

# The short ionizing photon mean free path at $z=6$ in Cosmic Dawn III, a new fully-coupled radiation-hydrodynamical simulation of the Epoch of Reionization

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## ABSTRACT

Recent determinations of the mean free path of ionising photons (mfp) in the intergalactic medium (IGM) at  $z = 6$  are lower than many theoretical predictions. In order to gain insight into this issue, we investigate the evolution of the mfp in our new massive fully coupled radiation hydrodynamics cosmological simulation of reionization: Cosmic Dawn III (CoDa III). CoDa III's scale ( $94^3 \text{ cMpc}^3$ ) and resolution ( $8192^3$  grid) make it particularly suitable to study the evolution of the IGM during the Epoch of Reionization (EoR). The simulation was performed with RAMSES-CUDATON on Summit, and used 131072 processors coupled to 24576 GPUs, making it the largest EoR simulation, and largest RAMSES simulation ever performed. A superior agreement with global constraints on reionization is obtained in CoDa III over CoDa II, especially for the evolution of the neutral hydrogen fraction and the cosmic photo-ionization rate, thanks to an improved calibration, later end of reionization ( $z = 5.6$ ), and higher spatial resolution. Analyzing the mfp, we find that CoDa III reproduces the most recent observations very well, from  $z = 6$  to  $z = 4.6$ . We show that the distribution of the mfp in CoDa III is bimodal, with short (neutral) and long (ionized) mfp modes, respectively, due to the patchiness of reionization and the co-existence of neutral versus ionized regions during the EoR. The neutral mode peaks at sub-kpc to kpc scales of mfp, while the ionized mode peak evolves from  $0.1 \text{ Mpc/h}$  at  $z = 7$  to  $\sim 10 \text{ Mpc/h}$  at  $z = 5.2$ . Computing the mfp as the average of the ionized mode provides the best match to the recent observational determinations. The distribution reduces to a single neutral (ionized) mode at  $z > 13$  ( $z < 5$ ).

**Key words:** cosmology: reionization – galaxies: high-redshift

## 1 INTRODUCTION

The Epoch of Reionization (EoR hereafter) began as the first ionising galactic sources started to ionize their immediate surroundings in the inter-galactic medium (IGM) some few hundred million years after the Big Bang. This epoch lasted approximately 600 Myr, until the reionization of the IGM was complete at some point between  $z \approx 6$  and  $z \approx 5.3$  (Bosman et al. 2021, Bo21 hereafter). Constraining

this distant epoch offers unique insight into the formation of the first galaxies and stars, and is an important step in bridging the gap between our knowledge of 'modern' galaxies, and the first moments after the Big Bang. Indeed, the rising and expanding UV background during the EoR may suppress star formation in low mass galaxies (Ocvirk et al. 2016, 2020; Dawoodbhoy et al. 2018, the former two will be called Oc16 and Oc20 from hereon). This in turn motivated efforts to investigate and predict possible signatures of the EoR in

populations of galaxies of the lowest mass, which are best observed in the Local Group (Ocvirk & Aubert 2011; Iliev et al. 2011; Ocvirk et al. 2013, 2014; Dixon et al. 2018).

Due to the very nature of the EoR and the extreme distances involved, direct observations of the reionizing sources as they drive reionization are extremely challenging. Despite this, over the past decades innovative indirect constraints on both the sources of reionization and on the IGM have emerged. Further, the future is bright as upcoming space and ground based observatories (e.g. the James Webb Space Telescope, the Nancy Grace Roman Space Telescope, or the Extremely Large Telescope) will improve our capability to target the drivers of reionization. At the same time, current and planned 21cm radio observations (e.g. EDGES, HERA, LOFAR, NenuFAR, SKA) may bring new constraints on the ionisation of the IGM during the EoR and at cosmic dawn. Thus, the study of the EoR appears to be set for rapid progress over the coming years. In preparation of this new era of EoR observations, the simulation community is hard at work making predictions for these new observational campaigns, and investigating the physical processes that drive the sources of reionization. However, the predictive power of these simulations relies on the quality of their agreement with existing observational constraints, some of which have proved difficult to match.

For instance, recent determinations of the mean free path of ionising photons (mfp hereinafter), at a higher redshift than ever before, have shown that models and simulations of reionization overestimate the mfp when  $z \approx 6$  (and possibly when  $5.24 \lesssim z \lesssim 6$ ), casting doubt on the realism of their portrayal of the ionisation state of the IGM and thus cosmic reionization as a whole (See Becker et al. 2021, Be21 from hereon). Already, new work has investigated the implications of these new data, finding that they require late and rapid reionization scenarios (Davies et al. 2021; Cain et al. 2021, Da21 and Ca21 from hereon). In fact, Ca21 have been able to obtain a reasonable agreement with both the new and old mfp constraints. We consider below these two recent works attempting to match the new very low mfp measurement of Be21 and show how using Cosmic Dawn III (CoDa III)<sup>1</sup> may improve upon them. Both studies above use a fairly low resolution simulation of the IGM ( $\sim 1\text{cMpc}$  cell size), and must recourse to complex sub-grid models, to:

- model the source population: Da21’s description of sources involves a range of parameters which fold in a number of complex and coupled aspects, such as the sensitivity of sources to SN and AGN feedback, their star formation efficiency, their escape fractions and the global dependence of these processes with respect to mass. However, as we show in Ocvirk et al. (2021)(Oc21 hereafter), radiative suppression of star formation in low mass haloes is crucial to obtaining a realistic Lyman-alpha forest after overlap. This regulation, for instance, is not included in Da21, and CoDa III improves on their approach by allowing this process to occur self-consistently thanks to the fully coupled radiation hydrodynamics (RHD) framework employed.
- set the transmission properties of the IGM sub-grid: Ca21 uses a sub-grid parameterization of the mean free path, which relies on simulations of irradiated patches (D’Aloisio et al. 2020). Such simulations do not include star formation, and one can therefore estimate that their densest patch structures would at some point form stars and therefore, both decrease their own mean free path and the mean free path around them.

Our approach circumvents the need for using such a sub-grid

model of the mean free path, as the whole volume of CoDa III is eligible to star formation provided the relevant criteria in density and temperature are met. Moreover, the mfp is self-consistently set in CoDa III by the physical state of the IGM, and is self-consistently affected by radiation received by sources near and far and the high-resolution hydrodynamical description of the IGM.

Beyond these two studies, it is desirable, in all cases, to deploy a fully coupled RHD formalism as we do here, in order to break free from the limitations imposed by the parameterization of the physical processes at hand as in Da21; Ca21, and check that the results they claim can be confirmed in more self-consistent simulations where more physics are resolved and therefore do not require such a level of sub-grid modelling. In this direction, the THESAN project (Kannan et al. 2021; Garaldi et al. 2021) has recently performed a series of AREPO-RT (Kannan et al. 2019) simulations of the EoR. While they reach high spatial resolution inside of galaxies, CoDa III improves on their approach in at least 2 aspects: their fiducial run, THESAN-1, stops at  $z=5.5$ , whereas we were able to go beyond this redshift, down to  $z=4.6$ , and as a result compare CoDa III mfp with observations in a larger redshift range, which, most importantly, includes post-reionization measurements as well. Also, THESAN-1 uses a typical speed of light reduction of 0.2, which can have a strong impact on the post-reionization residual neutral hydrogen fraction (Ocvirk et al. 2019), and to some extent change the timing of reionization (Deparis et al. 2019), complicating the interpretation of their simulation results. To avoid such difficulties, Cosmic Dawn III uses the full speed of light thanks to the GPU-optimized radiative transfer module CUDATON (Oc16; Oc20).

First, we present our methodology, including the particularities of our simulation code RAMSES-CUDATON, the simulation setup, and the computational steps we take to derive the mfp. Then, we present the global properties of reionization in the CoDa III simulation, and the evolution of the mfp in CoDa III. Finally we conclude our work.

## 2 METHODS

### 2.1 Simulation

#### *Overview of RAMSES-CUDATON*

The CoDa III (Cosmic Dawn III) simulation was performed using the fully coupled radiation and hydrodynamics code RAMSES-CUDATON (presented in Oc16; Oc20). Here we briefly recall its main properties as well as details concerning its deployment.

RAMSES-CUDATON results from the coupling of the RAMSES code for N-body dark matter dynamics, hydrodynamics, star formation and stellar feedback (Teyssier 2002), with the radiative transfer module ATON (Aubert & Teyssier 2008), which handles the radiative transfer of ionising photons via the M1 method (Levermore 1984), hydrogen photo-ionisation and thermo-chemistry. Motivated by the important computational cost of radiative transfer, we accelerate the ATON module using GPUs (Aubert & Teyssier 2010), whilst the remaining RAMSES physics run on CPUs. The performance boost thus obtained allows us to run fully coupled simulations with a full speed of light, circumventing pitfalls encountered by certain reduced speed of light approaches (Gnedin 2016; Deparis et al. 2019), in particular on the residual neutral fraction after overlap (Ocvirk et al. 2019).

<sup>1</sup> More information can be found about the whole simulation suite and the CoDa project here: <https://coda-simulation.github.io/>.

### Improvements over our previous simulation CoDa II

For the most part, the code and simulation setup are as described in [Oc20](#), but with higher resolution. Other features of CoDa III which differ from past CoDa simulations were fully tested and calibrated by a large suite of smaller simulations of the same numerical resolution as CoDa III to ensure a good match to observational constraints on the EoR. While the chief purpose of these calibration runs was to prepare for CoDa III, the calibration runs themselves were novel enough to warrant new science as described in [Ocvirk et al. \(2021\)](#). Since the new features of CoDa III were already described there, we refer the reader to that paper for more detail. We quickly enumerate the novelties of CoDa III with respect to CoDa II hereafter.

