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The locations of features in the mass distribution of merging binary black holes are robust against uncertainties in the metallicity-dependent cosmic star formation history.

L. A. C. van Son,^{1,2,3} S. E. de Mink,^{3,2,1} M. Chruślińska,³ C. Conroy,¹ R. Pakmor,³ and L. Hernquist¹

¹ Center for Astrophysics | Harvard & Smithsonian, 60 Garden St., Cambridge, MA 02138, USA
 ² Anton Pannekoek Institute of Astronomy, Science Park 904, University of Amsterdam, 1098XH Amsterdam, The Netherlands
 ³ Max Planck Institute for Astrophysics, Karl-Schwarzschild-Str. 1, 85748 Garching, Germany

ABSTRACT

New observational facilities are probing astrophysical transients such as stellar explosions and gravitational wave (GW) sources at ever increasing redshifts, while also revealing new features in source property distributions. To interpret these observations, we need to compare them to predictions from stellar population models. Such models require the metallicity-dependent cosmic star formation history (S(Z,z)) as an input. Large uncertainties remain in the shape and evolution of this function. In this work, we propose a simple analytical function for S(Z,z). Variations of this function can be easily interpreted, because the parameters link to its shape in an intuitive way. We fit our analytical function to the star-forming gas of the cosmological TNG100 simulation and find that it is able to capture the main behaviour well. As an example application, we investigate the effect of systematic variations in the S(Z,z) parameters on the predicted mass distribution of locally merging binary black holes (BBH). Our main findings are: I) the locations of features are remarkably robust against variations in the metallicity-dependent cosmic star formation history, and II) the low mass end is least affected by these variations. This is promising as it increases our chances to constrain the physics that governs the formation of these objects.

1. INTRODUCTION

A myriad of astrophysical phenomena depend criti-23 cally on the rate of star formation throughout the cosmic 24 history of the Universe. Exotic transient phenomena, 25 including (pulsational) pair-instability supernovae, long 26 gamma-ray bursts and gravitational wave (GW) events 27 appear to be especially sensitive to the metallicity at 28 which star formation occurs at different epochs through-²⁹ out the Universe (e.g., Langer et al. 2007; Fruchter et al. 30 2006; Abbott et al. 2016). Gravitational astronomy in 31 particular has seen explosive growth in the number of 32 detections in the past decade (Abbott et al. 2018, 2020, 33 2021a), while theoretical predictions vary greatly due to 34 uncertainties in the aforementioned metallicity of star 35 formation (e.g., Santoliquido et al. 2021; Broekgaarden 36 et al. 2021). In order to correctly model and interpret 37 these observations, it is thus fundamental to know the 38 rate of star formation at different metallicities through-39 out cosmic history; i.e. the metallicity-dependent cosmic

Corresponding author: L. van Son lieke.van.son@cfa.harvard.edu

⁴⁰ star formation history (S(Z, z), see also the recent re-⁴¹ view by Chruślińska 2022). Throughout this work little ⁴² z refers to the redshift and Z to the metallicity of star ⁴³ formation.

It is difficult to observationally constrain the shape of S(Z,z) – (see e.g., Chruślińska & Nelemans 2019; Boco et al. 2021, for discussion of relevant observational caveats). Even at low redshifts, the low metallicity part of the distribution is poorly constrained (Chruślińska et al. 2021). Nonetheless, several methods exist to estimate the metallicity-dependent cosmic star formation history.

The first method is based on empirical scaling relations, linking galaxy properties like stellar mass M_{\star} , metallicity Z, and overall star-formation rate density SFRD(z), with the galaxy stellar mass function, GSMF (see e.g. Dominik et al. 2013). However, the applied methods to infer galaxy properties and subsequently scaling relations such as the MZ-relation differ greatly, which makes it difficult to interpret these results in a consistent way (e.g., Kewley & Ellison 2008; Maiolino & Mannucci 2019; Cresci et al. 2019). Moreover, observations are generally incomplete at high redshifts and low galaxy luminosity (e.g., Chruślińska et al. 2021).

One can also directly extract the metallicity65 dependent cosmic star formation history from cosmo66 logical simulations (e.g. Mapelli et al. 2017; Briel et al.
67 2022a). However, these simulations currently lack the
68 resolution to resolve the lowest mass galaxies, and their
69 variations in S(Z,z) span a smaller range than those ob70 served in observationally-based models (Pakmor et al.
71 2022).

Alternatively, one can combine analytical models for the observed overall star-formation rate density, SFRD(z), like those from Madau & Dickinson (2014) or Madau & Fragos (2017), and convolve this with an assumed function for the shape of the cosmic metallicity density distribution, such as was was done in e.g., Langer & Norman (2006) and the phenomenological model in Neijssel et al. (2019).

In this work we follow the latter approach and propose a flexible analytical model for $\mathcal{S}(Z,z)$ that can be fit to the output of both cosmological simulations, and observational data constraints where available. In contrast to earlier work, we adopt a skewed-lognormal distribution of metallicities that can capture the asymmetry in the low and high metallicity tails.

The purpose of this proposed form is twofold. First 88 of all, the form we propose allows for an intuitive inter-89 pretation of the free parameters. This allows us to get 90 better insight of the impact of changes in these param-91 eters on the inferred ranges of astrophysical transients 92 (as we demonstrate in Section 4 using GW predictions as 93 an example). By adopting an analytical, parametrized ₉₄ form for S(Z,z), the large uncertainties can be system-95 atically explored. Secondly, both the large complica-96 tions in observational constraints, and the many uncer-97 tainties in cosmological simulations call for a generalised 98 form of S(Z,z) that can be easily updated when new in-99 formation becomes available. In particular, the advent 100 of observations with the James Webb Space Telescope promises a new era of high-redshift metallicity studies 102 of previously unexplored regimes (e.g., Sanders et al. 103 2022). We hope that this form will facilitate the flexibility needed to keep up with observations. The model 105 described in this work is incorporated in the publicly ¹⁰⁶ available 'Cosmic Integration' suite of the COMPAS code. ¹ We describe our model for $\mathcal{S}(Z,z)$ in Section 2. We 108 fit our model to the star-forming gas in the Illustris 109 TNG100 simulation in Section 3, and demonstrate an 110 example application of our model by systematically 111 varying the parameters that determine the shape of $_{112}$ $\mathcal{S}(Z,z)$ and investigate their impact on the local distribution of merging BBH masses in Section 4. We summarise our findings in Section 5.

Throughout this work, we adopt a universal Kroupa initial mass function (Kroupa 2001) with the mass limits $0.01-200\mathrm{M}_{\odot}$ and a flat $\Lambda\mathrm{CDM}$ cosmology with $\Omega_{\mathrm{M}}=0.31,~\Omega_{\Lambda}=0.69$ and $H_0=67.7\mathrm{km\,s^{-1}\,Mpc^{-1}}$ (Planck Collaboration et al. 2020).

