Effect of Separate Initial Conditions on the Lyman-α Forest in Simulations

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Accepted XXX. Received YYY; in original form ZZZ

ABSTRACT

Using a set of high resolution simulations, we quantify the effect of species specific initial transfer functions on probes of the IGM via the Lyman-α forest. We focus on redshifts 2−6, after H i reionization. We explore the effect of these initial conditions on measures of the thermal state of the low density IGM, the curvature and Doppler width cutoff. We also examine the matter and flux power spectrum, and potential consequences for constraints on warm dark matter models. We find that the curvature statistic is at most affected at the ≈ 2% level at z = 6. The Doppler width cutoff parameters are affected by ≈ 5% for the intercept, and ≈ 8% for the fit slope, though this is subdominant to sample variation. The flux power spectrum is at most affected by ≈ 5% at high redshift and small scales. We discuss numerical convergence with simulation parameters.

Key words: software; simulations – methods: numerical – cosmology: theory – intergalactic medium – quasars: absorption lines

1 INTRODUCTION

The intergalactic medium (IGM) occupies the space between galaxies and galaxy clusters, and houses the majority of baryonic matter in the universe. The major phase changes in the history of the IGM are fairly well understood, with recombination (H i) and quasars (Madau et al. 1999; McQuinn et al. 2009; Haardt & Madau 2012) for H i and He(II) reionization, respectively. The ionization state is well understood, as the neutral fraction is set by the equilibrium between photoionizations and recombinations. All of this makes the IGM, and especially the low density IGM, a valuable probe of the post-reionization universe (z < 6) and the scales probed make it useful for both astrophysics and cosmology.

Conveniently, there are numerous observations probing intergalactic gas at 2 < z < 6. Generally, these are observations of the Lyman-α forest, the series of absorption features blueward of the rest-wavelength Lyman-α emission observed in quasar spectra (Gunn & Peterson 1965). A single forest spectrum is a one-dimensional map of the gaseous structure along that line of sight, making it a useful probe of structure formation. Knowledge of the large scale structure, either through the flux power spectrum or the inferred matter power spectrum, constrains warm dark matter (WDM) models (Viel et al. 2005; Walther et al. 2019). In addition to probing structure formation, the Lyman-α forest can be used to measure the thermal state of the IGM, leading to a set of measurements describing the thermal history of the IGM. Using the thermal and ionization history of the IGM, one can test models of the makeup and evolution of the ionizing background, and thus infer properties of the ionizing sources and sinks over time (Boera et al. 2019)

There are several ways in which Lyman-α forest spectra are processed to constrain cosmological models and the thermal state of intergalactic gas. Cosmological contexts generally make use of the flux power spectrum from a sample of Lyman-α forest spectra (Zaldarriaga et al. 2001; Palanque-Delabrouille et al. 2013; Nasir et al. 2016; Boera et al. 2019). The flux power is the Fourier transform of the flux over-density, \( \delta_F = F/F_0 - 1 \). The flux power spectrum is sensitive to cosmological parameters on large scales.
(\(k < 0.02\) s/km for velocity wavenumber \(k\)), and constrains small scale smoothing at higher \(k\) (Kulkarni et al. 2015). For example, smoothing is enhanced in WDM models, leading to a reduction in power above some critical value of \(k\), (dependent on the mass of the WDM particle). This makes the flux power spectrum a robust tool for constraining WDM models (Walther et al. 2019).

The spectral statistics used in determining the thermal state of the IGM are more varied. Common methods include statistics which encapsulate an entire forest spectrum (Theuns & Zaroubi 2000; Theuns et al. 2002; Zaldarriaga 2002; Lidz et al. 2010; Becker et al. 2011; Boera et al. 2014), as well as analyses which make use of absorption features from spectra decomposed via Voigt profile fitting (Schaye et al. 1999; Ricotti et al. 2000; Schaye et al. 2000; McDonald et al. 2001; Bolton et al. 2014; His et al. 2018). The small scale flux power spectrum and the distribution of flux are also used to constrain the IGM thermal state (Zaldarriaga et al. 2001; Gaikwad et al. 2020).

The Lyman-\(\alpha\) forest probes scales on which non-linear structure growth is important, and so cosmological hydrodynamic simulations of the IGM are necessary to build a map between model parameters and observations. These simulations require two components: collisionless cold dark matter modelled using N-body techniques, and collisional baryons which include pressure forces. One common simplification is that, although baryons are evolved hydrodynamically, the initial conditions for both species are identical, using the transfer function for the total matter fluid (Emerson et al. 2019).