- CoDa III uses a  $8192^3$  grid while CoDa II had a  $4096^3$  grid, for the same volume, meaning its physical resolution is a factor of two finer, and its mass resolution is eight times higher.

- We take a more detailed approach with respect to our source model than in the previous CoDa simulations. In CoDa III, each stellar particle receives an ionising emissivity value based on its mass, age, and metallicity. We pre-compute emissivities using BPASS V2.2.1 [Eldridge & Stanway \(2020\)](#), considering that each stellar particle is a star cluster of about  $10^4 M_\odot$  forming over a few Myr as in [Oc21](#). As a result, in CoDa III individual stellar particles' ionising luminosities decrease more gradually and realistically than in CoDa II, where stellar particles had a fixed stellar luminosity until their massive stars went supernova, and their ionising luminosities were set to 0.

- We use a sub-grid stellar escape fraction of  $f_{\text{esc}}^{\text{sub}} = 1$ , whereas we used  $f_{\text{esc}}^{\text{sub}} = 0.42$  in CoDa II, i.e. all photons produced by the stellar particles in CoDa III are released in the host cell.

- One of the main model differences with respect to CoDa II lies within the star formation sub-grid model. In CoDa III, for a gas cell to form stars, we not only require that it be dense enough, but also that it be cooler than  $2 \times 10^4$  K. This additional temperature threshold for star formation has been widely used in similar simulations before CoDa III including CoDa I ([Ocvirk et al. 2016](#)) and others (e.g. [Dubois & Teyssier 2008](#)). Its physical interpretation is as follows: gas cells hotter than the threshold are so because of shocks, usually caused by supernovae, which are not favoured sites for star formation until they manage to cool back down to below the  $2 \times 10^4$  K threshold.

We also found that including the temperature threshold allowed our simulations to achieve better agreement with the residual neutral fraction at the end of the EoR and with the ionisation rate of ionized regions, thus advocating its use in CoDa III. For more information and a comparison between star formation with, and without the temperature threshold, we refer the reader to [Oc21](#).

- Just as in CoDa I & CoDa II (the two previous Cosmic Dawn simulation projects), upon reaching 10 Myr of age, a mass fraction  $\eta_{\text{SN}} = 0.2$  of stellar particles detonates as supernovae. Each supernova event injects 51 ergs of energy for every  $10 M_\odot$  of progenitor mass into its host cell (using the kinetic feedback of [Dubois & Teyssier 2008](#)). After the supernova event, a long lived particle of mass  $(1 - \eta_{\text{SN}})M_{\text{birth}}$  remains. Unlike CoDa I and CoDa II, CoDa III features the standard RAMSES chemical enrichment<sup>2</sup>. Metals are produced by supernovae. A fraction  $y = 0.05$  of the total supernova mass is re-injected as metals. Metallicity is treated as a passive scalar, and metals are thus advected along with the gas.

- CoDa III features a physically motivated model for the formation and destruction of dust in galaxies on the fly, that we coupled to the ionizing radiative transfer of ATON ([Lewis et al. 2022](#), in prep). An independent paper on the dust model is also in preparation ([Dubois et al.](#)), but the reader can find details on its implementation in another branch of the RAMSES code in [Trebitsch et al. \(2021\)](#). The dust aspects of CoDa III will be analysed in a forthcoming paper, and can be left aside for the present study.

For quick reference, Table 1 recaps the essential physical and numerical parameters of CoDa III.

### Initial conditions & Cosmology

As in previous CoDa simulations, CoDa III's initial conditions were constrained so as to produce facsimiles of the progenitors of the Local Group (See [Sorce et al. 2016](#); [Sorce & Tempel 2018](#)) within the Constrained Local Universe Simulations project (CLUES<sup>3</sup>). We will use this unique opportunity to investigate the reionization of the Local Group in a forthcoming paper. For the present study and for the purpose of this paper, we can forgo the Local Universe aspect and treat CoDa III as a random realization of the Universe, as its mass function, for instance, is compatible with that of a random patch of Universe. The cosmology used ( $\Omega_\Lambda = 0.693$ ,  $\Omega_m = 0.307$ ,  $\Omega_b = 0.0482$ ,  $H_0 = 67.77 \text{ km s}^{-1} \text{ Mpc}^{-1}$ ,  $\sigma_8 = 0.829$ ,  $n = 0.963$ ) here is taken from the Planck 2014 constraints ([Planck14](#))<sup>4</sup>, as summarised in Table 1. The initial conditions were generated at  $z = 150$ .

### Deployment

CoDa III was run on Summit at the Oak Ridge National Laboratory / Oak Ridge Leadership Computing Facility. It was deployed on 131072 processors coupled with 24576 GPUs, distributed on 4096 nodes, and ran for  $\sim 10$  days, allowing CoDa III to reach a final redshift of  $z=4.6$ , i.e. sufficiently late after overlap that we can consider reionization complete and sample well into the post-overlap phase. Snapshots were written every  $\sim 10$  Myr, we use a subset of them to derive the properties of the IGM in the following section. Subsequent processing of the more than 20 PB of data outputs took place at the same facility on Andes and Summit.