2. A CONVENIENT ANALYTIC EXPRESSION FOR THE METALLICITY-DEPENDENT COSMIC STAR FORMATION HISTORY

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We write the metallicity-dependent cosmic star formation history as

$$S(Z, z) = SFRD(z) \times \frac{dP}{dZ}(Z, z)$$
 (1)

126 (similar to e.g., Langer & Norman 2006). The 127 first term is the star formation rate density, SFRD(z), 128 that is the amount of mass formed in stars per unit time 129 and per unit comoving volume at each redshift, z. The 130 second term, dP/dZ(Z,z), is a probability density dis-131 tribution that expresses what fraction of star formation 132 occurs at which metallicity, Z, at each redshift.

2.1. The cosmic metallicity density distribution

For the probability distribution of metallicities we draw inspiration from the approach by e.g., Neijssel et al. (2019) who used a log-normal distribution for their phenomenological model. Unfortunately, a simple log-normal distribution cannot capture the asymmetry that we see in the cosmological simulations, which show an extended tail in $\log_{10} Z$ towards low metallicity, combined with a very limited tail towards higher metallicity. To capture this behaviour we adopt a skewed-log-normal distribution instead. This is an extension of the normal distribution that introduces an additional shape parameter, α , that regulates the skewness (first introduced by O'Hagan & Leonard 1976).

The skewed-log-normal distribution of metallicities is defined as:

$$\frac{\mathrm{dP}}{\mathrm{dZ}}(Z,z) = \frac{1}{Z} \times \frac{\mathrm{dP}(Z,z)}{\mathrm{d}\ln Z}$$

$$= \frac{1}{Z} \times \frac{2}{\omega} \underbrace{\phi\left(\frac{\ln Z - \xi}{\omega}\right)}_{(a)} \underbrace{\Phi\left(\alpha\frac{\ln Z - \xi}{\omega}\right)}_{(b)}, \quad (2)$$

where (a) is the standard log-normal distribution, ϕ ,

$$\phi\left(\frac{\ln Z - \xi}{\omega}\right) \equiv \frac{1}{\sqrt{2\pi}} \exp\left\{-\frac{1}{2} \left(\frac{\ln Z - \xi}{\omega}\right)^2\right\}$$
 (3)

 $^{^{1}\} https://github.com/TeamCOMPAS/COMPAS/tree/dev/utils/CosmicIntegration$

 $_{152}$ and (b) is the new term that allows for asymmetry, which is equal to the cumulative of the log-normal dis- $_{154}$ tribution, Φ ,

$$\Phi\left(\alpha \frac{\ln Z - \xi}{\omega}\right) \equiv \frac{1}{2} \left[1 + \operatorname{erf}\left\{\alpha \frac{\ln Z - \xi}{\omega \sqrt{2}}\right\} \right]. \tag{4}$$

This introduces three parameters, α, ω and ξ , each of which may depend on redshift. The first parameter, α , is known as the "shape". It affects the skewness of the distribution and thus allows for asymmetries between metallicities that are higher and lower than the mean. The symmetric log-normal distribution is recovered for $\alpha=0$. The second parameter, ω is known as the "scale". It provides a measure of the spread in metallicities at each redshift. Finally, ξ , is known as the "location", because this parameter plays a role in setting the mean of the distribution at each redshift.

The location and the mean of the metallicity distribution—
168 To obtain a useful expression for the redshift dependence
169 of the "location" $\xi(z)$ we first express the expectation
170 value or mean metallicity at a given redshift

$$\langle Z \rangle = 2 \exp\left(\xi + \frac{\omega^2}{2}\right) \Phi\left(\beta \omega\right)$$
 (5)

172 where β is

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$$\beta = \frac{\alpha}{\sqrt{1 + \alpha^2}}.\tag{6}$$

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174 (For a more extended derivation of the moments of the 175 skewed-log-normal, see e.g., Wang et al. (2019).)

For the evolution of the mean metallicity with redshift we follow Langer & Norman (2006) and the phenomenological model from Neijssel et al. (2019) in assuming that the mean of the probability density function of metallogical icities evolves with redshift as:

$$\langle Z \rangle \equiv \mu(z) = \mu_0 \cdot 10^{\mu_z \cdot z},\tag{7}$$

where μ_0 is the mean metallicity at redshift 0, and μ_z determines redshift evolution of the location. Equating this to Equation 5, we get an expression for $\xi(z)$,

$$\xi(z) = \ln\left(\frac{\mu_0 \cdot 10^{\mu_z \cdot z}}{2\Phi(\beta\omega)}\right) - \frac{\omega^2}{2}.$$
 (8)

The scale (and variance) of the metallicity distribution—
We will also allow the "scale" ω to evolve with redshift in a similar manner,

$$\omega(z) = \omega_0 \cdot 10^{\omega_z \cdot z}.\tag{9}$$

where ω_0 is the width of the metallicity distribution at z=0, and ω_z the redshift evolution of the scale.

Note that the width, w(z) is not the same as the variance. The variance, $\sigma^2(z)$, can be expressed as

$$\sigma^2(z) = \omega^2(z) \left(1 - \frac{2\beta^2}{\pi} \right) \tag{10}$$

Asymmetry of the metallicity distribution: α —The skewness α could in principle also be allowed to evolve with redshift (e.g., $\alpha(z)=\alpha(z=0)10^{\alpha_z\cdot z}$). However, we find no significant improvement over the simpler assumption where alpha is kept constant. Note that the redshift evolution of the 'scale' (eq. 9), already captures similar behaviour in our current formalism. We therefore adopt $\alpha=\alpha(z=0)$ and $\alpha_z=0$.

In summary, Equation 2 becomes:

$$\frac{\mathrm{dP}}{\mathrm{dZ}}(Z,z) = \frac{2}{\omega(z)Z} \times \phi\left(\frac{\ln Z - \xi(z)}{\omega(z)}\right) \Phi\left(\alpha \frac{\ln Z - \xi(z)}{\omega(z)}\right)$$
(11)

where $\xi(z)$ and $\omega(z)$ are defined in Equations 8 and 9 respectively and we have assumed α to be constant.

2.2. The overall cosmic star formation rate density

For the star formation rate density, we assume the analytical form proposed by Madau & Dickinson (2014),

SFRD(z) =
$$\frac{d^2 M_{SFR}}{dt dV_c}(z) = a \frac{(1+z)^b}{1 + [(1+z)/c]^d}$$
 (12)

 $_{211}$ in units of $[M_{\odot}\,\mathrm{yr^{-1}\,cMpc^{-3}}]$. This introduces four $_{212}$ parameters: a which sets the overal normalisation and $_{213}$ which has the same units as SFRD(z) and b,c and d which are unitless and which govern the shape of the $_{215}$ overal cosmic star formation rate density with redshift.

Lastly, we combine equations 11 and 12 to form a full metallicity specific star formation rate density as described in equation 1.

220 3. FIT AGAINST COSMOLOGICAL SIMULATION

We fit our new functional form of $\mathcal{S}(Z,z)$ as defined by equations 1, 11 and 12 to the IllustrisTNG cosmological simulations. We simultaneously fit for the following nine free parameters $\alpha, \mu_0, \mu_z, \omega_0, \omega_z$, which govern the metallicity dependence and a,b,c and d, which set the overall star-formation rate density. Below we briefly discuss the IllustrisTNG simulations, and elaborate on our fitting procedure.