Before recombination, baryons couple to radiation, suppressing their clustering on sub-horizon scales and reducing clustering relative to the dark matter. After recombination, baryons fall into the potential well of the cold dark matter and so the linear transfer functions differ by \(< 1\%\) at \(z = 0\). The effect is larger at higher redshifts, \(z = 2\) - \(5\), where the Lyman-\(\alpha\) forest is a sensitive probe of the gas (Naoz & Barkana 2005). Bird et al. (2020) showed that separate transfer functions can affect the one-dimensional Lyman-\(\alpha\) forest flux power spectrum by \(5\) – \(10\%\) on scales \(0.001\) – \(0.01\) s/km in the redshift range \(2 < z < 4\).

The aim of this work is to determine whether species specific initial transfer functions have an appreciable effect on probes of the Lyman-\(\alpha\) forest. We use the simulation technique developed in Bird et al. (2020), which reproduces the theoretical offset between the dark matter and baryon power (Angulo et al. 2013), to model separate initial transfer functions. Recently, Rampf et al. (2020) (see also Hahn et al. 2020; Michaux et al. 2020) resolved this discrepancy by perturbing the particle masses, in agreement with the results from Bird et al. (2020). We will examine the effect of these initial conditions on measures of the thermal state of the IGM; the curvature (Becker et al. 2011) and Doppler width cutoff (Schaye et al. 1999). We also examine the effect on the matter and flux power spectrum, which could have consequences for warm dark matter models (Narayanan et al. 2000). The simulations we use are higher resolution than in Bird et al. (2020), allowing us to better probe smaller scales.

In Section 2 we outline the simulations and artificial spectra used throughout. In Section 3 we discuss the methods used to calculate each measure of the IGM, as well as the results of those calculations. Measures of the thermal history of the IGM, including the curvature and the Doppler width cutoff are covered in sections 3.1 & 3.2, respectively. The WDM relevant measures are examined in Sections 3.3 (flux power spectrum) and Section 3.4 (matter power spectrum). In Section 4 we summarize and conclude. We include Appendix A, which discusses numerical convergence with box size, resolution, and number of artificial spectra used.

We assume throughout a flat ΛCDM cosmology with \(\Omega_0 = \Omega_b + \Omega_{CDM} = 0.288, \Omega_b = 0.0472, h = 0.7, n_s = 0.971\), and \(\sigma_8 = 0.84\) (consistent with 9-year WMAP results Hinshaw et al. 2013).

2 SIMULATIONS

Our set of hydrodynamical simulations were performed using the N-body and smoothed particle hydrodynamics (SPH) code MP-Gadget\(^1\), described in Bird et al. (2018, 2019). MP-Gadget is a fork of Gadget-3, itself the descendent of Gadget-2 (Springel 2005). Initial conditions are generated with MP-GenIC, the initial conditions generator packaged with MP-Gadget. The initial power spectrum is generated with the Boltzmann code CLASS (Lesgourgues 2011).

Two sets of simulations are used throughout this work. Both sets of simulations use a glass to initialize the baryons and a grid to initialize the CDM (a glass procedure is then applied to the combined distribution to minimize CDM-baryon overlap). Simulations using offset grids for both particle species (which is common in the literature) introduce a spurious growing mode to the CDM-baryon difference. This can be avoided by using a glass to initialize the baryons (Yoshida et al. 2003; Bird et al. 2020). The first set uses a single transfer function for both species. The second set uses separate, species specific, transfer functions. The phases of the Fourier modes are identical, leading to the same realisation of cosmic structure on scales larger than the particle grid.

Gas is assumed to be in ionization equilibrium with a uniform ultraviolet background using the model of Faucher-Giguère et al. (2009)\(^2\). Faucher-Giguère (2020) recently updated their UV background model and showed that simulations using uniform UV backgrounds do not accurately model the timing and photoheating associated with reionization. In our simulations reionization has completed by \(z = 6\) (the average neutral hydrogen fraction in low density regions of our simulations is less than \(1\%\)). Our results are generated in the redshift range \(2 < z < 6\), after hydrogen reionization. We do not implement He\(\upalpha\) reionization because the scale of our simulation box size is smaller than a typical He\(\upalpha\) bubble (Upton Sanderbeck & Bird 2020), leading to an effectively instantaneous reionization.