## 2.2 Computing the mean free path of ionising photons

To compute the mfp, we employ three approaches:

- First, we employ a method (called average transmission method from hereon) inspired by [Kulkarni et al. \(2016\)](#). For a given simulation snapshot, we draw 1024 lines of sight (LoS) across the whole simulation box in one direction. Our LoS are evenly separated so as to evenly sample the box.

For each LoS, we then compute the transmitted flux at  $912 \text{ \AA}$  as a function of position along the LoS  $x$ . These can then be averaged into one average transmitted flux  $F(x)$ , from which we obtain  $\lambda_{\text{AT}}$  by fitting it with Eq. 1 for the parameter  $\lambda$ :

$$F(x) = F_0 \exp\left(-\frac{x}{\lambda}\right) \quad (1)$$

where  $F_0$  is a normalisation parameter, equivalent to a flux incident

<sup>2</sup> for clarification: this is not a new code feature, but was not activated at run time in the previous simulations, for simplicity.

<sup>3</sup> <https://www.clues-project.org/cms/>

<sup>4</sup> these constraints are compatible with subsequent Planck publications

Setup	
Grid size & Dark matter particle number	8192 <sup>3</sup>
Box size	94.43 cMpc
Force resolution	
...comoving	11.53 ckpc
...physical (z = 6)	1.65 kpc
Dark matter particle mass	$5.09 \times 10^4 M_\odot$
Average cell gas mass	$9.375 \times 10^3 M_\odot$
Stellar particle mass	11 732 $M_\odot$
Star formation & feedback	
Density threshold for star formation	$50 < \rho_{\text{gas}} >$
Temperature threshold for star formation	$2 \times 10^4 \text{ K}$
Star formation efficiency $\epsilon_\star$	0.03
Massive star lifetime	10 Myr
Supernova energy	$10^{51} \text{ ergs}$
Supernova mass fraction, $\eta_{\text{SN}}$	0.2
Supernova ejecta metal mass fraction	0.05
Radiation	
Stellar ionising emissivity model	BPASS V2.2.1 binary (from Eldridge & Stanway 2020)
Stellar particle sub-grid escape fraction, $f_{\text{esc}}^{\text{sub}}$	1.0
Effective photon energy	20.28 eV
Effective HI cross-section (at 20.28 eV)	$2.493 \times 10^{-22} \text{ m}^2$
Reionization	
CMB electron scattering optical depth, $\tau_{\text{es}} (z = 14)$	0.0497
reionization mid-point, $z_{\text{re}}, 50\%$	6.81
reionization complete, $z_{\text{re}}, 99.99\%$	5.53

**Table 1.** Overview of the CoDa III simulation.

where  $x = 0$ , that is free during the fit. For key redshifts, we check that our results are converged with respect to the number of lines of sight, and find no significant difference in our result with 8x or 64x more lines of sight. In order to mimic the small number statistics regime of the observations, we draw samples of only 13 LoS (the same LoS sample size as in Be21, at  $z=6$ ) from our full sample of 1024. We repeat this  $10^5$  times, and our final  $\lambda_{\text{AT}}$  result is then the median of these  $10^5$  realizations. Also of interest, this approach yields the standard deviation of this set of mfp.

- Second, in order to access the distribution of mfp belonging to individual lines of sight ( $\lambda_{\text{los}}$  hereafter), we fit Eq. 1 to the transmitted flux of every LoS individually. We can then also compute the mean, median, and spread of the resulting distribution at every redshift. The results from bad fits (reduced  $\chi^2 > 1.0$ ) are discarded.

- Third, as we will see in Sec. 3.2, our  $\lambda_{\text{los}}$  are divided into two families that reside in neutral, and ionized areas of the IGM. We can easily isolate the evolution of the  $\lambda_{\text{los}}$  from the ionized regions so as to more closely mimic the observational context of the measurement of mfp, since such measurements cannot be performed in still neutral medium. To this end, for every redshift we divide the distribution of  $\lambda_{\text{los}}$  in two modes, at the approximate position of the minimum of the distributions and therefore the transition between the modes, and consider only the long mode of the distribution, corresponding to ionized LoSs. We refer to this approach as the ionised method. We use the notation  $\lambda_i$  to refer to mfps computed in this manner.

