Separate Universe Consistency Relation and Calibration of Halo Bias

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Linear halo bias is the response of dark matter halo number density to a long wavelength fluctuation in the dark matter density. Using abundance matching between separate universe simulations which absorb the latter into a change in the background, we test the consistency relation between the change in a one point function, the halo mass function, and a two point function, the halo-matter cross correlation in the long wavelength limit. We find excellent agreement between the two at the 1% level for average halo biases between 1 ≤ b1 ≤ 4 and no statistically significant deviations at the 4–5% level out to θ ≈ 8. Halo bias inferred assuming instead a universal mass function is significantly different and inaccurate at the 10% level or more. The separate universe technique provides a way of calibrating linear halo bias efficiently for even highly biased rare halos in the ΛCDM model. Observational violation of the consistency relation would indicate new physics, e.g. in the dark matter, dark energy or primordial non-Gaussianity sectors.

I. INTRODUCTION

Dark matter halos, which host observable galaxies and galaxy clusters, are biased tracers of the underlying dark matter density field of the large-scale structure of the Universe. Therefore understanding the mass, redshift, and scale dependence of halo bias is important for extracting cosmological information, on e.g. dark energy, massive neutrinos and the statistics of the primordial perturbations. From ongoing and future wide-area galaxy surveys such as the Dark Energy Survey, Dark Energy Spectrograph Instrument, the Subaru HSC/PFS Survey, and ultimately LSST, Euclid and WFIRST, we are able to probe the large scale density fluctuation of the dark matter, dark energy or primordial non-Gaussianity sectors.

In this paper we consider a related but alternative way of understanding and calibrating linear halo bias. As in the peak-background split approach, linear halo bias is modeled as the response of the number density of halos, or halo mass function, to a change in the background dark matter density field. Unlike the universal mass function implementation, this linearized change in the background is modeled throughout the whole past temporal history of the density fluctuation using the separate universe simulation approach developed in Refs. [22, 33, 34, 35]. The induced change in the mass function yields the response of halo number densities to the background dark matter density, or “response bias”. Defined in this way, the response bias is quite general in a sense that it does not assume the universality of halo mass function and it includes all the effects of mergers and mass accretion that are correlated with the background density mode. It can also be easily extended to baryonic and galaxy formation effects using simulations that include them.

We furthermore use a consistent set of simulations to address whether the response bias matches the clustering bias, and also compare the results with the fitting formula of clustering bias in Ref. [22]. Observational violation of this consistency relation would indicate new physics where the dark matter, dark energy, primordial non-Gaussianity or other effects provide alternate means of producing a mass function response to the dark matter density fluctuation.

The outline of this paper is as follows. In §I we define response bias and clustering bias in a ΛCDM cosmology, give a brief review of the separate universe simulation, and then propose the abundance matching method for calibrating the response bias. We present results and tests of the consistency of response and clustering biases in §II. We discuss the results in §IV. In the Appendices, we present robustness checks on the bias results and compare them with inferences from the universal mass func-
tion assumption.

II. HALO BIAS

A. Halo response vs. clustering bias

Dark matter halos of a given mass $M$ are biased tracers of the underlying dark matter density field. On large scales where the dark matter density fluctuations $\delta = \delta \rho_m / \rho_m$ are still in the linear regime $|\delta| \ll 1$, we can think of biasing as the linearized response of the halo number density to changes in the dark matter density, implicitly of some linear wavenumber $k$,

$$b_1(M) \equiv \frac{d \delta_h}{d \delta} = \frac{d \ln n_{n,M}}{d \delta},$$

where the mass function $n_{n,M}(M)$ is the differential number density of halos per logarithmic mass interval. We will call this quantity the “response bias”.

This definition of linear density bias is quite general as it includes any effect that is correlated with the change in $\delta$, as designated by the total derivative in Eq. (1). For example the halo density in a given mass range can change due to mass accretion, minor mergers, and major mergers. A change in $\delta$ could also be correlated with changes in the dark energy or massive neutrino density that could likewise influence halo numbers through their impact on the history of structure formation, e.g. the halo accretion and merger history [4, 38–41]. Intrinsic non-Gaussian correlation between long wavelength initial curvature fluctuations and small scale power in the density field can also change the response in a scale dependent way [2].