Star formation is implemented using the standard approach for Lyman-\(\alpha\) forest analyses. Gas particles in the simulations are turned into stars using a simple density-based method: when they reach an overdensity \(\rho/(\rho_0) > 1000\), but remain at a temperature \(T < 10^5\), they are turned into stars (Viel et al. 2004). Our simulations do not include black hole or supernovae feedback. The set of high-resolution simulations include our main simulations as well as volume-fixed and (gas mass) resolution-fixed simulations. The latter two are used to check numerical convergence, discussed in Appendix A. All simulations start at \(z = 99\) and have periodic boundaries. Box volume, particle number, and gas particle mass resolution are reported in Table 1. The gas particle mass resolution is set so that the higher redshift Lyman-\(\alpha\) forest is resolved (Bolton & Becker 2009).

Lyman-\(\alpha\) absorption spectra are generated by sending random

\(1\) https://github.com/sbird/MP-Gadget3

\(2\) Specifically the 2011 update. https://galaxies.northwestern.edu/uvb-fg99/
skewers through the simulation box using Fake Spectra Flux Extractor Bird (2017), described in Bird et al. (2015). Our analysis uses 5,000 randomly placed skewers, which are generated for each snapshot, leading to a large set of 1 km s$^{-1}$ pixel width neutral hydrogen absorption spectra for redshifts in the range $2 < z < 6$.

### 3 METHODS & RESULTS

In this section we examine the effect using species-specific initial conditions has on two commonly studied properties of the IGM, both of which use Lyman-α forest spectra. The first is the temperature-density relation of the low density IGM, which is generally parameterized as

$$T(\Delta) = T_0 \Delta^{-1},$$

where $\Delta$ is the matter overdensity, $T_0$ is the temperature at mean density ($\Delta = 1$), and $\gamma - 1$ is the power-law index (Hui & Gnedin 1997; McQuinn & Upton Sanderbeck 2016). Throughout we focus on redshifts after H reionization ($z \leq 6$), where adiabatic cooling and photoheating dominate the thermal state. This is the regime where the temperature-density relation parameterized above is generally valid (though it is not best described with a single temperature-density relation during He ii reionization (Trac et al. 2008; Furlanetto & Oh 2009; Upton Sanderbeck & Bird 2020). We focus on two measures which probe the temperature-density relation of the IGM: the curvature (3.1) and the Doppler width cutoff (Section 3.2).

The second property is the matter power spectrum of the IGM, which can constrain dark matter models, especially warm dark matter through its effect on structure formation. The matter power spectrum of the dim and diffuse IGM is not directly accessible. However, the flux power spectrum is a good proxy and allows constraints to be placed on the thermal free-streaming of dark matter and thus a potential WDM particle mass. We examine the effect species specific initial conditions have on both the Lyman-α flux power spectrum (Section 3.3) and matter power spectrum (Section 3.4).

#### 3.1 Curvature

The curvature statistic introduced in Becker et al. (2011) has an approximately one-to-one relationship with the temperature of the IGM at an optimal overdensity. The temperature at the mean density can then be inferred using a temperature-density relationship slope calibrated from simulations. The curvature is essentially the second derivative, or curvature, of the flux. Specifically, it is given by $\kappa \equiv F''/(1 + F'^2)^{3/2}$ and traces the ionized fraction of hydrogen. Higher temperature gas will show more thermal broadening in the absorption features of the spectra, while lower temperature gas will retain more small-scale spectral features. Because the curvature summarizes the entire spectrum it does not require decomposing.

![Figure 1](image.png)

**Figure 1.** Example of the curvature measurement. Top: spectrum with noise (black) and the smoothed cubic spline fit to it (green). Middle: The region enclosed in the dotted box in the top panel, renormalized into 10 Mpc h$^{-1}$ sections and rescaled such that the set of all these sections have the same mean flux across simulations. Bottom: the curvature of the middle panel. The single value reported for such a section is the mean absolute curvature value in regions where the renormalized and rescaled flux lies between 0.1 $< F < 0.9$.

spectra into individual absorbers, making it useful up to higher redshifts than the Doppler width cutoff method (Section 3.2).

The simulated spectra are processed, and the curvature calculated following the general procedure in Becker et al. (2011):

(i) Gaussian noise is added to the spectra such that the $S/N \sim 20$, then a cubic b-spline is fit to the flux iteratively. The initial break point spacing between the piecewise b-spline is set at 50 km s$^{-1}$ and additional points are added to improve the fit until either a minimum resolution is reached (10 km s$^{-1}$) or the fit converges (the $\chi^2$ value between spline and spectra changes by less than 3 between break point additions). The resulting spline, an example of which can be seen in the top panel of Figure 1, is used in place of the spectrum for the rest of the analysis.