### 3 RESULTS

#### 3.1 Global properties of the IGM during the EoR

The top left panel of Fig. 1 shows the evolution of the average volume weighted neutral fraction of hydrogen ( $\langle x_{\text{HI}} \rangle$ ) in CoDa III and CoDa II, along with a range of constraints. In both simulations,

$\langle x_{\text{HI}} \rangle$  starts to drop noticeably between  $z = 10$  and  $z = 9$ . However, in CoDa III, reionization ends later and less abruptly than in CoDa II, only finishing by  $z \approx 5.6$  ( $\approx 6$  in CoDa II). Further, in CoDa II the final average value of the neutral fraction is far lower than in CoDa III. This latter difference is due to the combination of the new star formation sub-grid model and improved resolution, as explained in Oc21. Considering this, along with the rather late reionization obtained (compared to the canonical value of  $z=6$  for the end of reionization in use since Fan et al. 2006), CoDa III is in much better agreement with the constraints from the transmission in the Lyman- $\alpha$  forest (and modelling) on  $\langle x_{\text{HI}} \rangle$  after reionization. In particular, the agreement with the data from Bo21 is excellent. The match with constraints from Becker et al. (2015) is also remarkable in CoDa III after the ankle of the  $\langle x_{\text{HI}} \rangle$  curve, although Becker et al. (2015) favours slightly earlier reionization than in CoDa III. Finally we find that the older constraints from Fan et al. (2006) are disfavored both by the more recent determinations of Bo21 and Becker et al. (2015), and our own simulations. The bottom left panel of Fig. 1 shows the evolution of the average ionised fraction of Hydrogen ( $x_{\text{HII}}$ ) on a linear scale, along with the same constraints. CoDa III is in better agreement with a greater fraction of the collection of constraints for  $x_{\text{HII}} \gtrsim 0.1$  than CoDa II. Overall the agreement of CoDa III with modern constraints on the evolution of the progress of reionization is very good.

The top right panel of Fig. 1 shows the evolution of the ionisation rate in ionized regions ( $\langle \Gamma_{\text{HII}} \rangle$ ) in both CoDa III and CoDa II. In the former,  $\langle \Gamma_{\text{HII}} \rangle$  rises rapidly by roughly a factor of 10 between  $z = 7$  and  $z = 5.5$ , after which the slope becomes shallower. CoDa III's  $\langle \Gamma_{\text{HII}} \rangle$  is a very good fit to the mix of observational constraints available, and a great improvement on the  $\langle \Gamma_{\text{HII}} \rangle$  from CoDa II, which overshoots all constraints for the presented redshift range. This excess is symptomatic of CoDa II's excessive ionisation of the IGM (see Oc20; Oc21, for discussions about this). As with  $\langle x_{\text{HI}} \rangle$ , the origin of this improvement lies both in the switch to a late reionization calibration and in the improved star formation sub-grid model, as well as increased resolution (as discussed in Oc21).

The bottom right panel of Fig. 1 shows that although reionization ends later in CoDa III, the optical depth due to scattering on free electrons seen by the Cosmic Microwave Background remains compatible with the constraints given by the latest Planck results (Planck18), demonstrating that a late reionization scenario may still yield a high enough electron scattering optical depth<sup>5</sup>.

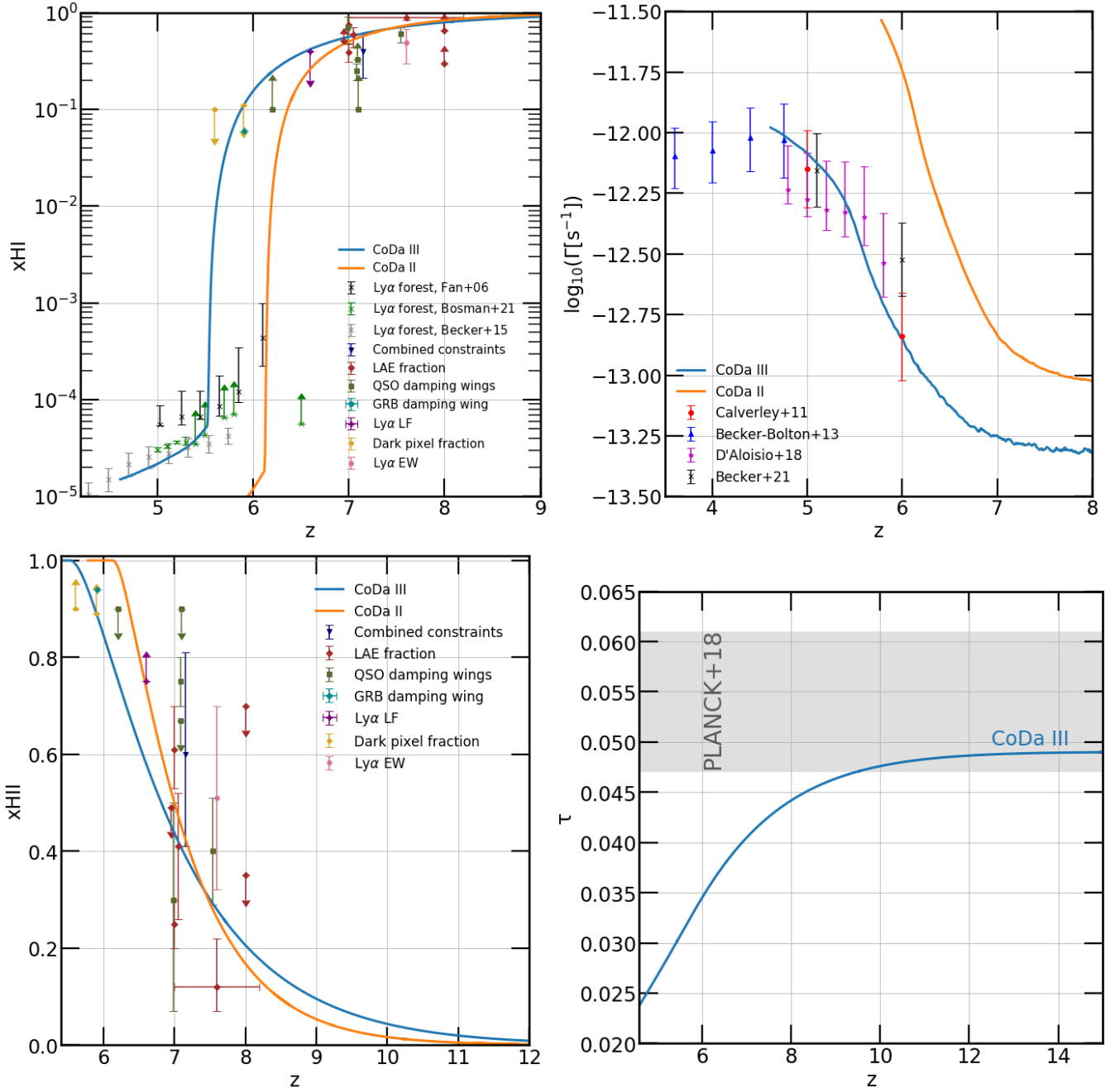
Overall reionization in CoDa III reaches a better agreement with observational constraints on the IGM and other works from the literature than CoDa II did, signalling a marked improvement in our description of reionization.