On the other hand, we can define the linear density bias directly via cross-correlation of halos with the cold dark matter density field:

$$b_1(M) = \lim_{k \to 0} \frac{P_{h\delta}(k; M)}{P_{\delta\delta}(k)},$$

where

$$\langle \delta_h(k)\delta(k') \rangle = (2\pi)^3 \delta(k-k')P_{h\delta}(k),$$

$$\langle \delta^*(k)\delta(k') \rangle = (2\pi)^3 \delta(k-k')P_{\delta\delta}(k).$$

We will call this form for $b_1$ “clustering bias”. Eqs. (1) and (2) characterize the same physical quantity since the mass function response can come from any effect that is correlated with $\delta$. Uncorrelated changes in the halo density, e.g. from stochasticity in the bias, can affect the autocorrelation of halos but by definition do not change the cross-correlation.

In this paper we focus on the most fundamental response, that of the direct influence of the long wavelength dark matter density fluctuation on the halo number density in the $\Lambda$CDM cosmology with Gaussian initial conditions. The critical assumption that we seek to test is the extent to which this local number density depends only on the local mean dark matter density. In this case the equivalence of Eqs. (1) and (2) forms a consistency relation between the change in a one point function, the halo mass function, and a two point function, the halo-matter cross correlation in the long wavelength limit. Validation of this consistency relation would allow two alternate means of calibrating bias in simulations. Observational tests of this consistency can in principle uncover new physics beyond $\Lambda$CDM where the dark matter, dark energy or primordial non-Gaussianity provide alternate means of producing a mass function response to $\delta$.

Specifically, as detailed in the next section, we will use separate universe (SU) simulations to test this consistency relation. In this approach, the fluctuation in the dark matter density is characterized by changes to cosmological parameters or spatially constant background densities to match the mean fluctuation $\delta_b = \delta$. This should be compared with the well-known peak-background or universal mass function approach to quantifying $b_1$ through the mass function $n_{n,M}$. Here it is assumed that the mass function can be described as a universal function of the peak height $\nu = \delta_c/\sigma(M)$, the ratio of the collapse threshold of halos $\delta_c$ relative to the rms linear density fluctuations in a radius that encloses the mass $M$ at the background density $\sigma(M)$. Changing the collapse threshold via shifting the background $\delta_c \to \delta_c - \delta_b$ then changes the number density of halos, providing an approximation for $b_1$ through Eq. (1).

Both the separate universe and the universal mass function approach seek to characterize the response bias through replacing $\delta$ with a change in the background $\delta_b$. However the former does not rely on the existence of a universal mass function or the idea of a strict threshold for collapse of dark matter halos. All types of responses of the mass function to the background, including the highly nonlinear processes of the merger history of halos etc., are automatically included in the simulations. Although we only test $N$-body effects and dark matter halos here, this in principle applies to baryonic effects and galaxy tracers through simulations that incorporate them. We present the separate universe approach in the main text and its comparison to the universal mass function approach to [13].

B. Separate universe technique

To calibrate numerically the response of halo mass function to a background mode, we use the separate universe (SU) simulation technique [32–35]. We follow Ref. [32] and refer the reader there for details.

In summary, the long-wavelength density fluctuation $\delta_b$ is absorbed into the background density $\bar{\rho}_{mW}$ of a separate universe:

$$\bar{\rho}_{mW} = \bar{\rho}_m(1 + \delta_b),$$

where the quantities with subscript “W” denote the quantities in separate universe.
The separate universe consequently has a different expansion history, and accordingly we need to change cosmological parameters for the flat ΛCDM cosmology, to the first order of \( \delta_b \), as

\[
\frac{\delta h}{h} = \frac{H_0 W - H_0}{H_0} = -\frac{5\Omega_m \delta_b}{6D},
\]

where the linear growth rate is normalized as \( \lim_{a \to 0} D = 1 \). Since \( \delta_b / D \) is independent of time the SU is characterized by a simple constant shift in parameters. Similarly the other parameters need to be changed to

\[
\frac{\delta \Omega_m}{\Omega_m} = \frac{\delta \Omega_{\Lambda}}{\Omega_{\Lambda}} = -\delta K = -2 \frac{\delta h}{h}.
\]

Thus in the presence of a \( \delta_b > 0 \), the properties of smaller scale structures including the abundance of halos experience the accelerated growth of a closed universe.