(ii) The spline is then renormalized by breaking it into 10 Mpc h$^{-1}$ sections and dividing by the maximum value in that section. This normalizes the measure and avoids uncertainties due to continuum finding.

(iii) Each of these sections is then rescaled such that the mean flux of the entire set of sections is consistent with the model from Kim et al. (2007), given by an effective optical depth, $\tau_{\text{eff}} = 0.0023(z + 1)^{3.65}$.

The result of steps (ii) and (iii) are shown in the middle panel of Figure 1. Note that the values used in the processing outlined above (e.g. the S/N, $\chi^2$ convergence value, etc.) are chosen either to agree with Becker et al. (2011), to be reasonable in regards to observation, or simply to fit the artificial spectra well.

The curvature is then calculated, using only flux in the range $0.1 < F < 0.9$. The bottom panel of Figure 1 shows an example of the curvature, before restricting the flux range. For each section the mean absolute curvature is returned, $\eta = \langle |\kappa| \rangle$, and the average of $\eta$ for each redshift is shown in Figure 2 (top), along with the fractional difference between the two (e.g. $\frac{|x_1 - x_2|}{x_2 - 1}$) in percentage (bottom). The squares (blue) show the results for the simulation which uses separate initial transfer functions, and the triangles (brown) show

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### Table 1. Simulations

| Simulation | Box Volume | N | $M_{gal}$ (M$_{\odot}$) |
|------------|------------|---|------------------------|
| Main       | (20 Mpc h$^{-1}$)$^3$ | 2 x 1024$^3$ | 9.8 x 10$^4$ |
| Fixed Volume | (20 Mpc h$^{-1}$)$^3$ | 2 x 512$^3$ | 7.8 x 10$^3$ |
| Fixed Resolution | (10 Mpc h$^{-1}$)$^3$ | 2 x 512$^3$ | 9.8 x 10$^3$ |

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3 https://github.com/sbird/fake_spectra
the simulation which uses the same transfer function. The difference between the two is remarkably small, peaking at $< 2\%$ at $z = 6$.

For convergence testing, noise is not added to the spectra, though the spectra are still renormalized and rescaled. Convergence of the curvature is discussed in Appendix A, and shown in Figure A1 for simulation parameters, and in Figure A4 (top panel) for convergence with number of sight lines used.

3.2 Doppler Width Cutoff

Another method used to determine the thermal state of the IGM, first introduced in Schaye et al. (1999), is fitting the lower cutoff in the Doppler width ($b$) of spectral features as a function of their neutral hydrogen column density ($N_{\text{HI}}$). Theoretically, an absorber has a minimum Doppler width, i.e. due entirely to thermal broadening with no additional effects such as broadening from a velocity gradient. The minimum will depend on the temperature of the absorber, $b_{\text{therm}} = \sqrt{2k_b T/m}$, where $k_b$ is the Boltzmann constant, $T$ the temperature, and $m$ the proton mass. The temperature depends on the density, with higher density clouds having a higher temperature and thus a broader spectral profile. As the true density of an absorber is not observable, the column density of the absorber and its Doppler width are measured from simulated spectra. Using simulations and observations of the $N_{\text{HI}} - b$ cutoff parameters, the temperature-density relation is calibrated and the physical density inferred from the column densities (Schaye 2001).

This method requires decomposing spectra into features, with widths and amplitudes corresponding to the Doppler width and column density of the associated absorbers. We decompose our artificial spectra, which are the optical depths ($\tau$) along a line of sight through the simulations, into individual features by fitting the flux ($F = e^{-\tau}$) using Voigt profiles. Each feature in the flux, starting with the highest peak in the optical depths, is fit, masked, and removed. Specifically, the mask extends to minima that are at least 8% smaller in flux (at continuum level) on either side of the peak, which reduces over-fitting. The masked region is subtracted and the next highest peak is fit using the resulting spectrum. Features are fit until no point in the spectrum is higher than 0.01% of the highest initial peak. Note that the simulation box has periodic boundaries, so each peak is centered before the fitting takes place (to account for absorbers lying across the edge of the box).