3.1. IllustrisTNG Cosmological simulations

Although here, we only fit our model to the TNG100 simulation, our prescription can be easily be used to fit other simulated or observational data of the metallicity-dependent cosmic star formation history².

² We provide a Jupyter notebook to facilitate this fit here: https://github.com/LiekeVanSon/SFRD_fit/blob/main/ src/scripts/Notebooks/Fit_model_to_sfrdzZ.ipynb

The IllustrisTNG-project (or TNG in short) considers galaxy formation and evolution through large-scale cosmological hydrodynamical simulations (Springel et al. 2018; Marinacci et al. 2018; Nelson et al. 2018; Pillepich et al. 2018a; Naiman et al. 2018; Nelson et al. 2019a; Pillepich et al. 2019). Such simulations provide the tools to study parts of the Universe that are not easily accessible by observations. In particular of interest for this work, they simulate the high redshift enrichment of galaxies and the tail of low metallicity star formation at low redshift.

The models implemented in the publicly available 245 TNG simulations (Nelson et al. 2019b)³ have lead to 247 many successes. These models where calibrated at the 248 resolution of the TNG100 simulation, hence TNG100 is 249 expected to provide the best overall agreement to global ₂₅₀ properties (like the star formation rate density). This why we adopt the TNG100 simulation as our fiducial simulation. For a more extended discussion focused 253 on the processes that govern the creation, distribution 254 and mixing of metals in in the TNG simulations, we re-255 fer to Pakmor et al. (2022). In short, star formation in 256 the TNG simulations is calibrated against the Kennicutt-Schmidt relation (Schmidt 1959; Kennicutt 1989), 258 using an effective equation of state (Springel & Hern-259 quist 2003). The stellar metallicity yields are an up-260 dated version of the original Illustris simulations as de-261 scribed in Pillepich et al. (2018b). Star particles deposit 262 metals into the gas through type Ia and type II super-263 novae, as well as through asymptotic giant branch stars. ²⁶⁴ The TNG simulations have been shown to match obser-²⁶⁵ vational constraints on the mass-metallicity relation of galaxies up to z=2 (Torrey et al. 2019), as well as iron abundances (Naiman et al. 2018), metallicity gradients within galaxies at low redshift (Hemler et al. 2021), and 269 the reduction of star formation in the centers of star-270 forming galaxies (Nelson et al. 2021). Several studies 271 have used the TNG simulations to make predictions for 272 astronomical transient sources (e.g. Briel et al. 2022a; 273 Bavera et al. 2022; van Son et al. 2022a). Out of the four $\mathcal{S}(Z,z)$ variations explored, Briel et al. (2022a) find 275 that TNG provides one of the best agreements between 276 observed and predicted cosmic rates for electromagnetic 277 and gravitational-wave transients, when combined with their fiducial binary population synthesis model.

On the other hand, large uncertainties and crude approximations remain in all contemporary cosmological simulations, thus also in the TNG simulations. Generally, some of the chemical evolution of galaxies in

283 cosmological simulations is unresolved, and thus de-284 pends strongly on the implemented 'sub-grid physics'. 285 A known uncertainty is that dust is not included in the 286 TNG simulations, which could mean that metallicity of 287 the star-forming gas is overestimated. Feedback from ac-288 tive galactic nuclei is not well understood theoretically 289 and is described in an approximate manner (Springel 290 et al. 2005; Weinberger et al. 2017). Furthermore, all 291 stellar winds mass loss from massive stars, binary inter-292 actions and their ionising effects are ignored (e.g. Dray 293 et al. 2003; Smith 2014; Götberg et al. 2020; Doughty & ²⁹⁴ Finlator 2021; Farmer et al. 2021; Goswami et al. 2022). ²⁹⁵ Moreover, the uniform ionising UV background is turned 296 on abruptly at z=6. This crucially impacts the amount 297 of low metallicity star formation at high redshift as it 298 allows small galaxies to produce more stars than what 299 would be expected for a gradually increasing UV back-300 ground that reaches full strength at z=6. All these 301 uncertainties underline the need for a flexible approximation of the S(Z,z), that can be easily updated when 303 cosmological models and sub-grid physics are updated.

3.2. Choices and binning of the data

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We fit equation 1 to the metallicity-dependent star formation rate of the star-forming gas in the TNG100 simulation. For this we use a binned version of the TNG data $\mathcal{S}(Z,z)_{\mathrm{sim}}$. We consider metallicities between $\log_{10}Z=-5$ to $\log_{10}Z=0$ in 30 bins, where we use $\log_{10}Z_i$ to refer to the logarithmic centres of the bins. We ignore star formation in metallicities $\log_{10}Z\leq-5$ as this accounts for less than 1% of the total cosmic star formation rate in these simulations. We consider bins in redshifts between z=0 and z=10, with a step size of dz=0.05, where z_i refers to the centres of the bins.

3.3. Optimisation function

To find a solution we use a method based on the sum of the quadratic differences between the simulations and our fit function. Using a vanilla χ -squared approach does not serve our purposes very well as it does a poor job in fitting regions where the star formation is very low. Using a χ -squared approach on the logarithm of the function instead places far too much weight on trying to fit the star formation rate in regions where the rate is very low or not even significant. After experimenting, we find that the following approach gives us satisfactory results.

We first consider a given redshift z_j . For this redshift z_j we compute the sum of the squared residuals between the cosmological simulation and our fit. This is effectively the square of the l^2 -norm:

$$\chi^2(z_j) \equiv \sum_{Z_i} \left(\mathcal{S}(Z_i, z_j)_{\text{sim}} - \mathcal{S}(Z_i, z_j)_{\text{fit}} \right)^2. \tag{13}$$

³ https://www.tng-project.org/

Here, the variable Z_i runs over all metallicity bins. We are particularly interested in properly fitting the low metallicity star formation at high redshifts. At high redshifts, the overall star-formation rate density is generally lower. To ensure that our fitting procedure gives sufficient weight to the behaviour at all redshifts, we introduce a penalisation factor to somewhat reduce the contribution of redshifts where the peak of cosmic star formation occurs, while increasing the weight at redshifts where the overall star-formation rate density is lower. To achieve this we divide $\chi^2(z_j)$ by the star formation $\sum_{Z_i} \mathcal{S}(Z_i, z_j)$ per redshift bin before adding the contribution of all redshifts. Our final expression for the cost function reads

$$\chi = \sum_{z_j} \frac{\chi^2(z_j)}{\sum_{Z_i} \mathcal{S}(Z_i, z_j)}$$
 (14)

To minimize this cost function, we use scipy optimize.minimize from SciPy v1.6.3 which mplements the quasi-Newton method of Broyden, Fletcher, Goldfarb, and Shanno (BFGS, Nocedal & Wright 2006).

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3.4. Resulting S(Z, z)

Our best fitting parameters are listed in Table 1. With these fit parameters, $\chi^2(z_j)$ is smaller than $2 \cdot 10^{-4}$ at any given redshift. To evaluate our fit, we show the residuals in Appendix A. We will refer to the $\mathcal{S}(Z,z)$ with the parameters listed in Table 1 as our fiducial model.