#### 3.2 Results: the mean free path of ionising photons

We now move to our titular subject: the mean free path of ionising photons. Fig 2 shows the evolution of mfp over time in CoDa III. Observations from Worseck et al. (2014) and Be21 show that the mfp increases over time for  $z < 6$ . The full blue line with errorbars shows that in CoDa III,  $\lambda_{\text{AT}}$  increases from  $\approx 1 \text{ cMpc h}^{-1}$  at  $z \approx 6$  to  $\approx 20 \text{ cMpc h}^{-1}$  at  $z \approx 4.6$ . In fact,  $\lambda_{\text{AT}}$  grows faster between  $z \approx 5.75$  and  $z \approx 5.2$ , allowing CoDa III to match the newest low mfp from observations at  $z = 6$  (Becker et al. 2021) and the high observed

<sup>5</sup> An even higher optical depth may still be achieved by adding the contribution from mini-halos at  $z \geq 15$ , adding an extra  $\Delta\tau_{z \geq 15} \approx 0.008$ , that are not treated in this work but suggested by Ahn & Shapiro (2021).



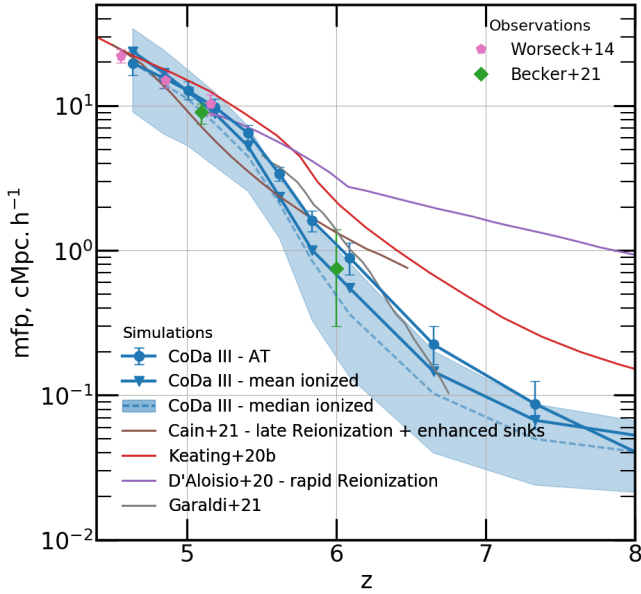


**Figure 1.** *Top left:* Volume weighted average neutral fraction along with a collection of constraints including Fan et al. (2006); Becker et al. (2015); Bosman et al. (2021); Ouchi et al. (2010); McGreer et al. (2015); Totani et al. (2016); Wang et al. (2021); Āurovčková et al. (2020); Bañados et al. (2018); Schroeder et al. (2013); Mortlock et al. (2011); Tilvi et al. (2014); Pentericci et al. (2014); Schenker et al. (2014); Ono et al. (2012); Mason et al. (2018); Hoag et al. (2019); Greig & Mesinger (2017); Jung et al. (2020). *Top right:* Ionisation rate in ionized regions when compared to constraints from Calverley et al. (2011); Becker & Bolton (2013); D'Aloisio et al. (2018); Becker et al. (2021). *Bottom Left:* Volume weighted ionised fraction. *Bottom Right:* Optical depth to CMB photons due to scattering by free electrons, compared to the Planck collaboration results Planck18. CoDa III is in very good agreement with constraints on the history of ionisation of the IGM as well as on the ionization rate, whilst remaining compatible with the optical depth due to electron scattering measured by Planck, despite a rather late end of reionization. Overall the improvement over CoDa II is very significant.

mfp at  $z \lesssim 5.25$ , whereas most other theoretical work has tended to overshoot the observed mfp at  $z=6$ . Because of the stronger evolution of the mfp in CoDa III, we report values that are significantly lower than in other theoretical work for  $z \gtrsim 6$ , where observations are very challenging. This points to substantially different progressions of

reionization in the IGM of these other simulations, feasibly implying differences in ionising emissivities and source populations.

