at $u_{||} = x$ is pushed so far into the wing that there are essentially no atoms with speeds fast enough to absorb at the Doppler shifted resonance line, i.e. $f \approx \exp(-u_{||}^2 / (a^2 + x^2))$. Therefore, we may simply draw from a proper Gaussian with a slight modification – the peak is shifted by $x^{-1}$. We demonstrate this by finding the local extrema in the core:

$$\frac{df(u_{||})}{du_{||}} \propto u_{||} (1 + a^2 + (x - u_{||})^2) - x \approx u_{||} x^2 - x = 0$$

$$\Rightarrow \quad u_{||,\text{max}} = \frac{1}{x} \; \text{ (24)}$$

Here we have assumed $|x| \gg 1 > u_{||}$. It is straightforward to show $f''(u_{||}) \approx -2x^{-2} < 0$ so this is a local maximum as expected. Therefore, for $x \gtrsim 9$ we draw from a Gaussian with mean $x^{-1}$.

The intermediate region is problematic for either of these methods. Therefore, we follow Zheng & Miralda-Escudé (2002) and use the piecewise comparison function:

$$g(u_{||}) \propto \begin{cases} g_1 = 1/ [a^2 + (x - u_{||})^2] & u_{||} \leq u_0 \\ g_2 = e^{-u_{||}^2 / [a^2 + (x - u_{||})^2]} & u_{||} > u_0 \end{cases} \; \text{ (25)}$$

where $u_0$ is a separation parameter and the corresponding acceptance fraction is $\exp(-u_{||}^2)$ for $g_1$ and $\exp(u_0^2 - u_{||}^2)$ for $g_2$. We now restrict the discussion to positive $x$, which is possible because $f(-x, u_{||}) = f(x, -u_{||})$ allows us to recover velocities drawn from negative $x$. The probability that a velocity is less than $u_0$ is

$$p = \frac{\int_{-\infty}^{u_0} g(u_{||})du_{||}}{\int_{-\infty}^{\infty} g(u_{||})du_{||}} = \frac{\theta_0 + \pi/2}{\left( 1 - e^{-u_0^2 / a^2} \right) \theta_0 + \left( 1 + e^{-u_0^2 / a^2} \right) \pi/2} \; \text{ (26)}$$

where

$$\theta_0 = \tan^{-1} \left( \frac{u_0 - x}{a} \right) \; \text{ (27)}$$

If $p < R$, a univariate, then $\theta$ is drawn uniformly from the interval $[\theta_0, \pi/2]$, otherwise $\theta \in [-\pi/2, \theta_0]$. Finally, a velocity candidate,

$$u_{||} = a \tan \theta + x \; , \; \text{ (28)}$$

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure2}
\caption{The relative per cent error, $100 [1 - x_{\text{cw,approx}}/x_{\text{cw}}]$, is shown in green. The yellow curve in the insert is $x_{\text{cw,approx}}$ as given by Equation (21). All curves cover a temperature range of $T \in [1, 10^3]$ K.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure3}
\caption{The distribution of parallel velocities $f(u_{||})$ as given by Eqn. (17) for different values of incoming frequency $x$. The profile resembles a Gaussian with a sharp peak around the point $u_{||} = x$. For large $x$ it becomes too improbable for atoms to have velocities high enough to Doppler shift into resonance so the peak at $u_{||} = x$ disappears and a shifted Gaussian is a good approximation. The frequencies sampled are $x = \{0, 1, 2, 3, 4.5, 10\}$.}
\end{figure}
is accepted if another univariate, \( R' \), is less than the acceptance fraction, i.e. \( \exp(-u^2_0) \) or \( \exp(u^2_0 - u^2_1) \) for each respective region.

The algorithm from Zheng & Miralda-Escudé (2002) works well as long as the probability of the two regions are balanced, i.e. in COLT we attempt to maintain \( p \approx \frac{1}{2} \). The reason for this is that \( u_0 \) controls the acceptance fraction, so if \( u_0 \) is too small then we do not gain much for larger \( x \) and conversely if \( u_0 \) is too large then we defeat the purpose for smaller \( x \). The exact value of \( p \) is very sensitive to both \( x \) and \( a \), so we can only hope for average acceptance rates to be reasonable given the variance in \( u_0(a, x) \). If we assume \( u_0 < x \) then to first order in \( a \) we have:

\[
p \approx \frac{a}{\pi} \frac{e^{u^2_0}}{u^2_0}.
\]

(29)

The behavior of this function is different for core and wing photons. In the core it is reasonable to assume a perturbation from the natural peak location and apply the transformation \( u_0 \rightarrow x - au_0 \) where \( u_0 = u_0(a, x) \) admits an analytic solution to the approximate balance of \( p \approx \frac{1}{2} \). Again, to first order in \( a \) Equation (29) becomes

\[
p \approx \frac{e^{u^2_0}}{\pi u^2_0} \approx \frac{1 - 2axu^2_0}{\pi u^2_0} \approx \frac{1}{2}.
\]

(30)

The solution in terms of \( u_0 = x - u'_0 \) is

\[
u_0,\text{core} \approx x - \frac{1/2}{x + 2e^{-x^2}} \approx x - \frac{1}{x + e^{1-x^2}/a}.
\]

(31)

where the final equality allows the approximation to extend to larger \( x \) and is used in COLT for \( 1 < x < x_{cw} \).

For the region in which the wing dominates, i.e. \( x > x_{cw} \), the algorithm suffers an identity crisis. As discussed earlier, the high-\( x \) behavior of \( f \) approaches a Gaussian distribution though each of the candidate \( u_0 \) samples are from a Lorentzian distribution. Therefore, the exact value of \( u_0 \) is less important as long as it is greater than \( x_{cw} \). We test various prescriptions for \( u_0(a, x) \), also varying initial frequency \( x \) and temperature \( T \), in order to minimize the average number of draws in a simulation. A linear function, matched to the previous region provides sufficient acceptance of candidate random numbers. We use the following separation constant for \( x_{cw} < x < 9 \), denoted the ‘wing’ region:

\[
u_0,\text{wing} \approx x_{cw} - x_{cw}^{-1} + 0.15 (x - x_{cw}).
\]

(32)

Figure 4 demonstrates the fractional probability \( p(a, x) \) for drawing \( u_0 < u_0 \) given \( u_0 \) with \( u_0,\text{core} \) for \( 1 < x < x_{cw} \) and \( u_0,\text{wing} \) for \( x_{cw} \leq x < 9 \). The efficiency of the algorithm is especially sensitive to frequency.

### 3.2.4 Core-skipping

In optically thick regimes photons spend much of their time undergoing core scatterings with negligible diffusion in physical or frequency space. These scatterings can be avoided by only selecting atoms with perpendicular velocity components greater than a critical frequency, i.e. photons have zero mean free path if \( u_{\perp} < u_{\text{crit}} \). Following Ahn et al. (2002) we employ the Box-Muller method to generate two independent draws according to:

\[
u_{\perp,1} = \sqrt{-2 \ln R_1} \cos 2\pi R_2,
\]

\[
u_{\perp,2} = \sqrt{-2 \ln R_1} \sin 2\pi R_2,
\]

(33)

Figure 4. The fractional probability \( p(a, x) \) that \( u_{\parallel} < u_0 \). This separation captures the behavior of \( g \) for frequencies above and below the transition frequency \( x_{cw} \). The axes are frequency \( x \) in \( (1, 10) \) and \( \log_{10} \) temperature \( T \) in \((1, 10^4) \) K.

where \( R_1 \) and \( R_2 \) are univariates. The speedup time achieved here is significant since the probability of drawing a wing photon is roughly \( P_{\text{wing}} \approx \int_{x_{cw}}^{\infty} \exp(-x^2) \, dx \approx 10^{-5} \) corresponding to skipping roughly \( 10^5 \) core scatterings.

The crucial problem is to find an appropriate value for the critical frequency \( x_{\text{crit}} \). COLT introduces an algorithm with core-skipping based on both local and nonlocal criteria. This is especially important for high resolution, adaptively structured grids where the range of densities may cover several orders of magnitude. We desire a local determination of \( x_{\text{crit}} \) that accelerates the code but does not artificially push photons too far into the wings. As noted by Laursen et al. (2009) the important parameter is the product \( \alpha_0 \) so we seek a relation of the form \( x_{\text{crit}}(\alpha_0) \). The model we consider for the near zone environment is that of an optically thick static uniform sphere. This is motivated by the idealized geometry and an analytic solution for the angular averaged intensity \( J \) at the surface first given by Dijkstra et al. (2006),

\[
J(\tau_0, a, x) = \frac{1}{8} \frac{\sqrt{\pi}}{6 \alpha_0} \, \text{sech}^2 \left( \frac{\sqrt{3} x^3}{54 \alpha_0} \right),
\]

(34)

which has been normalized to \( 1/4\pi \), reflecting an integration over solid angle. The peaks are located at \( x_p = +0.931 (\alpha_0)^{-1/3} \), which is derived by solving the equation \( \partial J / \partial x = 0 \), or equivalently \( \bar{x} \tanh \bar{x} = 1/4 \) with \( \bar{x} = \sqrt{\pi^3/54} x/a_0 \). Therefore, the peak heights correspond to \( J_p = J(x_p) = 0.0551 (\alpha_0)^{-1/3} \). We next expand Equation (34) around \( x = 0 \) and define \( x_{\text{crit}} \) for large \( \alpha_0 \) as the frequency where \( J \approx \frac{1}{8} \sqrt{\pi^3/54} x/a_0 + O(x^2) \) reaches a small fraction of \( J_p \), giving \( x_{\text{crit}} \approx \frac{1}{3} (\alpha_0)^{1/3} \text{percentage of } J_p \). Thorough tests demonstrate this expression for \( x_{\text{crit}} \) valid for all \( \alpha_0 > 1 \) (see Appendix A2). Furthermore, it has a negligible effect on the emergent spectrum but greatly reduces the computation time. In summary, COLT uses the following approximation:

\[
x_{\text{crit}} = \begin{cases} 0 & \text{for } \alpha_0 < 1 \\ \frac{1}{3} (\alpha_0)^{1/3} & \text{for } \alpha_0 \geq 1 \end{cases}
\]

(35)

If the photon is already in the wing we do not use a cutoff because there are no core scatterings to skip.