In Figure 1 we show our fiducial model at different redshifts and metallicities. We also show the overall starformation rate density SFRD(z) in Figure 2. In general,
our analytical model captures the metallicity-dependent
cosmic star formation history in the TNG100 simulations well (bottom panels of Figure 1). The skewedlog normal metallicity distribution is able to reproduce
the overall behaviour that is observed in TNG100 (bottom left panel, but cf. Pakmor et al. 2022, for an indepth discussion of low metallicity star formation in the
TNG50 simulation). Only minor features like the additional bump just above $\log_{10}(Z) = -2$ at redshift 2 are
missed. However, for our purposes, it is more important
to prioritise fitting the large scale trends, while we are
not so interested in smaller scale fluctuations.

Adopting a skewed-lognormal metallicity distribution allows for a tail of low metallicity star formation out to low redshifts. To emphasise the difference between a skewed-lognormal and a symmetric lognormal distribution, we show the phenomenological model from Neijssel

 $_{380}$ et al. (2019) in dotted grey. Their model falls within the $_{381}$ family of functions that is encompassed by our model $_{382}$ described in Section 2, but we note that their model is $_{383}$ distinctly different. 4

Although our model preforms well at reproducing the 385 large scale trends seen in TNG, we acknowledge that 386 more complex features as suggested by some observa-387 tional studies could be missed. One example is that 388 the SFRD(z) shape we adopt from Madau & Dickinson 389 (2014) does not account for starburst galaxies (see dis-390 cussion in Chruślińska et al. 2021). Moreover, our model 391 cannot capture inflection points in the mean metallicity, 392 because we assume both μ_0 and μ_z are constants with 393 redshift (equation 7). Contrarily, Chruślińska & Nelemans (2019) find an upturn in the amount of low metal-395 licity star formation above z = 4 if the power law of 396 the GSMF is allowed to evolve with redshift. Hence, 397 although our model is more broadly applicable than 398 previous models, in it's current form, it does not cap-399 ture the complete range of observationally-allowed varia-400 tions. Incorporating more complex functional forms for 401 our the mean metallicity could possibly capture such 402 behaviour, but this analysis is beyond the scope of this 403 paper.

404 4. APPLICATION: SYSTEMATIC VARIATIONS OF 405 $\mathcal{S}(Z,z)$ AND THE EFFECT ON THE MASS 406 DISTRIBUTION OF MERGING BBHS

We will now demonstrate the application of our analytical model by systematically varying the parameters in our fiducial S(Z,z) model, and investigate their effect on the local mass distribution of BBH mergers originating from isolated binaries.

We use the publicly available rapid binary population synthesis simulations presented in van Son et al. (2022b).⁵ These simulations were run using version v02.26.03 of the open source COMPAS suite (Riley et al. 2022)⁶. COMPAS is based on algorithms that model the evolution of massive binary stars following Hurley et al. (2000, 2002) using detailed evolutionary models by Pols et al. (1998). In particular, we use the simulations behind Figure 1 from van Son et al. (2022b), and we refer the reader to their methods section for a detailed description of the adopted physics parameters and as-

⁴ The phenomenological model from Neijssel et al. (2019) is recovered by adopting $\mu_0=0.035,~\mu_z=-0.23,~\omega_0=0.39,~\omega_z=0,~\alpha=0,~a=0.01,~b=2.77,~c=2.9$ and d=4.7.

⁵ Available for download at https://zenodo.org/record/7612755, see also the Software and Data section in the acknowledgements

⁶ https://github.com/TeamCOMPAS/COMPAS

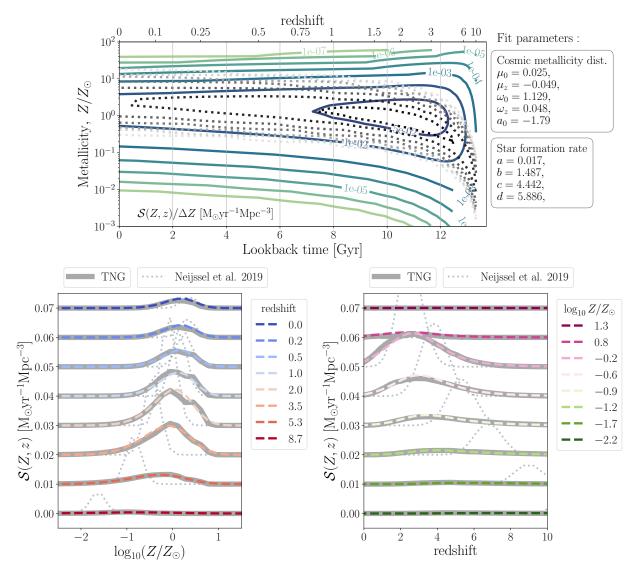


Figure 1. Our fiducial S(Z, z) model, adopting the best fitting parameters (listed on the top right) to fit the TNG100 simulations. The top panel shows the full two dimensional S(Z, z) linear in time. Contours range from $10^{-7} - 10^{-2} \text{M}_{\odot} \text{ yr}^{-1} \text{ Mpc}^{-3}$. The bottom left (right) panel shows slices of the distribution in redshift (metallicity). Each slice is displaced by $0.01 \text{M}_{\odot} \text{ yr}^{-1} \text{ Mpc}^{-3}$ (note the linear scale of S(Z, z) in the bottom panel). We show the TNG100 simulation data with thick gray lines. For comparison, we also show the phenomenological model from Neijssel et al. (2019) in all panels with grey dotted lines. The bottom panels show that our analytical model adequately captures the shape of the S(Z, z) from TNG100.

sumptions. Metallicities of each binary system were sampled from a smooth probability distribution to avoid artificial peaks in the BH mass distribution (e.g. Dominik et al. 2015; Kummer 2020). These simulations provide us with an estimate of the yield of BBH mergares ers per unit of star-forming mass and metallicity.

We combine the aforementioned yield with variations of the fiducial $\mathcal{S}(Z,z)$ model described in this work. By integrating over cosmic history, we obtain the local merger rates of BBH systems, which allow us to construct the distribution of source properties at every redistribution. We use the cosmic integration scheme that is part of the publicly available COMPAS suite, which includes the $\mathcal{S}(Z,z)$ model described in this work. The details of this framework are described in Neijssel et al. (2019), but also in van Son et al. (2022a), where more similar settings to this work are used.

4.1. Determining reasonable variations of S(Z,z)

⁷ We note that the rate in van Son et al. (2022b) is slightly higher than the fiducial rate presented in Figure 3 in this work. This difference is caused by the use of rounded parameter values of S(Z, z) in van Son et al. (2022b).

dP/dZ	description	best fit	SFRD(z)	best fit
			$\mathrm{M}_{\odot}\mathrm{yr}^{-1}\mathrm{Mpc}^{-3}$	
μ_0	mean metallicity at $z = 0$	0.025 ± 0.036	a	0.02 ± 0.072
μ_z	z-dependence of the mean	-0.049 ± 0.006	b	1.48 ± 0.002
α	shape (skewness)	-1.778 ± 0.002	c	4.44 ± 0.001
ω_0	scale at $z = 0$	1.122 ± 0.001	d	5.90 ± 0.002
ω_z	z-dependence of the scale	0.049 ± 0.009		

Table 1. Best fitting parameters for our S(Z, z) fit to TNG100 data.