These individual Voigt profiles are passed to a combined fit, which starts with the two most relevant peaks from the individual fitting, and gradually adds more peaks. This continues to add the next most relevant peak until the fit fails (the error between the spectrum and the fit is unable to converge to 25% of the largest peak in the spectrum), or the average improvement in fit from the previous two additional peaks is less than 2.5% per peak. The Voigt profiles for the peaks included in the final combined fit are retained, where the Voigt profile width is the Doppler width, $b$, and the Voigt profile normalized amplitude is the neutral hydrogen column density, $N_{\text{HI}}$.

Perfect spectra and flawless profile fitting are not possible – Figure 3 shows a clear trend in the minimum Doppler width with redshift, but there are points that lie below the visual cutoff. To best fit this minimum Doppler width cutoff, Schaye et al. (1999) developed an algorithm which fits the relation

$$\log_{10}(b) = \log_{10}(b_0) + (\Gamma - 1) \log_{10}(N_{\text{HI}}/N_{\text{HI},0}).$$

We follow most closely the algorithm choices used in Rudie et al. (2012), which added an initial rejection step. Our method is as follows:

(i) Features with column densities in $10^{12.5} < N_{\text{HI}} < 10^{14.5}$ are retained. Features with $b < 8 \text{ km s}^{-1}$ and $b > 100 \text{ km s}^{-1}$ are removed.

(ii) Features are rejected using the $\sigma$–rejection method from Rudie et al. (2012), in which features with $b < 40 \text{ km s}^{-1}$ are arranged by column density into 0.25 dex sized bins, then iteratively removed if they lie outside $2\sigma$ of the bin mean until no points are removed. Previously removed points which lie below this final mean are rejected from the final set.

(iii) Similar to the $\sigma$–rejection, the cutoff is fit by iteratively removing points and refitting. After an initial fit, points that lie more than $1\sigma$ above the fit are removed and the cutoff is fit with the reduced set of points. The fitting, removing, and refitting process is repeated until no more points meet the removal criteria. As a final step, points which lie more than $1\sigma$ below this converged fit are removed and one last fit is made.

Note that in the above algorithm the $\sigma$–rejection step uses the RMS deviation while the cutoff fitting step uses the mean absolute deviation and a column density normalization of $N_{\text{HI},0} = 10^{13.6}$, in agreement with Schaye et al. (1999) and Rudie et al. (2012).

An example of the cutoff fit can be seen in Figure 3. The results for the intercept, $b_0$, and slope, $\Gamma - 1$, of these fits for the main simulations are shown in the top panels of Figures 4 and 5. The bottom panels of these figures show the percent difference between the main simulations when the spectra used have not been rescaled (red), and when they have been rescaled (black). Difficulties with fitting Voigt profiles at higher redshift due to fewer unsaturated features (a lower ionized fraction) lead to a more ambiguous cutoff in the distribution, so we only attempt to fit a cutoff up to $z = 4$.

Our results agree closely with Rudie et al. (2012), for the redshifts in which we overlap that work. At $z = (2.4)$, Rudie et al. (2012) find a intercept and slope of $b_0 = 17.9$ and $\Gamma - 1 = 0.152$, respectively. At the same redshift we find $b_0 = 17.4$ and $\Gamma - 1 = 0.148$.

Figure 2. Results for the average curvature versus redshift. The curvature is robust up to higher redshift, hence the inclusion of redshifts up to $z = 6$. The agreement is extremely good, with a maximum difference of $< 2\%$ at redshift $z = 6$. The simulation box has periodic boundaries, so each peak is centered before the fitting takes place (to account for absorbers lying across the edge of the box).
0.153 for the case with separate transfer functions and \( b_0 = 17.1 \) and \( \Gamma - 1 = 0.154 \) when they are the same. Additionally, Rudie et al. (2012) split their sample into lower \((z = (2.3))\) and higher \((z = (2.7))\) redshift bins. Their results in these bins agree with the trend we see in both parameters, \( b_0 \) increasing with time and \( \Gamma - 1 \) decreasing with time.

Hiss et al. (2018) did not find a consistent trend in either of the cutoff parameters, in some disagreement with the results found here. However, the values at lower redshift are similar, with Hiss et al. (2018) reporting \( b_0 = 18.2 \) and \( \Gamma - 1 = 0.14 \) at \( z = 2 \) and \( b_0 = 18.7 \) and \( \Gamma - 1 = 0.17 \) at \( z = 2.4 \). The difference in the two fit parameters brought about by the separate transfer functions is not consistent with redshift (it leads to increase at some times, and a decrease at others), indicating that the primary driver of any differences is due to the sample of spectral features used in the fit. This is further indicated by the continued variance in the fit parameters as the sample size is increased (see Figure A4, bottom two panels).