The final ingredient in Equation (35) to be explained is how to calculate the product \( \alpha_0 \). COLT employs a combination of local
and nonlocal estimates of how aggressive to be with core-skipping. As we cannot possibly predetermine the escape path of a given photon we instead place a conservative limit on $\alpha \tau_0$ for different lines of sight. The local criterion is computed on-the-fly, using the minimum optical depth to the edge of the current cell $\alpha \tau_{\text{cell}}$. However, in highly refined regions (perhaps with partial ionization) and for scattering events near cell edges this can be quite small, i.e. if $\ell_{\text{cell}}$ is the minimum distance to the cell boundary Equation (7) gives

$$\alpha \tau_{\text{cell}} = 85.56 \, T_4^{-1} \left( \frac{N_{\text{H}_1}}{\text{cm}^{-2}} \right) \left( \frac{\ell_{\text{cell}}}{\text{pc}} \right).$$

(36)

It is apparent that if $n_{\text{H}_1}$ is roughly constant then the only nonlocal quantity needed is the physical size of the system. Therefore, the minimum integrated column density along rays emanating from the scattering event sets up an effective sphere with the intensity of Equation (34). Rather than calculating this for every scattering we combine the cell-based determination with a nonlocal (NL) estimate:

$$\alpha \tau_{\text{NL}} \equiv \min \sum_{\text{path}} \alpha \tau_0,$$

(37)

where the path is followed as long as the relative change in neutral hydrogen density remains less than a prescribed threshold, i.e. $|\Delta n_{\text{H}_1}/n_{\text{H}_1}| < f_{\text{NL}} \sim 0.2$. A value of $f_{\text{NL}} = 0$ ignores the nonlocal scheme completely and setting $f_{\text{NL}} \sim 1$ is too aggressive, failing to even detect sharp ionization fronts. To avoid double counting the local contribution, the paths originate at the edge of each cell and proceed outward. In practice the paths include at least the six directions of the coordinate axes and possibly more to achieve greater angular coverage. The nonlocal estimate can be computed once for each cell as the initial conditions are read in. COLT currently uses the sum of the local determination $\alpha \tau_{\text{cell}}$ and the nonlocal estimate $\alpha \tau_{\text{NL}}$ as the value of $\alpha \tau_0$ used in Equation (35).

We note that other criteria could be used for estimating $\alpha \tau_0$. For example, the nonlocal integration might stop if the velocity gradient exceeds the threshold for Sobolev escape; however, in most cases this is a secondary factor with little affect on core-skipping. Finally, additional local distances may be used in certain cases. Of special interest is to use the Jeans length to estimate core-skipping in idealized galactic setups. The Jeans length $\lambda_J \approx \sqrt{15k_B T/4\pi G\rho}$ acts as a physical upper limit for the size of a system with uniform density $\rho$. A primordial gas with mean molecular weight $\mu \approx 1.23 \, m_{\text{H}}$, mass fraction of hydrogen $X \approx 0.75$, and density $\rho \approx m_{\text{H}} n_{\text{H}_1}/X$ corresponds to a Jeans length of $\lambda_J \approx 0.75 \, \text{kpc} T_4^{1/2} (n_{\text{H}_1}/\text{cm}^{-3})^{-1/2}$ and a local $\alpha \tau_0$ of

$$\alpha \tau_J = 6.42 \times 10^4 \, T_4^{-1/2} \left( \frac{n_{\text{H}_1}}{\text{cm}^{-3}} \right)^{1/2},$$

(38)

so that $x_{\text{crit},J} \approx 8$ for $T = 10^4 \, \text{K}$ and $n_{\text{H}_1} = 1 \, \text{cm}^{-3}$.

3.2.5 Parallel implementation

Monte Carlo codes benefit greatly from parallel computation because each photon packet is an independent event. Therefore, the scalability is nearly linear. COLT uses the Message Passing Interface (MPI) libraries to implement dynamic load balancing between different processors. This is done because photons that undergo many scatterings take longer to escape. Therefore, the master process allocates a reasonable amount of work to each slave, e.g. $(1 − 10\%)$ of the photons)/(number of processors), until the required number of photons are assigned. The nonlocal determination of $\int d(\alpha x)$ for each cell, see Equation (37), is also performed with an efficient parallel computation.

4 TEST CASES

At this stage it is important to verify the code against known solutions. We choose tests that are complementary to each other in order to isolate certain key aspects of Ly$\alpha$ transport. The static test is the well-known Neufeld analytical solution for an optically thick homogeneous slab (Harrington 1973; Neufeld 1990). The dynamic test is that of an isotropically expanding sphere with different maximal velocities as described by Laursen et al. (2009).
3.1 Static test – the Neufeld profile

The angular averaged intensity \( J(\tau_0, a, x) \) for a static one-dimensional uniform slab was derived by Harrington (1973) and Neufeld (1990). Photons are injected at line centre at the origin and continuously scatter until escape occurs at a ‘centre-to-edge’ optical depth of \( \tau_0 \). When the bulk motion of the gas is set to zero, \( u_{\text{bulk}} = 0 \), and the recoil effect is ignored, \( q = 0 \), the emergent spectra are double-peaked and symmetric around the line-central frequency \( x = 0 \). The intensity at the surface is given by

\[
J(\tau_0, a, x) = \frac{1}{4\sqrt{\pi}} \frac{x^2 \sech{\frac{\pi^2}{54} x^3}}{a\tau_0},
\]

which has been normalized to \( 1/4\pi \), reflecting an integration over solid angle. The peaks are located at \( x_p = \pm 1.06642 (a\tau_0)^{1/3} \), which is derived by solving the equation \( \partial J/\partial x = 0 \), or equivalently \( x/\tanh{x} = 3/5 \). Therefore, the peak heights correspond to \( 10^3 J(\tau_0, a, x_p) = 45.074 (a\tau_0)^{-1/3} \).

As can be seen in Fig. 5, the agreement is quite good for high optical depths. The Neufeld approximation of Equation (39) fails to capture the correct spectra at lower optical depths because core scatterings also contribute to the spatial diffusion of Ly\(\alpha\) photons. This test has also been performed at other temperatures with similar results. Simulations of Ly\(\alpha\) scatterings through optically thick slabs help measure the effectiveness of the acceleration schemes.

3.2 Dynamic test – isotropic expansion of a uniform sphere

To test the code for the case of a nonzero gas bulk velocity we compare our results to previous simulations with isotropic expansion of a uniform sphere – see Zheng & Miralda-Escudé (2002); Dijkstra et al. (2006); Verhamme et al. (2006); Tasitsiomi (2006); Semelin et al. (2007); Laursen et al. (2009); Yajima et al. (2012). In general, velocity gradients affect Ly\(\alpha\) escape because photons are Doppler shifted out of line centre thereby reducing the effective optical depth. In general, even velocity fields on the order of the thermal velocity in photoionized gas (\( v_{\text{th}} \approx 10 \text{ km s}^{-1} \)) can change the emergent spectrum of Ly\(\alpha\) photons.

Following Laursen et al. (2009) we consider the intensity of an isothermal (\( T = 10^4 \text{ K} \)), homogeneous sphere of column density \( N_{\text{HI}} = 2 \times 10^{20} \text{ cm}^{-2} \) experiencing isotropic outflow. The Hubble relation gives the velocity \( v_{\text{bulk}}(r) \) of the gas at the position \( r \) from the centre of a sphere with radius \( R \):

\[
v_{\text{bulk}}(r) = Hr = \frac{v_{\text{max}}}{R} r
\]

where the Hubble-like parameter \( H \) sets the maximal velocity \( v_{\text{max}} \) at the edge of the sphere, i.e. \( v_{\text{max}} \equiv v_{\text{bulk}}(R) \). Figure 6 shows the result of this test which demonstrates excellent agreement with Laursen et al. (2009). The static case (\( v_{\text{max}} = 0 \)) also agrees with the analytical solution of Dijkstra et al. (2006) for a static, optically thick spherical “slab”. This test is also similar to that of Loeb & Rybicki (1999) who calculated the zero-temperature spectrum of a Ly\(\alpha\) source embedded in a neutral, homogeneous IGM undergoing Hubble expansion. Whereas a static solution produces two distinct peaks for blue and red modes of escape, the blue photons are continuously redshifted back to the core and the red mode becomes the only means of escape. This inevitably leads to free streaming on cosmological (> Mpc) scales. Unfortunately, there is no analytical solution for a medium possessing both thermal and bulk motions. Figure 6 illustrates the effect of increasing \( v_{\text{max}} \), which acts to suppress the blue peak until it disappears entirely by \( v_{\text{max}} \approx 200 \text{ km s}^{-1} \). At first the red peak is pushed further from line centre, however, past a critical \( v_{\text{max}} \) the peak approaches the centre again because the velocity gradient facilitates escape.