Table 2. Variations on S(Z,z). For every variation, we either swap the value of an individual $\mathrm{dP}/\mathrm{dZ}(Z,z)$ parameter, or exchange the set of four $\mathrm{SFRD}(z)$ parameters, and replace them by the the min/max values listed here. All other parameters are kept fixed at their fiducial value.

min 0.007 0.0	fiducial 0.025	max 0.035
	0.0_0	0.035
	0.0_0	0.035
0.0		
0.0	-0.049	-0.5
-6.0	-1.778	0.0
0.7	1.125	2.0
0.0	0.048	0.1
0.01, 2.60	(0.02, 1.48)	(0.03, 2.6)
5.20, 6.20)	4.44, 5.90)	3.3, 5.9)
	-6.0 0.7 0.0	-6.0 -1.778 0.7 1.125 0.0 0.048 0.01, 2.60 (0.02, 1.48

We consider variations in both the shape of the cosmic metallicity density distribution dP/dZ(Z,z), and the shape of the overall star-formation rate density, SFRD(z). To determine the range that is reasonably allowed by observations, we compare our variations to the observation-based S(Z,z) models described in Chruślińska et al. (2021). An overview of the explored variations is shown in Table 2. Below we explain how we arrive at these values.

For the cosmic metallicity density distribution, we 451 vary every parameter that determines the shape of 452 dP/dZ(Z,z) independently (three left-most columns of 453 Table 1, and top of Table 2), while keeping all other 454 parameters fixed at their fiducial value. For each vari-455 ation, we inspect the fraction of stellar mass that is 456 formed at low-metallicity ($Z<0.1Z_{\odot}$) versus the frac-457 tion of stellar mass that is formed at high-metallicity 458 ($Z>Z_{\odot}$), for all star formation that occurred be-

459 low a certain threshold redshift. We compare this to 460 the models from Chruślińska et al. (2021) in Figure 6 461 in Appendix B. We have chosen our variations such 462 that they span a reasonable range of cosmic metal-463 licity density distributions as allowed by observation-464 based and cosmological simulations-based models. We use the models 214-f14SB-BiC_FMR270_F0H_z_dM.dat, 302-f14SB-Boco_FMR270_F0H_z_dM.dat 467 Chruślińska et al. (2021)⁸ as a representation of a 468 very low and high metallicity star formation realisa-469 tion respectively. These models are the low and high 470 metallicity extreme under their fiducial SFR-metallicity 471 correlation, and so we will refer to them as Chr21_lowZ and Chr21_highZ respectively from hereon. The dif-473 ference between these models lies in the assumptions 474 in the underlying empirical galaxy relations. In gen-475 eral, low-mass galaxies contribute to low-metallicity 476 star formation and shift the peak of $\mathcal{S}(Z,z)$ to lower 477 metallicities. Chr21_lowZ is characterised by a star 478 formation-galaxy mass relation that is flat at high 479 galaxy masses (reducing the star formation rate for 480 the highest-mass galaxies), a galaxy stellar mass func-481 tion that evolves with redshift (predicting an increasing ⁴⁸² number density of low-mass galaxies), and a local galaxy 483 mass-metallicity relation as in Pettini & Pagel (2004). 484 This model further approximates the contribution of 485 starburst galaxies following Bisigello et al. (2018) and 486 Caputi et al. (2017). Assuming that starburst galax-487 ies follow the empirical fundamental metallicity relation 488 (leading to anti-correlation between the SFR and metal-489 licity), their inclusion tends to shift the peak of S(Z,z)490 to lower metallicities and broadens the low-metallicity 491 part of the distribution.

On the other hand, Chr21_highZ assumes the star formation—galaxy mass relation does not flatten towards

⁸ These models including a detailed description of their contents are publicly available at https://ftp.science.ru.nl/astro/mchruslinska/Chruslinska_et_al_2021/

higher galaxy masses, a galaxy stellar mass function where the slope for the low-mass end is constant over redshift, and a local galaxy mass-metallicity relation following Kobulnicky & Kewley (2004). Lastly, this model adopts the starburst prescription from Boco et al. (2021), which produces results that are similar to models without starburst galaxies.

For every variation of our model, we inspect both the full $\mathcal{S}(Z,z)$ and slices at redshifts z=0,0.5,3.0 and 6 by eye. At each slice we compare our model variation to Chr21_lowZ and Chr21_highZ, and ensure that none of our variations significantly exceeds these extremes in $\mathcal{S}(Z,z)$. This also serves as a sanity check for the overall star-formation rate density.

We also consider two variations of the overall star-508 formation rate density, SFRD(z), where we keep the metallicity distribution dP/dZ(Z,z) fixed, but vary all four SFRD(z) parameters at once (right two columns 512 of Table 1, and bottom of Table 2). We use Figure 11 513 from Chruślińska et al. (2021) to determine approximate 514 upper and lower bounds to the overall star-formation 515 rate density. We choose Madau & Fragos (2017) as an 516 approximation of the lower limit. For the upper limit, we use the upper edge of models that adopt starbursts following Bisigello et al. (2018) and Caputi et al. (2017) (SB: B18/C17), combined with a non-evolving low-mass 520 end of the galaxy stellar mass function (shown as a thick 521 brown line in Fig. 11 of Chruślińska et al. 2021, and 522 described in their table B1). To approximate these ₅₂₃ models, we fit equation 12 by eye to the broken power 524 law description of this model as presented in appendix 525 B1 of Chruślińska et al. (2021). We show all SFRD(z)526 variations in Figure 2.

528 4.2. The effect of the S(Z,z) on the primary masses of merging BBH

To isolate the effect of the S(Z,z) from the effects of different formation channels, we split the data from van Son et al. (2022a) between the stable mass transfer channel (e.g., van den Heuvel et al. 2017; Inayoshi et al. 2017; Bavera et al. 2021; Marchant et al. 2021; Gallegos-Garcia et al. 2021; van Son et al. 2022a), and the 'classical' common-envelope channel (or CE channel, Belczynski et al. 2016; Vigna-Gómez et al. 2018). These channels are distinguished based on whether the binary system has experienced a common envelope phase (CE channel) or only stable mass transfer (stable channel in short from now on).

In Figures 3 and 4, we show the resulting primary mass distribution of merging BBHs from the stable channel and CE channel respectively. The primary (sector ondary) component refers to the more (less) massive component of merging BBHs. Each panel varies one aspect of the S(Z,z). In the first five panels of Figures 3 and 4, we vary one of the parameters that determine the shape of the probability density distribution of metallicities, while keeping all other values fixed at their vary the shape of the overall star-formation rate densities, SFRD(z), to one of the variations shown in Figure 2, while keeping the probability density distribution of metallicities fixed.