Convergence of these results between the main simulations and fixed mass resolution and fixed volume simulations are discussed in Appendix A and can be seen in Figure A2. Convergence with number of sight lines used is also discussed in the Appendix and can be seen in Figure A4 (bottom two panels).

### 3.3 Flux Power Spectrum

Lyman–\( \alpha \) forest spectra from the IGM can also be used to constrain cosmologies alternative to ΛCDM. For example, a warm dark matter particle suppresses structure relative to CDM on scales smaller than the WDM particle free-streaming scale (Narayanan et al. 2000). Lyman–\( \alpha \) forest spectra probe the scales relevant to the WDM model and can be used to estimate the clumping of matter (the matter power spectrum) through the observed flux distribution (the flux power spectrum) (Viel et al. 2004). The flux power spectrum is \( P_F(k) = \langle \delta_F(k) \rangle \), where \( \delta_F(k) \) is the Fourier transform of the

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**Figure 3.** Examples of the distribution of column densities and Doppler widths at \( z = 2.4 \) from the main simulation with separate transfer functions. The green line is the best fit cutoff given by Equation 2 with \( b_0 = 17.4, \Gamma - 1 = 0.153 \).

**Figure 4.** Results for the minimum width, i.e. the intercept for the fitted cutoff. The simulation with separate transfer functions is in good agreement with the single transfer function simulation. The bottom panel shows the percent absolute difference between the scaled (black), and unscaled (red) results. At most the unscaled results differ by \( \approx 6\% \) at \( z = 4 \) and the scaled results differ by \( \approx 2\% \).

**Figure 5.** The same as Figure 4, but for the slope of the fitted cutoff. The agreement is good, peaking at \( \approx 8\% \) difference for both the scaled (at \( z = 3.2 \)) and unscaled results (at \( z = 2 \)).
flux excess, $\delta_F(k) = F(k)/\langle F(k) \rangle \sim 1$, and $L$ is the length of the sight lines in velocity space.

The effect of WDM on the flux power spectrum is to suppress high $k$ (> 0.01 s/km) power and marginally enhance low $k$ (< 0.01 s/km) power (Viel et al. 2013; Iršič et al. 2017a). The shape of the Lyman-α forest flux power spectrum can be used to measure the suppression scale, which directly constrains the WDM particle mass. The ever increasing number of observed quasar sight lines has meant that a statistically significant sample can be assembled to look at this effect (Iršič et al. 2017b; Walther et al. 2018).

These constraints rely on accurate modeling of the flux power spectrum in simulations using a CDM or WDM model, coupled with observed Lyman-α forest spectra. Figure 6 shows the effect of using separate transfer functions for baryons and CDM on the Lyman-α forest flux power spectrum. Shown is the percent change in the power spectrum when using separate transfer functions instead of a single transfer function. The effect is generally strongest at the high end of the $k$ range, with a decrease in power across all redshifts at $k < 0.02$ for the rescaled result. The effect increases with redshift, however both the rescaled and unscaled results remain at $\lesssim 5\%$ across the range of $k$ our simulations reliably probe.

While observations extending to the largest wave numbers used here are not presently available, we can compare the flux power spectrum we obtain from our simulations to currently available data where they overlap. Figure 7 shows our flux power spectrum at $z = 3$ and $z = 4$ compared to data taken from Iršič et al. (2017b). Their estimate of the Lyman-α contribution to their total flux power, as well as their total flux power, are shown with the reported errors. Our results show a small underestimate of the power in comparison with them, but are roughly consistent. To estimate the level of agreement, we interpolate our flux power spectrum onto the wave numbers of the Iršič et al. (2017b) data. We find that at most, our power spectrum differs by $\delta_F(k) \sim 2.5\sigma$ from their data (where the deviation is their reported statistical and systematic errors, added in quadrature). For most data points, the difference is within $1\sigma$. In terms of this deviation, the difference between the single and separate transfer function cases is $< 1\sigma$.

### 3.4 Matter Power Spectrum

The total matter power spectrum is affected only at the $1 \sim 2\%$ level at all scales probed with the simulations presented in this work ($k = 0.6 \sim 100$ h Mpc$^{-1}$). This is unsurprising, as the effect of the separate initial conditions is to decrease the power in the baryons, while retaining the behaviour at both higher redshift (for linear structure to dominate on a large range of scales) and at lower redshift (for baryons to collapse into non-linear structures at small scales). The offset is independent of $k$, and is consistent both with linear theory (O’Leary & McQuinn 2012) and with Bird et al. (2020).