5 FIRST GALAXY MODELS

Galaxy formation is a highly complex process; however, studying the formation and radiative transport in the first, comparatively sim-
ple, systems provides an ideal laboratory for the physics involved (Bromm & Yoshida 2011). We here employ two complementary methodologies to represent the structure and dynamics of a first galaxy for COOLT—first, in Section 5.1 we construct idealized analytic models of these galaxies, and second, in Section 5.2 we extract a virialized halo from an 

\[ 4\pi m_H \int_0^{r_{\text{edge}}} n_H(r) r^2 dr \]

\[ = 4\pi m_H n_{H,0} r_{\text{core}}^3 \left( \frac{n_{H,0}}{n_{H,\text{IGM}}} - \frac{2}{3} \right) . \]  

Equation (43) is a cubic polynomial in \( n_{H,0} \) whose solution is not particularly insightful. However, we may expand about large masses \( M_{H,\text{tot}} \) to consolidate the leading order terms. These terms provide a relative accuracy in \( n_{H,0} \) of better than 1 part per billion for masses larger than \( 10^6 \) M\(_\odot\). For the parameters chosen above this implies a central density of

\[ n_{H,0} \approx n_{H,\text{IGM}} \left( \frac{2}{9} + \frac{4}{27} \right) , \]

where we have introduced the dimensionless parameter:

\[ \chi \equiv \frac{n_{H,\text{IGM}}^{1/3}}{r_{\text{core}}} \left( \frac{M_{H,\text{tot}}}{4\pi m_H} \right)^{1/3} \]

\[ = 1088 \left( \frac{M_{H,\text{tot}}}{10^8 \text{ M}_\odot} \right)^{1/3} \left( \frac{r_{\text{core}}}{10 \text{ pc}} \right)^{-1} \left( \frac{1 + z}{11} \right)^{-1} . \]

This term may also be found by dropping the \( \frac{2}{3} \) term in Equation (43). The \( \chi \) parameter relates the (leading order) ratio of core and background densities via \( n_{H,0} \approx \chi n_{H,\text{IGM}} \) and the ratio of core and edge radii via \( r_{\text{edge}} \approx \chi r_{\text{core}} \). With this central density the optical depth to Ly\( \alpha \) scattering of the core region is at least \( r_{\text{core}} \sim n_{H,0} \sigma_0 r_{\text{core}} \sim 10^8 \), a value that would increase with a larger core radius, a lower temperature, or a more massive system.

We are primarily interested in the mass and density of hydrogen, therefore we decided to use \( M_{H,\text{tot}} \) in the comparison. The total or virial mass of the galaxy is larger for two main reasons: (i) The mass fraction of hydrogen to baryons is less than unity, i.e. \( X \approx 0.75 \). (ii) The contribution of baryonic mass is considerably less than the contribution of dark matter, which is usually more extreme in smaller galaxies. In fact, if a substantial amount of gas is lost through ram pressure stripping or supernova blowout, for example, the baryonic mass may be significantly below the cosmological baryon fraction of \( \Omega_b/\Omega_m \sim 16 \) per cent (Allen, Schmidt & Fabian 2002). At any rate we can reasonably relate the virial and total hydrogen masses by \( M_{\text{vir}} \sim 10 M_{H,\text{tot}} \).

5.1 Idealized models

We now explore idealized models for the first galaxies at redshift \( z \sim 10 \) in preparation for extractions from a cosmological simulation. The number density of hydrogen nuclei \( n_H \) is built up from the following assumptions: First, we require spherical symmetry so that \( n_H = n_H(r) \). Second, we adopt a power law density profile within the galaxy, i.e. \( n_H \propto r^{-\beta} \) out to the edge of the galaxy \( r_{\text{edge}} \) defined as the point where \( n_H \) equals the background IGM, \( n_{H,\text{IGM}} \). An isothermal law with \( \beta = 2 \) provides a good description of a virialized system (e.g. Binney & Tremaine 2008). Finally, we prefer a non-cuspy ‘core’ in the centre of the galaxy, meaning the density profile flattens off to a constant density \( n_{H,0} \) within a core radius of \( r_{\text{core}} \approx 10 \) pc. This is inspired by observations of low surface brightness galaxies that suggest a softening in the centre (Burkert 1995; de Blok et al. 2001; Kormendy et al. 2009). In summary, the model is piecewise in the radial coordinate \( r \) according to:

\[
n_H(r) = \begin{cases} 
n_{H,0} & \text{for } r \leq r_{\text{core}} = 10 \text{ pc} \\
n_{H,0} \left( \frac{r}{r_{\text{core}}} \right)^{-2} & \text{for } r_{\text{core}} < r < r_{\text{edge}} \\
n_{H,\text{IGM}} & \text{for } r \geq r_{\text{edge}}.
\end{cases}
\]  

(41)

Here \( n_{H,\text{IGM}} \) is the background atomic hydrogen number density derived from a \( \Lambda \)CDM model with cosmological parameters taken from the Planck Collaboration (2013), and incorporating constraints from the Wilkinson Microwave Anisotropy Probe (WMAP; Hinshaw et al. 2013), the South Pole Telescope (SPT; Keisler et al. 2011), and the Atacama Cosmology Telescope (ACT; Das et al. 2014). Specifically, the Hubble constant is taken to be \( H_0 = 67.8 \) km s\(^{-1}\) Mpc\(^{-1}\) while the fractional energy contributions of baryons, matter, and dark energy are \( \Omega_b = 0.0485, \Omega_m = 0.307, \) and \( \Omega_\Lambda = 0.693, \) respectively. Therefore, \( n_{H,\text{IGM}} \) is \( \rho_{\text{c},\alpha} X \Omega_b (1+z)^3/m_H, \) or

\[ n_{H,\text{IGM}} \approx 2.5 \times 10^{-4} \left( \frac{1+z}{11} \right)^3 \text{ cm}^{-3} , \]

(42)

where \( X \approx 0.75 \) is the mass fraction of hydrogen and \( \rho_{\text{c},\alpha,0} \equiv 3H_0^2/(8\pi G) \) is the critical energy density at present.

Furthermore, the edge of the galaxy is given by solving the equation \( n_H(r_{\text{edge}}) = n_{H,\text{IGM}} \), which yields a radius of \( r_{\text{edge}} = r_{\text{core}} (n_{H,0}/n_{H,\text{IGM}})^{1/2} \). The density parameter \( n_{H,0} \) is then found by normalizing the overall mass of hydrogen in the galaxy \( M_{H,\text{tot}} \) to some value, e.g. \( 10^6 - 10^8 \) M\(_\odot\) for an atomic cooling halo.

The total mass is given by the integral

\[
M_{H,\text{tot}} = 4\pi m_H \int_0^{r_{\text{edge}}} n_H(r) r^2 dr
\]

\[ = 4\pi m_H n_{H,0} r_{\text{core}}^3 \left( \frac{n_{H,0}}{n_{H,\text{IGM}}} - \frac{2}{3} \right) . \]  

(43)

5.1.1 Structure and evolution of the ionized region

The model above did not include an ionized region around a central star cluster. This is important because Ly\( \alpha \) photons can easily escape such regions. Furthermore, a Strömgren analysis suggests that the ionized region may be on the order of \( r_{\text{core}} \) for a reasonable set of parameters:

\[
R_S = \left( \frac{3}{4\pi} \frac{N_{\text{ion}}}{n_{\text{H}} n_{\text{e}} n_{\text{B}}} \right)^{1/3} \approx 15 T_4^{1/4} N_{\text{ion},51}^{1/3} n_{100}^{-2/3} \text{ pc} , \]

(46)

where we have defined normalized values for ionizing photon rate \( N_{\text{ion}} \) (in \( 10^{51} \text{ s}^{-1} \)) and density \( n_{100} \equiv n/100 \text{ cm}^{-3} \). The normalization used for \( N_{\text{ion}} \) is a plausible guess at the rate expected from the starbursts residing in the first galaxies (see Section 5.3 for further discussion). The expression was simplified by approximating the total Case B recombination rate by \( \alpha_\text{B} \approx \)
Therefore, the late scenario corresponds to a time when the biconic region out to $r_{\text{edge}}$ is fully ionized – see Fig. 7 for an edge-on view of the column density through one such halo.

\begin{figure}
\centering
\includegraphics[width=0.5\textwidth]{L7_Model}
\caption{Neutral hydrogen column density $N_{\text{H}}$, for a “Late” model at a source redshift of $z = 9$ with $M_{\text{H, tot}} = 10^7 M_\odot$. The spatial scale, in physical kiloparsecs and arcseconds, are provided. The edge-on view of the halo demonstrates the hourglass ionization structure of these models.}
\end{figure}

The central starburst provides a feedback mechanism on the host galaxy. In order to motivate a spherically symmetric velocity law we consider the relative strength of the gravitational force $F_{\text{grav}}$ to the radiation force $F_{\text{rad}}$ in the single-scattering limit. Both forces scale as $1/r^2$ so their ratio is typically of order

\[ \frac{F_{\text{rad}}}{F_{\text{grav}}} \approx \frac{L_\alpha \sigma_T}{4\pi c m_\text{H} GM_*} \approx 0.3 \left( \frac{Y}{10^3} \right)^{-1}, \tag{48} \]

where $L_\alpha$ and $M_*$ are respectively the total luminosity and mass of the entire cluster. The normalization is chosen to correspond to the mass to light ratio for Pop III stars, i.e. $Y \approx 10^3$ (see Section 5.3). For simplicity Equation (48) assumes a point source. In reality, the ratio decreases radially from the centre of the gravitational potential as the dark matter halo mass dominates the gravitational force. However, we also consider a force multiplier $M(t) = k t^{-\alpha}$ originating from many resonant and optically thin lines, where $k \approx 1/30$, $\alpha \approx 0.7$, and $t$ is either the electron-scattering optical depth $\int_0^\infty \sigma_T \rho dr$ or the Sobolev optical depth $\sigma_T \rho v_{\text{esc}} |dv/dr|^{-1}$ in static or expanding media, respectively (CAK; Castor et al. 1975).