The first thing we note is that the location of the 559 features in the primary mass distribution are robust ₅₆₀ against variations in S(Z,z). For the stable channel, 561 two features are visible in all variations: a peak at $_{562}~M_{\rm BH,1} \approx 9 {
m M}_{\odot}$ and a bump at $M_{\rm BH,1} \approx 22 {
m M}_{\odot}$. Two 563 more features are visible in at the high mass end for almost all S(Z,z); a knee at $M_{\rm BH,1} \approx 35 {\rm M}_{\odot}$ and another 565 bump at $M_{\rm BH,1} \approx 45 {\rm M}_{\odot}$. Although the locations of 566 these features are constant, the features themselves can 567 disappear for variations that suppress the rate of high 568 mass BHs (e.g., dashed lines in the top panels of Fig. 569 3). Similarly, the CE channel displays a kink in the dis-570 tribution at about $9M_{\odot}$, and a peak at approximately $_{^{571}}$ $M_{\rm BH,1}$ \approx $17 \rm M_{\odot}$ for all variations. The latter peak is 572 the global peak of the mass distribution in almost all 573 variations.

The finding that the locations of features in the mass 575 distribution do not change for different $\mathcal{S}(Z,z)$ is con-576 sistent with earlier work. Recent work by Chruślińska 577 (2022) showed that, when comparing two very different models of S(Z,z) (their Figure 5), the location of the 579 peaks remains the same, even though the normalisation 580 between the two BBH merger rates is completely dif-581 ferent. Furthermore, Broekgaarden et al. (2021) show 582 the probability distribution of chirp masses for BBHs 583 in their Fig. 4. Although features can disappear when the S(Z,z) prohibits the formation of certain (typically 585 higher) mass BHs, the location of features remains the 586 same. This implies that the locations of features in 587 the mass distribution of BBHs are determined by the 588 formation channel and its underlying stellar and binary 589 physics. The locations of features could therefore serve 590 as sign posts of the underlying physics.

Second, we see that the low mass end of the primary mass distribution is relatively robust against variations in S(Z,z). To quantify this, we annotate the ratio between the maximum and minimum rate at three

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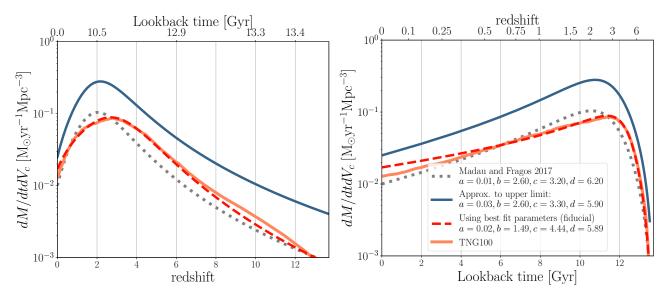


Figure 2. Comparison of several overall star-formation rate densities, SFRD(z), with redshift (left panel) and with lookback time (right panel). The solid orange and dashed red lines respectively show the star formation data from TNG100 and our corresponding fit adopting eq. 12 (fiducial model). The dotted gray and solid blue lines are variations of eq. 12 used to approximate the lower and upper edge of possible star-formation histories. The dotted gray line shows the model from Madau & Fragos (2017), while the solid blue line mimics the behaviour of the powerlaw-fit to the SB: B18/C17 variations with a non-evolving low-mass end of the galaxy stellar mass function from Chruślińska et al. (2021).

⁵⁹⁶ reference masses; $M_{\rm BH,1}=10,25,~{
m and}~40{
m M}_{\odot}.$ At $M_{\rm BH,1}=10{\rm M}_{\odot}$, we find that the rate changes by at 598 most a factor of about 3.7 for the stable channel, and 599 at most about a factor of 3.8 for the CE channel. On 600 the other hand, the change in rate at $M_{\rm BH,1}=40{
m M}_{\odot}$ 601 can be as high as a factor of about 200 and 150 for the 602 stable and CE channels, respectively. The lowest mass 603 BHs are least affected by the S(Z,z) because they can be formed from all metallicities above $Z \gtrsim 10^{-3}$ (see 605 e.g., Figures 7 and 13 from van Son et al. 2022a). The for rate of star formation at metallicities above $\gtrsim 10^{-3}$ is 607 observationally relatively well constrained for redshifts 608 below 0.5 (which comprises the past 5 Gyr of star for-609 mation). This is reflected in the top panel of Figure 610 6: all models show that 10% or less of the stellar mass ₆₁₁ was formed at a metallicity below $Z/10 \approx 0.0014$, or 612 in other words, about 90% or more of the stellar mass $_{613}$ was formed at a metallicity above $\mathbb{Z}/10$. Hence the low-614 est mass BHs derive from the least uncertain parts of the S(Z,z). The low-mass end of the mass distribution 616 of merging double compact objects will also provide a 617 particularly powerful cosmological constraint in the era 618 of third generation gravitational wave telescopes (María 619 Ezquiaga & Holz 2022). Our finding that the low mass 620 end is more robust against variations in $\mathcal{S}(Z,z)$ supports 621 this claim.

Parameter variations that affect shape of S(Z, z) at low redshift primarily change the normalisation of the mass distribution. This is the case for variations of the

625 width of the cosmic metallicity density distribution at $_{626}$ z=0 (ω_0) , the mean metallicity of the cosmic metal-627 licity density distribution at z=0 (μ_0), and the skew-628 ness of the cosmic metallicity density distribution (α , 629 left columns of Figures 3 and 4). To emphasise this 630 point, we annotate the total BBH merger rate at redshift $_{631}$ 0.2, $\mathcal{R}_{0.2}$, in the legends of Figures 3 and 4 (0.2 is the 632 redshift where the observations are best constrained Ab-633 bott et al. 2021b). Variations that increase the amount 634 of star formation at low metallicity (i.e. for a low mean 635 metallicity $\mu_0=0.007$ and a wide metallicity distribu-636 tion $\omega_0 = 2.0$) increase the predicted BBH merger rate. 637 This is consistent with other work that finds merging 638 BBHs form more efficiently at low metallicities (e.g. Bel-639 czynski et al. 2010; Stevenson et al. 2017; Mapelli et al. 640 2017; Chruślińska et al. 2019; Broekgaarden et al. 2021). 641 A more skewed cosmic metallicity density distribution 642 pushes the peak of the distribution to higher metallici-643 ties and thus forms more stars at high metallicity when 644 compared to a symmetric distribution. Hence, the local 645 rate of BBH mergers is lower for the skewed distribu-646 tion ($\alpha = -6$) with respect to the symmetric variation 647 ($\alpha = 0.0$).