### 4 SUMMARY & CONCLUSIONS

In this work we have explored how switching from a single initial transfer function (for both baryons and CDM) to species specific transfer functions affects properties of the IGM. Using a set of high

![Figure 6](https://example.com/figure6.png)
resolution simulations, we have quantified the effect this change has on probes of the IGM via the Lyman-α forest. The main simulations presented here differ only in the transfer functions used; one uses a single transfer function, the other follows Bird et al. (2020), adopting species specific transfer functions. Our work is motivated by simulations generally not matching the theoretical offset between baryon and cold dark matter power. Artificial spectra were extracted from snapshots in the $2 < z < 6$ range and statistics relevant to the thermal history of the IGM and WDM models were calculated. We did not include a WDM model in any of the simulations — cold dark matter is assumed throughout — thus the results are approximations to the level of effect one should expect due to this change to the simulations. Below we summarize the main results of this work.

- The curvature statistic is relatively unaffected by the use of the species specific initial transfer functions, with a peak difference of $< 2\%$ at $z = 6$.
- The Doppler width cutoff fit parameters converge less well with number of sight lines used (see Figure A4) and simulation parameters. This is likely due to the fitting method being more sensitive to the inclusion or omission of data points. Regardless, the effect on these parameters is larger than for the curvature, at most $\approx 5\%$ for the fit intercept and $\approx 8\%$ for the fit slope.
- The flux power spectrum is affected more at high $k$ ($k > 0.05$ $\text{s/km}$) and redshift ($z > 2$). However, the enhancement to the power is at most $\approx 5\%$ for $z > 2$ and $\lesssim 1\%$ at $z = 2$.

For measures of the thermal state of the IGM, the effect of the separate transfer functions is either small ($\sim 1\%$ for the curvature) or subdominant to the sample used (Doppler width cutoff). It is therefore not a necessary inclusion at the current level of precision for these statistics.

The flux power spectrum is relatively unaffected on the scales and times which are currently well observed, however our results indicate that it may become important on smaller scales or higher redshift. This may indicate that using separate transfer functions may be important for future observations and surveys. However, the effect is most pronounced at early times and on small scales, which may become important on smaller scales or higher redshift. This may indicate that using separate transfer functions may be important for future observations and surveys. However, the effect is most pronounced at early times and on small scales, which may become important on smaller scales or higher redshift. This may indicate that using separate transfer functions may be important for future observations and surveys. However, the effect is most pronounced at early times and on small scales, which may become important on smaller scales or higher redshift. 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The future study of the IGM will be predicated on measuring absorption spectra at higher redshifts and at higher resolution using large optical and infrared telescopes in conjunction with broader surveys such as the James Webb Space Telescope (Becker et al. 2019). Given the ever increasing sample size and quality of IGM observations, it is paramount that simulations keep pace by improving their precision and modeling. The adjustment to the initial conditions in simulations explored here is one such improvement, but there are others which should be implemented as well, for example the modeling of He $\upiota$ reionization (Upton Sanderbeck & Bird...
2020). Improved simulations, in concert with future observations, will push the study of the IGM into the reionization epoch as it occurs, leading to a greater understanding of this relatively recent major phase transition, as well as the formation of the first galaxies and their subsequent evolution.

ACKNOWLEDGEMENTS

This material is based upon work supported by the National Science Foundation Graduate Research Fellowship under Grant No. DGE-1326120. SB and PUS were supported by NSF grant AST-1817256. Computing resources were provided by NSF XSEDE allocation AST2000018. The authors acknowledge the Frontera computing project at the Texas Advanced Computing Center (TACC) for providing HPC and storage resources that have contributed to the research results reported within this paper. Frontera is made possible by National Science Foundation award OAC-1818253. URL: http://www.tacc.utexas.edu

REFERENCES

Angulo R. E., Hahn O., Abel T., 2013, MNRAS, 434, 1756
Becker G. D., Bolton J. S., Haehnelt M. G., Sargent W. L. W., 2011, MNRAS, 410, 1096
Becker G., D’Aluisio A., Davies F. B., Hennawi J. F., Simcoe R. A., 2019, BAAS, 51, 446
Bird S., 2017, FSFE: Fake Spectra Flux Extractor (ascl:1710.012)

APPENDIX A: CONVERGENCE

We check the convergence of our simulations with box size and mass resolution by running an additional four simulations. For both the separate and same transfer function cases we run a fixed volume simulation (with a smaller box). The simulation volume, particle
number, and mass resolution can be seen in Table 1. The mass resolution used in the main simulations agrees with Becker et al. (2011), which previously showed convergence for the curvature at that resolution. Bolton et al. (2014) showed convergence for the $N_{\text{HI}} - b$ cutoff parameters using the same set of simulations.