The multiplier can amplify the scattering efficiency by many orders of magnitude. Thus, the luminosities considered here ($\gtrsim 10^7 L_\odot$) may be capable of sustaining radiation-driven winds (Wise et al. 2012a). Indeed, the Ly$$\alpha$ line alone may be responsible for much of the opacity these winds require (Dijkstra & Loeb 2008, 2009).

The CAK theory uses mass conservation and momentum balance to arrive at a ‘beta law’ for the radial velocity profile

\[ v(r) = v_\infty \left( 1 - \frac{R_*}{r} \right)^{1/2}, \tag{49} \]

where $R_*$ is the size of the source. The terminal velocity $v_\infty$ is typically larger than the escape velocity $v_{\text{esc}}$ by a factor of a couple. Plausible values for our models are obtained by requiring that the mass loss rate $M = 4\pi r^2 \rho v$ be less than the maximally efficient mass loss for single scattering $M_{\text{max}} v_\infty = L_\alpha / c$ for which the radiation momentum is imparted entirely to the gas. In the halo’s isothermal region, i.e. $r_{\text{core}} < r < r_{\text{edge}}$ the velocity approaches $v_\infty$ and $\rho \propto r^{-2}$ so

\[ v_\infty \approx \left( \frac{4\pi m_\text{H} M_\text{tot}^2 n_{\text{H, IGM}}}{10^7 M_\odot} \right)^{-1/6} \sqrt{\frac{L_\alpha}{c}}, \]

\[ \approx 10 \left( \frac{M_\text{tot}}{10^7 M_\odot} \right)^{-1/3} \left( L_\alpha \frac{11}{10^7 L_\odot} \right)^{1/2} \text{km s}^{-1}. \tag{50} \]

In principle, multiple scattering in the optically thick environment could boost $v_\infty$ by a factor of the square root of the optical depth, or at least an order of magnitude. However, for simplicity our wind models all assume the velocity profile of Equation (49) with $R_* = 1$ pc, the approximate size of the central star cluster, and $v_\infty = 10$ km s$^{-1}$, a value comparable to the thermal velocity $v_{\text{th}}$.

The density and velocity profiles considered here are not self-consistent in the dynamical sense. However, our simplified $\beta$-model, calibrated in the above fashion, should give us a rough window into the otherwise extremely complex physics of galactic winds (e.g. Veilleux, Cecil & Bland-Hawthorn 2005). This also avoids overconstructing models that are already quite idealized.
Table 1. Classification scheme for the idealized galactic models.

| Classification | Velocity | H II Scenario | \( M_{\text{H}, \text{tot}} \) [M\(_\odot\)] |
|----------------|----------|---------------|--------------------------------------|
| SE [5–8]       | Static   | Early         | \( 10^5 \)–\( 10^8 \)               |
| SL [5–8]       | Static   | Late          | \( 10^5 \)–\( 10^8 \)               |
| WE [5–8]       | Wind     | Early         | \( 10^5 \)–\( 10^8 \)               |
| WL [5–8]       | Wind     | Late          | \( 10^5 \)–\( 10^8 \)               |

5.1.3 Model parameter space

The various galactic models we consider are based on the following physical quantities: (i) The velocity structure as either static or with a radial wind. (ii) The H II structure as either an early or late ionization scenario. (iii) The total mass of hydrogen in the halo \( M_{\text{H}, \text{tot}} \) chosen as either \( 10^5 \), \( 10^6 \), or \( 10^7 \) M\(_\odot\). For clarity we describe the model classifications summarized in Table 1:

- **S** ⇒ “Static” – The bulk velocity of every cell is zero.
- **W** ⇒ “Wind” – A radiation-driven wind assuming the velocity profile of Eq. (49) with \( R_\alpha = 1 \) pc and \( v_\infty = 10 \) km s\(^{-1}\).
  - Note: For simplicity we chose the same \( v_\infty \) for all models although it could very well be larger by a factor of a few.
- **E** ⇒ “Early” – The density profile of Eq. (41) is modified to have zero neutral hydrogen density within a Strömgren sphere of radius \( R_S = r_{\text{core}} \) at the centre of the galaxy.
- **L** ⇒ “Late” – The density profile of Eq. (41) is also modified to have zero neutral hydrogen density within a bipolar cone of opening angle \( \theta = 30^\circ \) out to \( r_{\text{edge}} \).

5–8 ⇒ \( M_{\text{H}, \text{tot}} = 10^5 \)–\( 10^8 \) M\(_\odot\) – These models allow us to explore the effect of mass, or column density, on Ly\(\alpha \) escape. \( M_{\text{vir}} \) is roughly an order of magnitude larger.

These models are intended to test the basic physics involved with Ly\(\alpha \) transport under the conditions discussed above, and we consider more realistic conditions from a cosmological simulation in Section 5.2.

5.1.4 Refinement criteria

The above models require accurate spatial discretization with a dynamic range of several orders of magnitude. Because we work primarily with cosmological simulations utilizing adaptive mesh refinement (AMR) we also incorporate the AMR grid structure into these idealized models. This has the dual benefit of (i) efficiently characterizing the field information even with ionization fronts or high density formations and (ii) unifying the data structures and ray tracing algorithms for both idealized setups and extractions from hydrodynamical simulations. In order to map the analytic conditions onto an AMR grid we first construct a Cartesian grid with dimensions \( \{x, y, z\} \in (-2r_{\text{edge}}, 2r_{\text{edge}}) \). This choice for the box size is somewhat arbitrary but provides enough of a buffer from the IGM to redistribute any remnant Ly\(\alpha \) core photons that might have escaped through the bipolar cavity. At this point we recursively refine the grid structure until the following criteria are all met: (i) Density – the cell dimensions must be smaller than the Jeans length \( \lambda_J \) by a factor of \( N_3 \), i.e. \( \Delta x_{\text{cell}} N_3 \leq \lambda_J \). A choice of \( N_3 = 64 \) was implemented in the models. (ii) Velocity gradient – the cell must be smaller than the Sobolev length \( \lambda_S \) by a factor of \( N_8 \), i.e. \( \Delta x_{\text{cell}} N_8 \leq \lambda_S \). A choice of \( N_8 = 32 \) was made to avoid unresolved Doppler shifting from continuous Sobolev escape. (iii) Geometric – refine based on whether a cell is within a specified volume or if the boundary of a geometric shape passes through the cell. For example, the shape of the edge of the galaxy was resolved by requiring that cells containing points where \( r = r_{\text{edge}} \) satisfy \( \Delta x_{\text{cell}} N_G \leq r_{\text{edge}} \). The chosen value was \( N_G = 64 \). Similarly for \( r_{\text{core}} \). The refinement criteria for the boundary of the ionized cone in the “Late” scenario was chosen to be \( 512 \Delta x_{\text{cell}} \leq r_{\text{edge}} \).
5.2 First atomic cooling haloes

The analytic models considered above inform us about key aspects of Lyα line transfer in the first galaxies, testing our methods and sensitivity. However, we can push these questions further by employing \textit{ab initio} cosmological simulations as post-processing initial conditions for \textsc{COLT}. We examine one cosmological simulation in this paper, and analyze additional cases in a follow-up study. In this section we summarize the simulation described by Safranek-Shrader et al. (2012, hereafter SS12), in preparation for the radiative transfer calculations of Section 6.3. The simulation of SS12 uses the hydrodynamical/N-body code FLASH (Fryxell et al. 2000) to evolve cosmological initial conditions through the nonlinear collapse of structure formation in a (1 Mpc)$^3$ comoving volume. The first galaxy model we study with \textsc{COLT} is an extraction of a virialized halo at redshift $z = 13.8$ with $R_{\text{vir}} \approx 600$ pc and $M_{\text{vir}} = 2.1 \times 10^7$ $M_{\odot}$, corresponding to $M_{H,\text{tot}} = 2.6 \times 10^6$ $M_{\odot}$ for comparison with our idealized models.