Changing the overall star-formation rate density (SFRD(z), bottom right panels of Figures 3 and 4) also affects the normalisation of the mass distribution, but has a smaller effect than the width and the mean of the cosmic metallicity density distribution at z = 0 (ω_0 and μ_0). This underlines the importance of the amount of

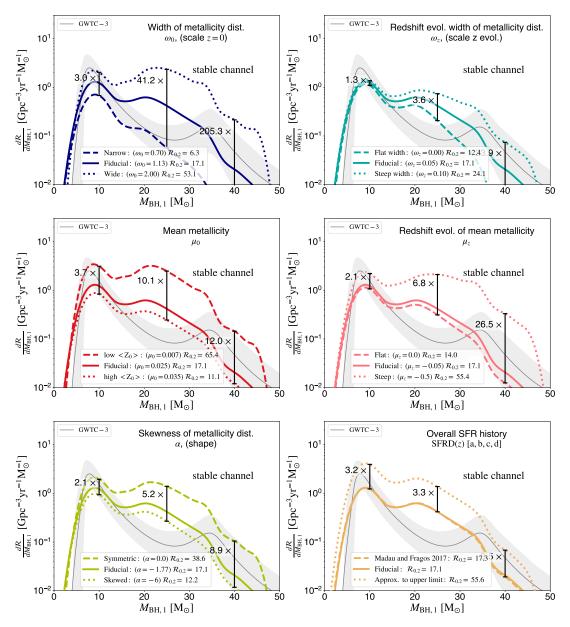


Figure 3. The primary mass distribution of merging BBH systems from the stable mass transfer channel for several variations in S(Z,z). The first five panels show variations of the cosmic metallicity density distribution dP/dZ(Z,z), eq. 11, (parameters listed in the first three columns of Table 1), where we vary one parameter at a time while keeping the rest fixed at their fiducial value. The bottom right panel shows variations in the magnitude of the star formation rate with redshift; i.e. SFRD(z). For the latter we vary the four fiducial parameters of SFRD(z) simultaneously (last two columns of Table 1). All panels are shown at a reference redshift of z=0.2, with the corresponding predicted BBH merger rate indicated in the legend. For reference, we show the power-law + peak model from Abbott et al. (2021b) in grey. We annotate the relative change in the rate at three reference masses: $10M_{\odot}$, $25M_{\odot}$ and $40M_{\odot}$.

formation (e.g., Chruślińska 2022), and is furthermore in line with findings from Tang et al. formation (2020). As discussed in Section 4.1, we use Madau & Fragos (2017) and the solid blue line in Figure 2 as an approximate lower and upper bound to the SFRD(z) respectively. The overall cosmic star formation rate density from Madau & Fragos (2017) is very similar to our fiducial model (Figure 2), and the differences be-

tween the resulting mass distributions are correspondingly small. Our approximation of the upper limit to the allowed SFRD(z) leads to an overall increase of the BBH merger rate by a factor of about 3.

Parameters that change the evolution of the metallicfor ity distribution dP/dZ(Z,z) with redshift, such as the redshift dependence of the with and mean; ω_z and μ_z for (top right and centre right panels of Figures 3 and 4)

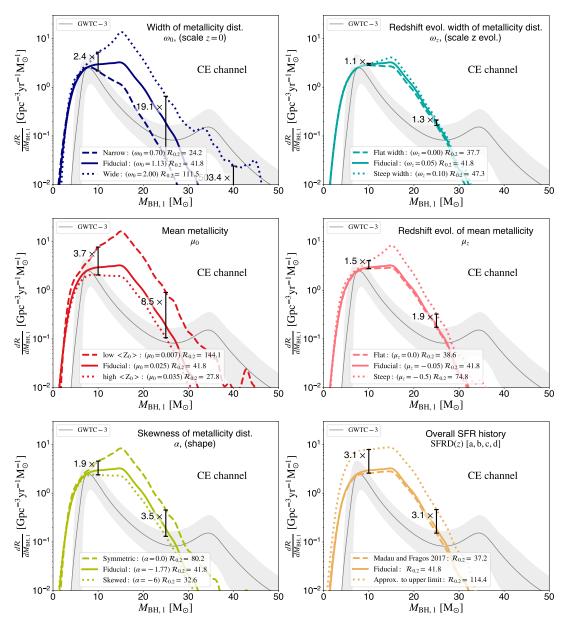


Figure 4. Same as Figure 3, but for the Common Envelope channel. These figures show that the low mass end of the primary mass distribution is least affected by the adopted S(Z, z). Moreover, the *location* of features in the mass distribution are robust against all explored variations.

primarily affect the high mass end of the stable channel. We understand this as an effect of the different delay time distributions for both formation channels. Since both, ω_z and μ_z influence the amount of low metallicity stellar mass formed at high redshifts they will mostly affect systems with longer delay times. The stable channel has been shown to produce more high mass BHs with longer delay times when compared to the CE channel (van Son et al. 2022a; Briel et al. 2022b). Hence we find these variations affect the slope of the high mass end of the BBH mass distribution for the stable channel, while they have a relatively small impact on the CE channel.

5. DISCUSSION & SUMMARY

We present a flexible analytic expression for the metallicity-dependent cosmic star formation history, S(Z,z) (equations 1, 11 and 12). An analytical expression allows for controlled experiments of the effect of S(Z,z) on dependent values, such as the rate and mass distribution of merging BBHs. The model presented in this work adopts a skewed-lognormal for the distribution of metallicities at every redshift (dP/dZ(Z,z)).

The model can capture the general behaviour of cosmological simulations, such as TNG100—Our analytical expression

for S(Z,z) is composed of a cosmic metallicity density distribution that is determined by a mean, scale and skewness and their redshift dependence, as well as parameters governing the overall star-formation rate density. We fit our analytical expression for S(Z,z) to the star-forming gas in the TNG100 simulation, and provide the best fit parameters in Table 1. We show that our model captures the shape and general behaviour of the cosmological simulations well (Figure 1). Although our model is more broadly applicable than previous models, we acknowledge that it does not capture the complete range of observationally-allowed variations in it's current form. Incorporating more complex functions for the redshift evolution of the metallicity could solve this issue, but this is left for future research.

The model allows for a controlled experiment on the effect of S(Z,z) on the local distribution of merging BBH—As an example, we use our model to calculate the local rate and mass distribution of the more massive components from merging BBHs $(M_{\rm BH,1})$ in Figures 3 and 4. We systematically vary all five parameters that shape the cosmic metallicity density distribution, and explore two additional variations of the overall star-formation rate density SFRD(z). Our main findings are as follows:

- The locations of features in the distribution of primary BH masses are robust against variations in S(Z,z). The location of features in the mass distribution of BHs could thus be used as sign posts of their formation channel.
- For all variations, the low mass end of the mass distribution is least influenced by changes in the S(Z,z). This is because the lowest mass BHs can be formed from all metallicities above $Z\gtrsim 10^{-3}$, for which the star formation rate is relatively well constrained in the recent Universe. This suggests that the lower end of the BH mass distribution (component masses of $\leq 15 {\rm M}_{\odot}$) is potentially very powerful for constraining the physics of the formation channels, irrespective of the cosmic star formation rate uncertainties.
- The metallicity distribution of star formation at low redshift primarily impacts the normalisation of the BBH merger rate. Changing the overall star-formation rate density, SFRD(z) also affects the rate, but to a lesser degree. This shows that low-metallicity star formation at low redshifts domi-

nates the overall normalisation of the BBH merger rate.

• Parameters that influence the redshift evolution of the mean and the width of the metallicity distribution affect the slope of the high mass end of the primary BH mass distribution for the stable channel. This reflects the longer delay times of the stable channel with respect to the CE channel.