Already, previous work (Da21; Ca21) has highlighted that the latest determinations of mfp by Be21 point to a late and rapid reionization, which CoDa III matches. However, unlike in Cain et al.



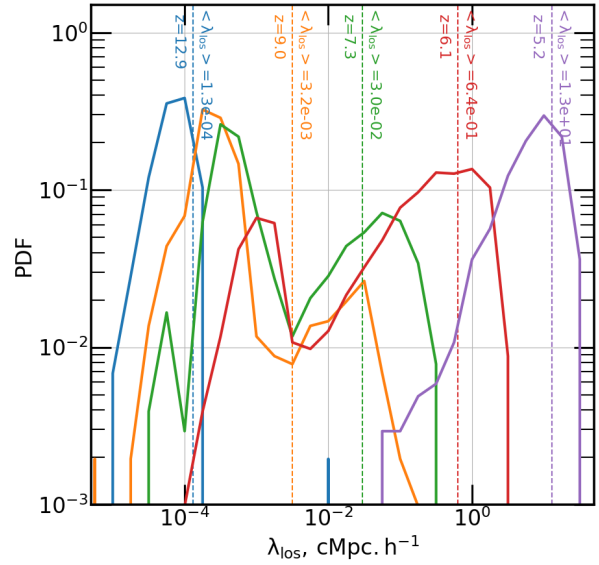
**Figure 2.** Evolution of the mean free path with redshift in CoDa III, and comparison to observational constraints from (Worseck et al. 2014; Becker et al. 2021) and previous simulation results from the literature (Keating et al. 2020; D’Aloisio et al. 2020; Cain et al. 2021; Garaldi et al. 2021). The blue graphics show results from CoDa III. The full blue line with circles and errorbars show the median and 25<sup>th</sup> – 75<sup>th</sup> percentile region for  $\lambda_{AT}$ . The full blue line with triangles shows the mean  $\lambda_i$ , the blue dashed line and blue region show the median and 25<sup>th</sup> – 75<sup>th</sup> percentile region  $\lambda_i$ . The median mean free path in CoDa III is in good agreement with existing observational constraints from  $z = 4.5$  till  $z = 6$ .

(2021) we do not need to invoke unresolved photon sinks in order to obtain our agreement with the observed mfp.

The THESAN simulation (Garaldi et al. 2021) also finds a good agreement with the  $z = 6$  data point from Be21, however, unfortunately, the simulation ended too soon to comment on their agreement with lower redshift constraints, and it is therefore difficult to gauge the overall success of their simulation in reproducing the evolution of the properties of the IGM over the whole EoR, down to the post-overlap regime. In any case, it is possible that fully coupled RHD simulations are better able to match the mfp constraint from Be21 at  $z = 6$  than post-processing or modelling methods, perhaps because of the more consistent treatment of the radiative-hydrodynamical interactions in the IGM and possible radiative feedback in galaxies, and/or the superior resolution.

In order to gain further insight into what drives the mfp measured in CoDa III, we show the distribution of individual LoS mfp (i.e.  $\lambda_{los}$ ) at several redshifts in Fig. 3. At  $z = 12.9$ , before reionization is fully underway, the distribution of  $\lambda_{los}$  has a single mode near  $10^{-4} \text{ Mpc h}^{-1}$ . Although this is shorter than the simulation’s cell size, it is physical: indeed, the general formula for the mean free path of ionising photons reads  $1/\sigma\rho_{HI}$ , where  $\sigma$  is the interaction cross-section and  $\rho_{HI}$  the number density of neutral hydrogen atoms. In the dense, neutral high-redshift Universe before reionization, mean free paths shorter than our cell size naturally occur and are fully consistent with the measurements presented here.