SS12 examine the formation and fragmentation conditions for a star cluster inside a cosmological atomic cooling halo, i.e. a system with virial temperature $T_{\text{vir}} \gtrsim 10^4$ K such that Lyα line cooling is enabled. These systems are important for the first galaxies because Lyα line cooling is much more efficient than cooling by molecular hydrogen or metal lines, and catalyzes the star formation process. Figure 8 shows the neutral hydrogen column density $N_{\text{H}}$, line of sight velocity $v_{\lambda}$, and ambient gas temperature $T$ of the cutout region. The filamentary, irregular nature of the gas is apparent, stressing the need for more realistic conditions than analytic models may allow. For simplicity we assume the stellar population of this galaxy has had no significant feedback on its galactic surroundings, thereby isolating the radiative transfer effects as originating from a Lyα source within a cosmological environment harboring gas accretion inflow. We will analyze additional haloes for which feedback is accounted for with greater sophistication in a follow-up paper. Finally, we also test cutouts of varying sizes within the (1 Mpc)$^3$ comoving volume, or $(67.5 \text{ kpc})^3$ physical volume in Appendix A3. We find minimal differences between the emergent flux densities $f_{\lambda}$, especially for the larger cutouts.

5.3 Properties of the central starburst

We now clarify the assumptions regarding the central starburst luminosity and stellar properties. The initial mass function (IMF) of a cluster depends on the metallicity of the population, where more massive Pop III stars are distributed with a top-heavy IMF and Pop II stars display a normal IMF biased toward low-mass stars. For simplicity, we assume a Pop III starburst with a top-heavy IMF, although a significant fraction of the first galaxies may typically already be populated by metal enriched Pop II stars, or a mixture of populations (Johnson et al. 2008; Greif et al. 2010; Ritter et al. 2012; Wise et al. 2012b; Muratov et al. 2013; Ritter et al. 2014). The Lyα luminosity, $L_{\text{Ly} \alpha}$, depends on the Pop III star formation efficiency, $\eta_* \equiv M_* / M_{\text{gas}}$, where $M_*$ is the mass in Pop III stars and $M_{\text{gas}}$ is the total baryonic mass in the host halo. For ease of comparison we assume a fixed star formation efficiency of $\eta_* = 0.01$ for both the idealized models and the cutout simulation of SS12. The assumption that the cluster consists of Pop III stars with a top-heavy IMF sets the ionizing photon rate to $N_{\text{ion}} \sim 10^{48}$ $(M_* / M_{\odot})$ s$^{-1}$. However, if metal enriched Pop II stars were present the rate would be an order of magnitude lower (Bromm, Kudritzki & Loeb 2001; Schaerer 2002). The luminosity in Lyman-α is (Dijkstra 2014)

$$L_{\text{Ly} \alpha} = 0.68 \ h \nu_0 \left(1 - f_{\text{esc}}^{\text{ion}} \right) N_{\text{ion}}$$

$$\approx 5 \times 10^8 \left( \eta_*/0.01 \right) \left( \frac{M_{\text{vir}}}{10^7 M_{\odot}} \right) L_{\odot},$$

(51)

where $h\nu_0 = 10.2$ eV and $f_{\text{esc}}^{\text{ion}}$ is the fraction of ionizing photons escaping the central starburst region, which we assume to be zero. Because Equation (51) scales with $N_{\text{ion}}$, if one assumes a Pop II IMF the radiative transfer calculations of Section 6, including flux and surface brightness, scale down by roughly a factor of ten compared to the Pop III case if $\eta_*$ would remain the same as before. Again, we emphasize that the Lyα flux and intensity profiles throughout this paper are scale free because the radiative transfer is decoupled from the hydrodynamics. The choice of a fixed star formation efficiency serves as the primary normalization for our profiles and fundamentally captures the basic idea that source luminosity should depend on halo mass. The one per cent star formation efficiency is admittedly an optimistic value that represents a likely upper limit on the prospects of detecting Lyα photons from Pop III sources. A comprehensive list of the properties of the central starburst is given in Table 2.

6 RADIATIVE TRANSFER CALCULATIONS

The output from \textsc{COLT} can be viewed as a redistribution of Lyα photons in both frequency and spatial position. In this section we describe the next-event estimator method for calculating surface brightness profiles (Section 6.1) and the results from each of the first galaxy models described above (Sections 6.2 and 6.3).

6.1 Surface brightness construction

The first galaxies are positioned near the horizon of the currently observable Universe and therefore appear as very small and faint...
objects. The observability of individual galaxies depends on both the details of Lyα transfer and the sensitivity of the instruments. If a galaxy is completely unresolved we may only be able to measure a single integrated flux. However, if the feature of interest is spatially resolved we may also measure the surface brightness. Therefore, COLT calculates the line of sight surface brightness using the next-event estimator method, similar to that of Tasitsiomi (2006) and Laursen et al. (2009). For each scattering we ask what is the probability that the photon would have been scattered toward a given line of sight and how the intervening medium would have attenuated the hypothetical signal. For anisotropic scattering the proper phase function $W(\theta)$ from Equation (18) quantifies the probability of being scattered into the line of sight. Additionally, the optical depth integrated to the edge of the computational domain diminishes the photon’s absolute weight by a factor of $e^{-\tau_{esc}}$. If each photon originally has equal weight, i.e. $L_{Ly\alpha}/N_{\text{ph}}$, where $L_{Ly\alpha}$ is again the total Lyα luminosity and $N_{\text{ph}}$ is the number of photon packets, then a square CCD grid composed of pixels each subtending a solid angle $\Omega_{\text{pix}}$, observing a source at a luminosity distance $d_L$, receives a total binned surface brightness of

$$S_{\text{Bpix}} \equiv \frac{\Delta E}{\Delta v \Delta \lambda \Delta \Omega} = \frac{L_{Ly\alpha}/N_{\text{ph}}}{4\pi d_L^2 \Omega_{\text{pix}}} \sum W(\theta)e^{-\tau_{esc}}. \space (52)$$

The summation is over all scatterings of all photons within the pixel range. In Equation (52), the phase function $W(\theta)$ is set to unity for isotropic scattering. At the relevant wavelengths the typical pixel size of JWST instruments ranges from $\Omega_{\text{pix, NIRCam}} \approx 10^{-3}$ arcsec$^2$ for photometry to $\Omega_{\text{pix, NIRSpec}} \approx 0.1$ arcsec$^2$ for spectroscopy.

The surface brightness may be calculated on the fly for any prescribed direction. In practice, however, we find it more efficient to ray trace along the six coordinate axes, yielding six orthogonal
The Lyα signature of the first galaxies

Figure 10. Radial surface brightness profiles for each of the different mass models. The color scheme and intrinsic halo parameters are the same as that of Fig. 9 (i.e. $\eta_z = 0.01$ and $z = 9$). For the anisotropic L–models there is a distinct feature at the edge radius corresponding to the hourglass ionization effect, where $r_{\text{edge}} \approx 1.09$ kpc for the 5–models, $r_{\text{edge}} \approx 2.35$ kpc for the 6–models, $r_{\text{edge}} \approx 5.05$ kpc for the 7–models, and $r_{\text{edge}} \approx 10.88$ kpc for the 8–models. The “Late” models are more extended than the bottled-up “Early” models.

observers for the faces of a cube. Furthermore, due to the severe exponential damping with even moderate optical depths we only continue to ray trace as long as $\tau_{\text{sec}} \lesssim 50$, which is conservatively large but still accelerates the process significantly. The line of sight flux is calculated with the same method but without the ‘per solid angle’, i.e. $\frac{\Omega}{\Omega_{\text{pix}}}$. COLT produces spatial and frequency bins for $\Sigma W(\theta)e^{-\tau_{\text{sec}}}$ which is multiplied by $L_{\text{Ly}\alpha}/[4\pi N_{\text{ph}}(1+z)^3206265^2\Omega_{\text{pix}}]$, and integrated over frequency to obtain intensity $^3$ SB, expressed in units of erg s$^{-1}$ cm$^{-2}$ arcsec$^{-2}$, or by $L_{\text{Ly}\alpha}/[4\pi N_{\text{ph}}\alpha_{\text{bin},\text{obs}}d_L^2]$ and integrated over the field of view to obtain flux density $^3$. Here $\Delta \lambda_{\text{bin},\text{obs}}$ corresponds to the observed wavelength bin size; throughout this paper we use a Doppler resolution of about $\Delta v \approx 10 \text{ km s}^{-1}$, corresponding to a spectral resolution of $R \equiv \lambda/\Delta \lambda \approx 30,000$, which is achievable with next-generation large-aperture ground-based infrared observatories equipped with adaptive optics. Our results may be degraded by a factor of $\sim 30$ for comparison with the NIRSpec instrument aboard the JWST.