The flexibility of the model presented in this work can capture the large uncertainties that remain in the shape and normalisation of the metallicity-dependent cosmic star formation history. Our hope is that this expression will provide a useful starting point for making predictions and comparisons with observations.

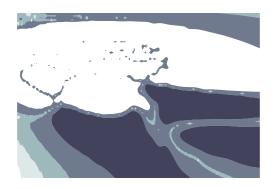
The authors acknowledge partial financial support from the National Science Foundation under Grant No. (NSF grant number 2009131 and PHY-1748958).", the Netherlands Organisation for Scientific Research (NWO) as part of the Vidi research program Bin-Waves with project number 639.042.728 and the European Union's Horizon 2020 research and innovation program from the European Research Council (ERC, Grant agreement No. 715063). This research was supported in part by the National Science Foundation under Grant No. NSF PHY-1748958.

SOFTWARE AND DATA

All code associated to reproduce the data and plots in this paper is publicly available at https://github. com/LiekeVanSon/SFRD_fit. The data used in this work is available on Zenodo under an open-source Creative Commons Attribution license at 10.5281/zen-ro odo. 7612755. All observationally constrained models of the $\mathcal{S}(Z,z)$ from Chruślińska et al. (2021) can be found online at: https://ftp.science.ru.nl/astro/mchruslinska/Chruslinska_et_al_2021/.

This research has made use of GW data provided by the Gravitational Wave Open Science Center (https: //www.gw-openscience.org/), a service of LIGO Laboratory, the LIGO Scientific Collaboration and the Virgo Collaboration. Further software used in this work: Python (Van Rossum & Drake 2009), Astropy (Astropy Collaboration et al. 2013, 2018) Matplotlib (Hunter 2007), NumPy (Harris et al. 2020), SciPy (Virtanen et al. 2020), ipython/jupyter (Perez & Granger 2007; Kluyver et al. 2016), Seaborn (Waskom 2021) and hdf5 (Collette et al. 2019).

A. EVALUATING OUR FIT; THE SQUARED RESIDUALS



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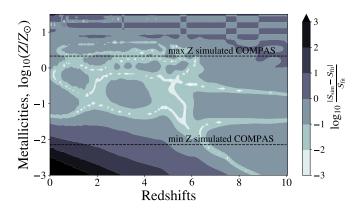


Figure 5. log of the residuals (left), and log of the relative error (right) between the TNG100 data and our best-fitting model. We show the minimum and maximum metallicity used in COMPAS simulations with dashed lines in each plot.

In the left panel of Figure 5, we show the log of the absolute residuals. The square of the residuals 788 is used in the cost function, equation 14, to optimise our fit. We observe that the maximum residuals appear near the peak of star formation at high metallicities. The log of the relative errors (defined $\frac{|\mathcal{S}\text{sim}-\mathcal{S}\text{fit}|}{S_{--}}$), is shown in the right-hand panel of Figure 5. The relative errors generally exhibit an opposite trend with respect to the residuals. The relative errors are largest in regions of very low-792 metallicity star formation at low redshift. This occurs due to the very low star-formation rate in this $_{793}$ regime (of the order $10^{-8}
m M_{\odot}\, yr^{-1}\, Mpc^{-3}$ for the TNG simulations and $10^{-11}
m M_{\odot}\, yr^{-1}\, Mpc^{-3}$ in our model ₇₉₄ fit). Another regime where the relative error becomes large is at very high metallicities (about 10 times Z_{\odot}). In this regime, the TNG data is very sparse and contains regions where the rate abruptly drops 796 to zero. To avoid sharp features in the data, we use interpolated TNG data to produce the fit. We note that we chose to minimise the squared residuals (which is similar to minimising the mean squared error) in favour of minimising, for example, the relative error, to prevent overfitting such regions of very low star-formation rate. For the illustration purposes in this work, we are most interested in closely fitting the S(Z,z) between the minimum (10⁻⁴) and maximum (0.03) metallicities that can be simulated with COMPAS (or more generally, with population synthesis simulations). For applications that focus on extremely low ($< 0.01 Z_{\odot}$) or extremely high ($\sim 10 \times Z_{\odot}$) metallicity star formation, a different cost function would be more appropriate.

B. DETERMINING REASONABLE VARIATIONS OF THE S(Z,z)

To determine reasonable variations of our fiducial model for S(Z, z), we compute the fraction of low and high metallicity stellar mass formed for redshifts below z < 0.5, z < 3.0 and z < 10. We show the results in Figure 6, which is an adaptation of Fig. 2 in Pakmor et al. (2022), which in turn builds on Fig. 9 from Chruślińska & Nelemans (2019).

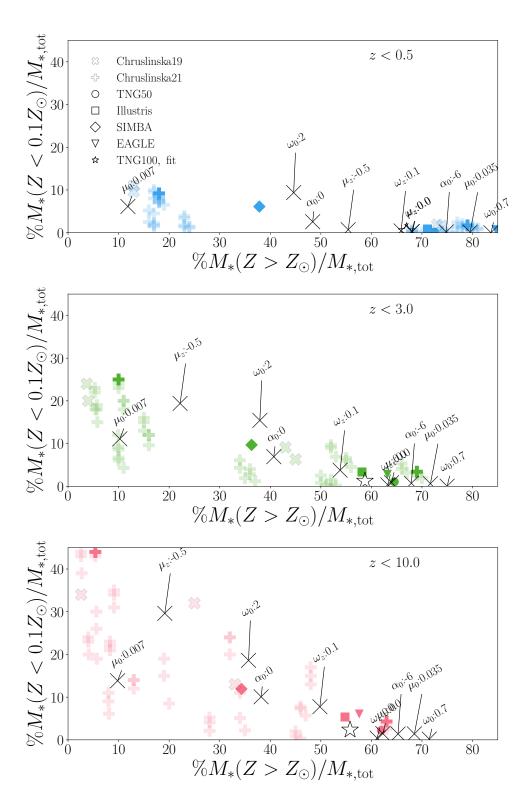


Figure 6. Percentage of stellar mass formed at low metallicity ($Z < 0.1Z_{\odot}$), versus high metallicity ($Z > Z_{\odot}$) for all star formation below a certain threshold redshift: z < 0.5 (top), z < 3.0 (middle) and z < 10 (bottom). Data from observation-based variations are shown with semi-transparent thick crosses, (Chruślińska & Nelemans 2019) and semi-transparent thick plus signs (Chruślińska et al. 2021), the low- and high-metallicity extremes are indicated with opaque symbols. For data from cosmological simulations, we follow Pakmor et al. (2022) and show Illustris (Vogelsberger et al. 2014, squares), Simba (Davé et al. 2019, diamonds), EAGLE (Schaye et al. 2015, triangles), TNG50 and TNG100 (Springel et al. 2018, filled and open circles respectively). Black thin crosses display variations of the cosmic metallicity density distribution that is part of our fiducial S(Z,z). The parameter that is varied with respect to the fiducial and its new value are annotated. This shows that our S(Z,z) variations span the range of reasonable cosmic metallicity density distributions as determined by observation-based and cosmological simulations-based models.

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