Figure A1 shows the fractional difference as a percentage between each of the main simulations, and the two associated convergence simulations (called $\delta$ in this, and the next two figures) for the curvature. The curvature calculated here uses spectra without added noise, obviating the need for a spline fit. Otherwise, the calculation is the same as that outlined in Section 3.1 (spectra are renormalized into 10 Mpc/h sections and the mean flux is rescaled). The curvature is well converged, with a difference of $\lesssim 1\%$ for three of the four checks, and $\sim 5\%$ for the case using separate transfer functions and a lower mass resolution (the fixed volume case).

Figure A2 shows the convergence for the two fit parameters of the $N_{\text{HI}} - b$ cutoff. As this method uses a population of features taken from each set of spectra, renormalizing between different volume simulations is not necessary. The logarithmic intercept, $b_0$, is well converged, with an absolute difference of $< 10\%$ at all redshifts. The logarithmic slope, $\Gamma - 1$, is less well converged, remaining within an absolute difference of $< 20\%$ at all redshifts except $z = 2.4$, where the fixed volume simulation using a single transfer function is $> 30\%$. However, this is not unexpected for two reasons. The first is that saturated lines make the Voigt fitting less reliable and lead to larger scatter and less accurate cutoff fits, especially at higher redshifts, $z > 3.2$. The second is that this is a fit to a set of data, i.e. features in the spectra, and so the amount of data used to make the fit affects the result. This can be seen in the bottom two panels of Figure A4, where the convergence with the number of sight lines used is shown. In contrast with the flux power spectrum and curvature, these fit parameters do not completely converge, instead exhibiting some variance all the way up to the inclusion of all 5,000 sight lines.

Figure A3 shows the convergence for the flux power spectrum at the two redshifts which span our analysis. We are well converged at low $k (< 0.05)$ for all simulations and redshifts. At $z = 6$ we are well converged ($< 20\%$) for three cases, while the fixed volume simulation (gas particles have 8 times larger mass than the main simulation) with separate transfer functions is not well converged beyond $k \approx 0.05$. The shaded regions in Figure 6 which indicate the trusted $k$ range for each redshift are based on this. At $z = 2$ we are well converged across the range ($k < 0.1 h$ Mpc$^{-1}$) explored here.

The matter power spectrum is converged with gas mass resolution at all redshifts ($2 < z < 6$) and scales ($k = 0.6 - 100 h$ Mpc$^{-1}$) such that the difference between the higher and lower resolution simulations is $\lesssim 20\%$. Convergence with box volume is similarly converged in the range $k = 10 - 100 h$ Mpc$^{-1}$, and less well ($\approx 30\%$) from $k = 0.6 - 10 h$ Mpc$^{-1}$.

Finally, we check the convergence of the curvature, flux power spectrum, and $N_{\text{HI}} - b$ cutoff fit parameters with the number of sight lines used in each of their calculation. Figure A4 shows this convergence for two selected redshifts from the main simulation using separate transfer functions. Each statistic is calculated in the same way as in the main analysis, but using only the corresponding fraction of the 5,000 sight lines available (e.g. the 0.2 value for the $N_{\text{HI}} - b$ cutoff fit parameters use only features from the first 1000 random sight lines). While the curvature is insensitive to the number of sight lines used (beyond ~ 50 sight lines), the flux power spectrum depends strongly on the number, and the $N_{\text{HI}} - b$ cutoff fit parameters continue to fluctuate even with a large number of sight lines. Note that the convergence of the flux power spectrum shows the maximum difference between consecutive power spectra (the difference between the spectrum with $x$ sight lines and the
Figure A3. Convergence of the flux power spectrum with simulation box volume and gas mass resolution. At early times we are converged with volume and gas mass resolution. At late times the convergence breaks down for the fixed volume, separate transfer function simulation at wave numbers larger than \( \sim 0.05 \).

Figure A4. Convergence of curvature, flux power spectrum, and \( N_{\text{HI}} - b \) cutoff parameters with number of artificial spectra used. Shown here is the convergence for simulations with separate transfer functions. The flux power spectrum convergence shows the maximum change in the spectrum when additional sight lines are added. Note that the sight lines are randomly placed in the simulation box.

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