Transmission through the IGM depends on the local environment and details of reionization. Our treatment follows that of Madau & Rees (2000) who examine the effect of local H II bubbles on the red damping wing of the Gunn-Peterson (GP) trough. In essence, the IGM opacity removes Lyα photons with a single scattering out of the line of sight, resulting in a spatially extended Lyα halo (Loeb & Rybicki 1999). Normally the GP optical depth at line centre, $\tau_0(z) \approx 7 \times 10^9 [(1+z)/10]^{3/2}$, is large enough to remove any flux blueward of the Lyα line. However, if the Lyα emitter resides within an ionized patch on the order of $\sim 0.1 \text{ – } 1 \text{ physical Mpc}$ the radiation can redshift sufficiently far from resonance to avoid total suppression in the intervening IGM. In an Einstein–de Sitter universe with a completely neutral medium outside the ionized bubbles the optical depth of the red damping wing is (Madau & Rees 2000)

$$\tau_{\text{GP}} = \frac{\tau_0(z_{\text{em}})}{\pi R_{\alpha}^{-1}} \frac{\lambda_{\alpha}(1+z)}{\lambda_{\text{obs}}} \int_{x_{\text{obs}}}^{x_{\text{em}}} \frac{dx}{(1-x)^2 + R_x^2 x^2}$$,

with dimensionless parameters $R_{\alpha} \equiv \Lambda \lambda_{\alpha}/(4\pi c) \approx 2 \times 10^{-8}$, $x_{\text{obs}} = (1 + z_{\text{obs}})\lambda_{\alpha}/\lambda_{\text{obs}}$, and $x_{\text{em}} = (1 + z)\lambda_{\alpha}/\lambda_{\text{obs}}$. The limits

$^3$ The units of $L_{\text{Ly}\alpha}$ are erg s$^{-1}$, the factor $\frac{100 \times 60 \times 60}{206265}$ converts from radians to arcseconds, and $\epsilon_{\text{pix}}$ is the physical size of a pixel in cm. The redshift and pixel size dependence originates from considering that $d_L = (1+z)^2d_A$ and $\sqrt{\Omega_{\text{pix}}} = \epsilon_{\text{pix}}/d_A$ where $d_A$ is the angular diameter distance.

$^4$ The flux density is an observed quantity, therefore, we use the redshifted wavelength bin size, $\Delta \lambda_{\text{bin},\text{obs}} = (1+z)\Delta \lambda_{\text{bin}}$. 

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Figure 11. Integrated light within a given radius, $I(r) \propto \int_0^r \text{SB}(r') r' dr'$, for the 5– and 8–mass models, left and right respectively. The color scheme and intrinsic halo parameters are the same as Figures 9 and 10. The anisotropic L–models are much more extended than the E–models as can be seen by comparing the half-light radii, $R_{1/2}$, shown as extended colored ticks on the radial axis. The curves have been normalized to unity to allow for direct comparison.

Figure 12. Surface brightness profile for the WL7 idealized galaxy model at redshift $z = 9$, which has a “Wind” velocity profile, a “Late” anisotropic ionization scenario, and total mass of hydrogen $M_{\text{H, tot}} = 10^7 M_\odot$ so that $M_{\text{vir}} \approx 10^8 M_\odot$. The central starburst has a Pop III star formation efficiency of $\eta_* = 0.01$, which for this mass corresponds to a central starburst of $L_{\text{Ly}{\alpha}} = 3.9 \times 10^8 L_\odot$ (see Table 2 for more information). The galactic centre contains a Strömgren sphere within the core radius $r_{\text{core}} = 10$ pc and produces a biconic ionized cavity out to $r_{\text{edge}} \approx 5$ kpc where the density drops to that of the background $n_{\text{H, IGM}}$. The simulation region is roughly 20 kpc across which allows the local IGM to play an important role. Indeed, a lighthouse effect is apparent as photons preferentially escape through the bipolar lobe aligned with the $z$-axis and are scattered when they hit the neutral IGM. The intrinsic bolometric flux $F$ is given for each line of sight at the bottom of each panel.

of integration are set by a cutoff at the redshift of reionization $z_{\text{reion}}$ and the redshift $z_i$ to the edge of the H II region around the source. For simplicity, we employ this prescription for the IGM opacity, i.e. $\tau_{\text{IGM}} = \tau_{\text{GP}}^{\text{red}}$ in Equation (52).

6.2 Idealized models

The freedom to change one parameter at a time allows us to perform a direct comparison between various idealized first galaxy models. We discuss the line flux and surface brightness profiles, employing the S–W, E–L, and $M_{\text{H, tot}}$ nomenclature, introduced above.

Figure 9 demonstrates how line flux changes between the halo models. Some of the most apparent trends are:

- Static profiles are symmetric about the Ly$\alpha$ line centre whereas moderate radiation-driven winds generate considerably more red photons than blue ones. This scenario would facilitate Ly$\alpha$ escape and reduce the fraction of photons subject to Gunn-Peterson absorption. On the other hand cosmological inflow models might produce the opposite effect, creating more extended profiles.
- The “Late” ionization models lead to a distinctive sharp drop near line centre. Ionized pockets prove to be a very efficient mode
of escape. Indeed, there would be a third peak at line centre if it were not for the neutral IGM surrounding these models.

- The bolometric flux for a given “Late” anisotropic model is larger when observed face-on (z) than edge-on (xy). See Table 3 for the line of sight flux normalized for comparison against the angular averaged flux of the same model. The most dramatic difference is for the WL8 model, where the viewing angle can lead to a dynamic range of $\sim 10$ km s$^{-1}$ or $\sim 0.04 (1 + z)$ Å, which explains the deviation from the lower (red) least squares fit. The cosmological simulation of Safranek-Shrader et al. (2012) is plotted as a gray circle with a vertical line to represent the uncertainty. SS12 is consistent with a relatively isotropic ionization scenario. To guide the eye we have included power law fits for selected models.

The spatial distribution of the photons is apparent in the radial surface brightness profiles of Fig. 10, the light enclosed within a given radius of Fig. 11, and the line of sight intensity maps of Fig. 12. The main qualitative features involve the hourglass effect. Indeed, there would be a third peak at line centre if it were not for the neutral IGM surrounding these models.

- The bolometric flux for a given “Late” anisotropic model is larger when observed face-on (z) than edge-on (xy). See Table 3 for the line of sight flux normalized for comparison against the angular averaged flux of the same model. The most dramatic difference is for the WL8 model, where the viewing angle can lead to a dynamic range of $\sim 10$ km s$^{-1}$ or $\sim 0.04 (1 + z)$ Å, which explains the deviation from the lower (red) least squares fit. The cosmological simulation of Safranek-Shrader et al. (2012) is plotted as a gray circle with a vertical line to represent the uncertainty. SS12 is consistent with a relatively isotropic ionization scenario. To guide the eye we have included power law fits for selected models.

The spatial distribution of the photons is apparent in the radial surface brightness profiles of Fig. 10, the light enclosed within a given radius of Fig. 11, and the line of sight intensity maps of Fig. 12. The main qualitative features involve the hourglass effect. Areas within the extended ionized regions are darker because the Ly$\alpha$ photons only scatter once they reach the neutral gas at the boundaries. Therefore, Ly$\alpha$ surface brightness images highlight sharp ionization fronts. In addition, the “Late” scenarios produce more extended profiles due to this effect.

Finally, we illustrate some observable trends between these idealized first galaxy models. Figure 13 shows the location of the red peak, $v_{\text{red peak}}$, in Doppler velocity units from line centre, i.e. $\Delta v = c\Delta \lambda / \lambda$, which increases as a function of mass. A power law fit of the data shows that $v_{\text{red peak}}$ is twice as sensitive to mass for “Early” models than for “Late” models. Figure 14 shows the qualitative differences of the flux properties listed in Table 3. The anisotropic models appear more luminous when observed face-on (z) than edge-on (xy) by a factor of a few. Additionally, for “Wind” models the relative flux redward of line centre ($F_r / F_b \sim$ a few) is generally more exaggerated for the “Early” models. Finally, Figure 15 compares the half-light radius, $R_{1/2}$, which roughly follows the relation predicted by Equation (45) that $R_{1/2} \propto \chi \propto M_{H,tot}^{1/3}$. When appropriate we have included power law fits for selected models to guide the eye.

### 6.3 Realistic first galaxy

We now present the COLT output of the realistic cosmological simulation introduced in Section 5.2. Figure 16 shows the line of sight flux and radial surface brightness profiles for the six coordinate faces of the (67.5 kpc)$^3$ extraction region in physical units. The different sightlines are quite smooth and qualitatively similar. Likewise, the actual intensity images (see Fig. 17) also appear relatively isotropic and featureless despite the obvious inhomogeneous and anisotropic features illustrated by the column density (see Fig. 8) and surface brightness images (see Fig. 18) captured in the immediate vicinity of the galaxy, i.e. a few virial radii away. The dark fluffy streaks are clouds of neutral hydrogen blocking particular sightlines. The main distinguishing characteristic is that certain faces of the cube are significantly brighter than others, especially in the central $\approx 1$ kpc region. This is due to the inhomogeneous medium which provides preferred channels of escape. It is apparent from Fig. 14 that the deviation from isotropy for the SS12 model is not very pronounced compared to the idealized anisotropic models. In this particular case $|1 - F_r / F_b| \lesssim 0.2$, although smaller extraction cubes exhibit significant anisotropic variance in the emergent
spectra, especially when comparing opposite lines of sight, i.e. ±x, ±y, and ±z (see Appendix A3). Such line-of-sight difference is likely due to the location of the central starburst within the dense galactic environment. However, much of the relative variation between sightlines may wash out as we account for the additional diffusion required to escape the vast neutral IGM. Furthermore, looking at the temperature structure of Fig. 8 indicates that it may also be possible to experience a similar ‘temperature lighthouse effect’ where higher temperatures lead to channels of lower optical depths.