By  $z = 7.3$ , reionization is in full swing, and the distribution of  $\lambda_{los}$  is now bi-modal, displaying a short and a long mode. The short mode peaks around  $8 \times 10^{-4} \text{ Mpc h}^{-1}$  and seems to descend from the  $z = 12.9$  mode. However, approximately 30% of LoS



**Figure 3.** Distribution of  $\lambda_{los}$ . Dashed vertical lines show the distribution mean for each redshift. For readability, only a subset of redshifts roughly 200 Myr apart between  $z=12.9$  and  $z=5.2$  is shown. The  $\lambda_{los}$  are distributed in a neutral opaque mode of short mean free paths, and an ionised transparent mode of long mean free paths. The relative weight of these modes changes as reionization progresses.

are now scattered around a secondary, longer mode peaking near  $\lambda_{los}=10^{-1} \text{ Mpc h}^{-1}$ . This bi-modality reflects the co-existence of large fully ionized regions already by  $z = 7.3$ , when reionization is almost complete in half of CoDa III’s volume (about 40% ionized reading from the bottom left panel of Fig. 1). At  $z = 6.1$ , both modes have moved to slightly higher  $\lambda_{los}$  values ( $10^{-3} \text{ Mpc h}^{-1}$  for the short  $\lambda_{los}$  peak, and  $0.64 \text{ Mpc h}^{-1}$  for the long  $\lambda_{los}$  peak), and the relative weight between modes has swapped: now most LoS belong to the long  $\lambda_{los}$  peak.

By  $z = 5.2$ , reionization is complete, all of the LoS have been ionized and the short mode has disappeared in favour of the long mode. The evolution of the  $\lambda_{los}$  distribution reveals that the CoDa III  $\lambda_{los}$  evolves due to both gradual changes along every LoS (due to cosmic expansion driving the average physical density to decrease over time), and to rapid changes along short  $\lambda_{los}$  LoS due to reionization. The rapid increase of  $\lambda_{AT}$  in Fig. 2 between  $z = 6.1$  and  $z = 5.2$  could be driven by the disappearance of the shortest  $\lambda_{los}$  values as more and more LoS experience reionization.

Fig. 3 shows that the transition between the ionised mode of the  $\lambda_{los}$  distribution and the neutral mode occurs near  $10^{-2} \text{ Mpc h}^{-1}$ . Accordingly we select only those  $\lambda_{los}$  longer than this threshold for the ionised method. The blue solid curve with triangles in Fig. 2 shows the evolution of  $\lambda_i$  in CoDa III. For  $z > 5$ , both the mean and the median  $\lambda_i$  are lower than  $\lambda_{AT}$ . This makes our prediction based on the mean  $\lambda_i$  a better match to the  $z = 6$  constraint from Be21, and also shows that the average transmission method (measuring the mean free path from an average simulated transmission spectrum) is biased towards high transmissions and overestimates the median  $\lambda_{los}$  at the redshifts considered in Fig. 2. For  $z \leq 5$ , the mean  $\lambda_i$  is slightly above the constraints from Worseck et al. (2014), however

the median remains in very good agreement and there is a broad scatter, comparable to the error bar of [Be21](#).

#### 4 CONCLUSIONS

In this article, we have presented first results from our latest large scale simulation of the Epoch of Reionization, Cosmic Dawn III (CoDa III), the largest fully coupled RHD simulation of Reionization ever performed. It improves on our previous CoDa II simulation in many aspects, such as using a two times higher spatial resolution and 8 times higher mass resolution, as well as updates of the physical modules and sub-grid models, in particular star formation and stellar source modelling. We show that, thanks to these improvements, CoDa III compares much better than CoDa II with observational constraints of the high-redshift Universe, in particular the evolution of the neutral hydrogen fraction which sees a dramatic improvement, as well as the ionizing rate in ionized regions, while the evolution of the ionized fraction and the electron scattering optical depth are also in good agreement with the constraints available. Moreover, we showed that CoDa III is the first fully coupled radiative hydrodynamics simulation to reproduce the latest constraints on the ionising photon mean free path all the way from  $z = 6$  down to  $z = 4.6$  thanks to a late reionization ( $z_{\text{rei}} = 5.6$ ) and a rapid evolution of the ionising mean free path. In particular, CoDa III shows that the surprisingly low mean free path measured by [Be21](#) can naturally occur in a well-calibrated simulation of the EoR such as ours. The distribution of mean free paths during reionization is generally bi-modal, displaying a short, neutral mode and a long, ionized mode. Both modes shift to higher mfp as reionization progresses: The neutral mode peak shifts from sub-kpc to kpc scales of mfp, and the ionized mode peak from 0.1 Mpc/h (at  $z=7$ ) to  $\sim 10$  Mpc/h at ( $z = 5.2$ ). The balance of these modes reflects the degree of ionisation of the simulated volume. The bi-modal distribution reduces to a single short (long) mode before (after) reionization, respectively. Finally, by using 3 different methods for computing the mean free path from CoDa III, we show that the choice of the method is important. In particular, measuring the mean free path from an average transmitted flux stacking a number of lines of sight tends to overestimate the mean free path otherwise obtained as the average or the median of the mfp of individual lines of sight. Overall, CoDa III's description of reionization in the IGM appears to be a marked improvement over CoDa II, providing an adequate basis with which to perform a broad range of studies of the EoR, such as Lyman- $\alpha$  transmission in the IGM, but also of star formation suppression, and the ionising photons budget of galaxies.

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#### DATA AVAILABILITY

The authors will share the data used for this article upon reasonable request.

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