6.3.1 IGM Transmission

The observability of this particular galaxy model depends on the subsequent transmission through the IGM. In Fig. 16 we present the intrinsic flux density $f_{\lambda}$ (shown as semi-transparent curves) and three scenarios that include suppression from the IGM. All signals have been corrected for redshift and assume a $10^8 \, L_{\odot}$ source. The lower three sets of curves include a frequency dependent factor of $\exp(-\tau_{\rm GP})$ defined in Equation (53) using physical sizes for the local ionized bubble $R_{\rm H\beta}$ of 1 Mpc, 0.1 Mpc, and 0 Mpc, respectively. The $R_{\rm H\beta} = 0$ Mpc curves represent the worst case scenario of no H II region while the $R_{\rm H\beta} = 1$ Mpc curves are likely a best case scenario, under the assumption that the IGM is fully neutral outside the ionized bubble. At $z = 13.8$ the Ly$\alpha$
Figure 16. Line of sight flux density (left), radial surface brightness profile (middle), and bolometric flux (right) for the six coordinate faces of the (67.5 kpc)$^3$ physical extraction region, assuming a 10$^9$ L$_\odot$ source at $z = 13.8$. The specific flux in the left panel is calculated for a Doppler resolution of $\Delta v \approx 10$ km s$^{-1}$, corresponding to a spectral resolution of $R \equiv \lambda/\delta \lambda \approx 30,000$, achievable with next-generation large-aperture ground-based infrared observatories with adaptive optics. The light-shaded curves are intrinsic to the galaxy whereas the other three sets of curves include suppression from IGM opacity, i.e. a frequency dependent factor of $\exp(-r_l^{IG}/R)$ defined in Equation (53). The difference between the transmission models is the size of the local ionized bubble $R_{HI}$ which has a strong effect on the observed flux. Although Figures 8 and 18 demonstrate many distinct inhomogeneous features, e.g. obscuration from clouds or anisotropic excess intensity, the spatially averaged flux and radial surface brightness are quite similar across different sightlines. The middle panel illustrates the singular nature of the intrinsic Ly$\alpha$ source and the transition to an exponentially damped halo, which in this case roughly coincides with $SB \approx \exp(-r/12.5$ kpc). The right panel compares the effect of $R_{HI}$ on the total observed flux for comparison with JWST sensitivities.

Table 4. JWST instrument sensitivity for a 5$\sigma$ detection after 10$^6$ seconds of exposure time based on sensitivities assuming the G235M grating with the F170LP filter for NIRSpec and the F150W filter for NIRCam. Flux densities are related by $f_{\lambda} \approx (c/\lambda^2) f_{\nu}$, where $1$ Jy = 10$^{-23}$ erg s$^{-1}$ cm$^{-2}$ Hz$^{-1}$. Entries denoted by G06 represent values taken from Gardner et al. (2006), scaled from the quoted sensitivity based on a 10$^6$ seconds detection after 10$^6$ seconds.

| Instrument | $R$ | $\Delta \lambda$ | $\Delta \nu$ | $\Delta \Omega_{\text{pix}}$ | $f$ | $f_{\nu}$ | $f_{\lambda}$ | $SB$ |
|------------|-----|-----------------|-------------|-----------------|-----|-------------|-------------|-----|
| Units      | –   | Å               | Hz          | arcsec$^2$      | erg s$^{-1}$ cm$^{-2}$ | nJy        | erg s$^{-1}$ cm$^{-2}$ Å$^{-1}$ | erg s$^{-1}$ cm$^{-2}$ arcsec$^{-2}$ |
| NIRSpec    | 1000| 20              | $10^{11}$   | 0.1             | $8 \times 10^{-20}$ (G06) | 50          | $4 \times 10^{-21}$            | $8 \times 10^{-19}$ |
| NIRCam     | 4   | 4500            | $4 \times 10^{-3}$ | $10^{-3}$       | $2 \times 10^{-19}$ (G06) | 0.56 (G06) | $5 \times 10^{-23}$            | $2 \times 10^{-16}$ |

line is redshifted to 1.8 µm which will be detected by JWST with NIRSpec at a (medium) spectral resolution of $R \approx 1000$, corresponding to a Doppler velocity resolution of $\sim 300$ km s$^{-1}$. Therefore, if we assume a 5$\sigma$ signal after 10$^6$ seconds of exposure time the expected flux detection limit$^5$ for observations with the NIRSpec is $f_{\lambda, \text{NIRSpec}} \approx 4 \times 10^{-21}$ erg s$^{-1}$ cm$^{-2}$ Å$^{-1}$, or $f_{\nu, \text{NIRSpec}} \approx 50$ nJy (see Table 4; Figure 16; Gardner et al. 2006; Johnson et al. 2009; Pawlik, Milosavljević & Bromm 2011). For the most part only optimistic H II scenarios allow a significant detection of the Ly$\alpha$ line in the first galaxies. However, if the strength of the source is increased and redshift is decreased then possibly even the $R_{HI} = 0$ Mpc scenario may be observable. The NIRSpec instrument will have an integrated flux sensitivity of $f_{\lambda, \text{NIRSpec}} \approx 8 \times 10^{-20}$ erg s$^{-1}$ cm$^{-2}$ and therefore, a surface brightness sensitivity of $SB_{\text{NIRSpec}} \approx 8 \times 10^{-19}$ erg s$^{-1}$ cm$^{-2}$ arcsec$^{-2}$. The NIRCam instrument is capable of $f_{\lambda, \text{NIRCam}} = 0.56$ nJy photometry, or $f_{\nu, \text{NIRCam}} \approx 5 \times 10^{-23}$ erg s$^{-1}$ cm$^{-2}$ Å$^{-1}$, over $10^{-3}$ arcsec$^2$ pixels, providing an equivalent sensitivity of $SB_{\text{NIRCam}} \approx 2 \times 10^{-16}$ erg s$^{-1}$ cm$^{-2}$ arcsec$^{-2}$ and $f_{\lambda, \text{NIRCam}} \approx 2 \times 10^{-19}$ erg s$^{-1}$ cm$^{-2}$ for the 5 µm range of the F150W filter. See Table 4 for a summary of detection limits for NIRSpec and NIRCam aboard the JWST. Neither instrument is sensitive enough to detect Ly$\alpha$ emission from the SS12 first galaxy model without an additional boost from gravitational lensing.

6.3.2 Gravitational lensing to boost the Ly$\alpha$ luminosity

Currently, the Hubble Space Telescope (HST) is carrying out the Frontier Fields programme, which uses high-magnification foreground galaxy clusters to produce the deepest lensing observations to date. This method has the potential to sufficiently boost observed Ly$\alpha$ luminosities to detect high-z target galaxies. Zackrisson et al. (2012) explore the prospects of detecting Pop III galaxies behind the $z = 0.546$ galaxy cluster MACS J0717.5+3745. With a magnification $\mu \gtrsim 10$, the cluster is an ideal candidate for an even deeper JWST Frontier Field programme. The authors conclude that if $z \geq 0.1$ per cent of the available baryons are converted into Pop III stars, then one expects a statistically significant number of lensed Pop III galaxy images in a single JWST/NIRCam field. Therefore, even conservative Ly$\alpha$ galaxies with virial mass $M_{\text{vir}} \gtrsim 10^8$ M$_{\odot}$ and redshift $8 < z < 15$ may be observable with the JWST. However, current estimates are based on semi-analytic modeling of the

$^5$ See JWST sensitivity limits for detecting spatially unresolved line fluxes at www.stsci.edu/jwst/science/sensitivity.
Figure 17. Line of sight surface brightness profiles for the six coordinate faces of the entire \((1 \text{ Mpc})^3\) comoving volume or \((67.5 \text{ kpc})^3\) in physical units. On larger scales the IGM tends to smooth out the profiles so the viewing angle differences are less severe.
Figure 18. Line of sight surface brightness profiles for the six coordinate faces of the \( \sim (4 \text{kpc})^3 \) extraction region. The dark fluffy streaks are wisps or clouds of neutral hydrogen blocking the particular sightline. Artifacts of the next-event estimator method sometimes appear, which does not resolve intensity features on scales smaller than the intervening AMR grid structure. Although these features are smoothed out when considering larger volumes (cf. Fig. 17) and transmission through the IGM, such a halo could possible serve as an analog for resolved systems at lower redshifts.
transition from dark matter halo mass to total stellar luminosity (e.g. Safranek-Shrader et al. 2012). More precise Ly$\alpha$ fluxes from additional simulations would help provide input for the upcoming deep lensing searches.

7 SUMMARY AND CONCLUSIONS

Lyman-$\alpha$ emitting sources provide observational clues about the formation and evolution of distant galaxies. Future observatories, such as the JWST and large-aperture ground-based facilities, will help focus and extend our view into the high-z Universe. As we better understand the properties of Ly$\alpha$ radiative transfer we can more fully assess the potential of this probe of the cosmic dark ages. The modeling of both individual galaxies and the background emission from all Ly$\alpha$ sources is highly complementary at these redshifts. Here we have carried out an exploratory survey of Ly$\alpha$ and surface brightness profiles show unique aspects of Ly$\alpha$ emission. The modeling of both individual galaxies and the background emission from all Ly$\alpha$ sources is highly complementary at these redshifts.

The intervening IGM has a significant effect on the Ly$\alpha$ line flux prior to and during the epoch of reionization. We expect the Gunn-Peterson effect to eliminate the blue peak entirely and significantly destroy the signal out to at least $\Delta \nu \sim 500$ km s$^{-1}$, which corresponds to $\Delta \nu_{\text{obs}} \sim 20 (1 + z)/10$ $\AA$. The idealized models with “Late” type ionization are intrinsically peaked close to line centre; therefore, Ly$\alpha$ sources from $z \gtrsim z_{\text{crit}}$ associated with a highly anisotropic ionization scenario from the host galaxy may be nearly impossible to detect. However, the “Early” galaxy models with virial mass $M_{\text{vir}} \gtrsim 10^8 M_\odot$ have resonantly scattered far enough into the wings to possibly survive IGM transmission. This may be inferred from Fig. 16 for the post-processing results of the cosmological simulation described above (see also Fig. 9 for the idealized models). We note that our treatment of Ly$\alpha$ transmission through the IGM could be extended. The analytic prescription can hardly capture the details of the epoch of reionization (EoR). Indeed, the EoR was not instantaneous and inhomogeneous reionization boosts the Ly$\alpha$ visibility, especially if local H II patches are large enough for photons to redshift out of resonance. The IGM model we considered does not include line-of-sight overdensities (e.g. Damped Lyman-$\alpha$ systems, etc.), gravitational lensing, or realistic prescriptions for the ionizing background. The sum total of all such effects may produce a large variance in Ly$\alpha$ observations across different sightlines.

The specific flux detected from high-z Ly$\alpha$ sources depends on the spectral resolution and sensitivity of the instrument. Throughout this study we have presented numerical calculations of $f_\lambda$ with a resolution of $R \equiv \lambda/\Delta \lambda \approx 30,000$, achievable with next-generation large-aperture ground-based infrared observatories with adaptive optics. The NIRSpec instrument aboard the JWST is capable of obtaining $R \approx 1000$, so many of the Ly$\alpha$ profiles here marginally span ~ 10 wavelength bins. Furthermore, at $z = 9$ a physical size of 4 kpc corresponds to 1 arcsec, i.e. ~ 30 NIRCam pixels or ~ 3 NIRSpec pixels, thus the JWST also has sufficient angular resolution to consider surface brightness measurements and spatially varying spectral features. We anticipate ongoing and future deep field surveys which take advantage of Ly$\alpha$ selection for further spectroscopic follow-up. As seen from Fig. 16 the atomic cooling halo from SS12 with $M_{\text{vir}} = 2 \times 10^7 M_\odot$ at $z = 13.8$, with a Pop III star formation efficiency of $\eta_* = 0.01$, residing in a super bubble with $R_{\text{HII}} = 100$ kpc, and a boost from gravitational lensing is still a factor of 100 below the JWST detection limits for a 5$\sigma$ signal after 10$^3$ seconds of exposure time. Thus, extrapolation from our result implies that haloes with $M_{\text{vir}} < 10^8 M_\odot$ are generally too faint to be amenable to the detection of Ly$\alpha$ emission from stellar sources. More massive haloes, on the other hand, should be within reach for the JWST. Their observability is further boosted by the expected broader spectral profiles which are less susceptible to the opacity of the IGM.

With post-processing results from additional cosmological simulations of more evolved haloes we will be better equipped to discuss the observability of the Ly$\alpha$ signature of the first galaxies. Furthermore, additional processes not considered in this study may have an important effect on Ly$\alpha$ observations. For example, diffuse emission may account for a significant source of radiation and numerical methods should be developed to compute this directly from the conditions of the ambient gas.

Finally, we have not included dust in these models. The presence of high amounts of dust in quasars at $z > 6$ constrains the production timescale to $\lesssim 100$ Myr (e.g. Bertoldi et al. 2003). Therefore, the origin of high-redshift dust may be almost exclusively due to $\sim 8 - 40 M_\odot$ core-collapse supernovae (SNe; Gall et al. 2011). Current models based on chemical kinematics of $\lesssim 1000$ day old SNe ejecta predict the formation of a significant amount of silicate dust along with other metals (Dwek & Cherchneff 2011). However, it is unclear how much dust actually survives in these hostile environments (Gall et al. 2014). Dust grain destruction may be caused by shock-heating from the SN UV flash, hot gas in the reverse shock $\sim 10^4$ years after the explosion, or lower order effects such as radioactivity. Still, there is empirical evidence for resilient dust production in SN ejecta, e.g. observations of remnants with yields of $0.1 - 1 M_\odot$ (Matsuura et al. 2011; Gomez et al. 2012). This coincides with numerical simulations demonstrating rapid metal enrichment in young galaxies (e.g. Greif et al. 2010; Wise et al. 2012b). We expect to be able to model dust accurately by post-processing cosmological simulations that include models for metal enrichment. This may give additional insight and can be compared with models that assume mixed or clumpy distributions based on an intrinsic dust to gas mass ratio.

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APPENDIX A: ADDITIONAL DETAILS

A1 Calculation of $H(a, x)$

COLT uses the following approximation for $H(a, x)$:

$$H_{\text{approx}}(a, z) = \begin{cases} 
1 - a & \text{for } z \leq 3 \\
\frac{e^{-z}}{1 - a} \left[ A_0 + \frac{A_1}{z - A_2 + \frac{A_3}{z - A_4 + \frac{A_5}{z - A_6}}} \right] & \text{for } 3 < z < 25 \\
\frac{e^{-z} + a}{1 - a} \left[ B_0 + \frac{B_1}{z - B_2 + \frac{B_3}{z - B_4 + \frac{B_5}{z - B_6}}} \right] & \text{for } z \geq 25 
\end{cases}$$

where $z = x^2$ and the constants $A_i$ and $B_i$ are given in Table A1.

A2 Tests for $x_{\text{crit}}$

The expression $x_{\text{crit}} \propto (a\tau_0)^{1/3}$ is based on comparing an expanding of the analytical solution for a static uniform sphere to the height of its peak – see Equation (34). However, the constant of proportionality must be found by empirical tests. The tests were run on many different values of $a\tau_0$, however, we only show two to demonstrate the validity across the parameter space. The first is for $a\tau_0 = 1$, for which Equation (35) gives $x_{\text{crit}} = 0.2$, while the second is for $a\tau_0 = 10^5$, where $x_{\text{crit}} = 9.3$. As can be seen from Fig. A1, both values produce excellent results.

A3 Extraction size for the cosmological simulation

In order to test the grid structure of the cosmological simulation for edge effects and sensitivity to the extraction size we examine the emergent spectra for cubes with a centre to edge distance of 500 pc, 2 kpc, 8 kpc, and 32 kpc. The largest size represents the radiative transfer through the entire (1 Mpc)$^3$ comoving volume. Figure A2 demonstrates the convergence of the flux density $f_3$ toward that of the largest extraction, although there is still a significant variance across different lines of sight due to the inhomogeneous nature of the cosmic structure.

Table A1. Coefficients for the rational function approximation of the central ($x^2 \leq 3$) and intermediate ($3 < x^2 < 25$) regions of Equation (A1).

| $i$ | $A_i$ | $B_i$ |
|-----|-------|-------|
| 0   | 15.75328153963877 | 0.0003300469163682737 |
| 1   | 286.9341762324778 | 0.5403095364583999 |
| 2   | 19.05706709007019 | 2.676724102580895 |
| 3   | 28.22644101723441 | 12.82026082606220 |
| 4   | 9.52639980241186 | 3.21166435627278 |
| 5   | 35.29217026286130 | 32.032981933420 |
| 6   | 0.8681020834678775 | 9.0328158696 |
| 7   | -- | 23.7489999060 |
| 8   | -- | 1.82106170570 |

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Figure A1. Top panel: A test for $\alpha \tau_0 = 1$ designed to compare different values of $x_{\text{crit}}$. The converged solution (yellow histogram) is given by $x_{\text{crit}} = 0$ while a low value of $x_{\text{crit}} = 0.25$ provides excellent agreement and is shown in black. A sample of values which are too high and affect the emergent spectrum are $x_{\text{crit}} = \{0.5, 1, 2\}$ and are respectively given by orange, red, and purple dotted histograms. Bottom panel: Same as the top panel except for $\alpha \tau_0 = 10^5$. A value of $x_{\text{crit}} = 5$ is sufficiently converged for our purposes. An acceptable value of $x_{\text{crit}} = 10$ is given by a black line while non-converged values of $x_{\text{crit}} = \{15, 25, 35\}$ are again given by the orange, red, and purple dotted histograms. Here $\alpha \tau_0$ is large enough that the analytical solution of Eqn. (34) is accurate, so it is included as the green dashed line in the background. Both tests used $\sim 500,000$ photon packets.

Figure A2. A test to examine the effect of extraction size for the post-processing conditions of Safranek-Shrader et al. (2012). Solid curves represent the angular averaged spectra while the transparent curves show the observed flux as viewed along each each of the six coordinate axes. The red, blue, green and yellow curves represent the results from extraction cubes with a physical edge size of 1 kpc, 4 kpc, 16 kpc, and 67.5 kpc, respectively. The normalization is set by a $10^8 L_\odot$ source at $z = 13.8$. 

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