Finally, the separate universes have to be compared at the same time which corresponds to a different value of the scale factor

\[
a_W \simeq a \left( 1 - \frac{\delta_b}{3} \right).
\]

Because of this difference, the SU simulations are most naturally set up as a Lagrangian approach where the simulation volumes match in their comoving rather than physical volume (cf. [32] for an alternative method that matches physical volumes at a specific time). This splits the response of the mass function into two pieces. The first corresponds to the change due to the growth of structures, including processes such as shell crossing, mass accretion and merger of halos

\[
b_1^L(M) \equiv \frac{\partial \ln n_{\text{in,}M}^L}{\partial \delta_b} = \frac{\partial \ln n_{\text{in,}M}^L}{\partial \delta_b} \bigg|_{V_c},
\]

where \( |V_c| \) denotes the separate universe response at fixed comoving volume. “L” superscripts refer to that fact that this generalizes the concept of Lagrangian bias to the whole volume rather than individual N-body particles or halos. The second is due to the change in the physical volume and hence physical densities due to Eq. (7) or

\[
\frac{\partial \ln a_W^L}{\partial \delta_b} = -1.
\]

The sum of these two effects is then the Eulerian response bias

\[
b_1(M) \equiv b_1^L(M) + 1.
\]

It is important to note that this is a definition and hence is exact, rather than an approximation that relies on halo number conservation. This is the growth-dilation derivative technique developed in Ref. [33] as applied to the mass function response. Calibrating the response bias with separate universe simulations therefore amounts to determining the derivative of the Lagrangian mass function \( n_{\text{in,}M}^L \) with respect to the background density fluctuation \( \delta_b \) in Eq. (8).

\[
\text{FIG. 1.} \quad \text{Abundance matching relates the number density weighted bias above threshold mass } M_{\text{th}} \text{ to the shift of that threshold. The halo abundance above } M_{\text{th}} \text{ grows in proportion to the bias function when increasing } \delta_b, \text{ which we can compensate by moving } M_{\text{th}} \text{ accordingly. This figure graphically illustrates Eq. (13).}
\]

\[
C. \quad \text{Abundance matching}
\]

Much of the response of the Lagrangian mass function \( n_{\text{in,}M}^L \) to \( \delta_b \) comes from small changes in the mass of individual halos rather than a change in the net number of halos in the volume. Therefore measuring the response by binning halos into finite mass ranges is very inefficient (see § A.2), since the mass change associated with a small \( \delta_b \) only shifts the mass of halos near bin edges.

Given the pairs of SU simulations with the same Gaussian random fields, in principle the same halos could be identified in each and the response calculated from the average change in the mass. However, in practice the identity of halos can be easily affected by mergers. Even for those halos for which a one-to-one correspondence exists, their change in mass is not uniquely determined by \( M \) due to differences in the environment around halos of the same \( M \) which introduces scatter into the mapping. This suggests that we need to find a statistic that does not rely on a one-to-one correspondence between SU halos in mass whose ensemble average recovers the desired response in numbers.

Abundance matching of the cumulative number density or mass function of halos above a given mass threshold \( M_{\text{th}} \) provides such a statistic [42][43]. Defining

\[
n(M_{\text{th}}; \delta_b) \equiv \int_{M_{\text{th}}}^{\infty} \frac{dM}{M} n_{\text{in,}M}^L (M; \delta_b),
\]

we change the threshold \( M_{\text{th}}(\delta_b) \) to keep the cumulative number density in the comoving volume fixed when varying \( \delta_b \)

\[
\frac{dn(M_{\text{th}}; \delta_b)}{d\delta_b} = 0.
\]
We use \((\ldots;p)\) to denote a quantity for which we omit the parameter \(p\) where no confusion should arise.

Abundance matching balances two effects to keep the number density the same, as illustrated in Fig. [I]. The first is the boundary effect of halos moving across a threshold shifted by \(s\) due to the change in \(\delta_b\)

\[
d\ln M_{th} = s(M_{th}) d\delta_b.
\]

The second is the integrated change in the mass function itself, which is the effect we want to extract for estimating response bias. Abundance matching sets these to be equal:

\[
n_{in,M}(M_{th}) s(M_{th}) = \int_{M_{th}}^{\infty} \frac{dM}{M} \frac{\partial n_{in,M}^L}{\partial \delta_b},
\]

which also follows algebraically from Eq. [11] and Eq. [12].

Measuring the mass shift \(s\) associated with matching the abundance therefore provides a way of estimating the average response bias above threshold

\[
\bar{b}_{th}^L(M_{th}; \infty) = \frac{1}{n(M_{th})} \int_{M_{th}}^{\infty} \frac{dM}{M} \partial n_{in,M}^L \frac{\partial n_{in,M}^L}{\partial \delta_b}
\]

\[
= \frac{1}{n(M_{th})} \int_{M_{th}}^{\infty} \frac{dM}{M} \partial \ln n_{in,M}^L \frac{n_{in,M}^L}{n(M_{th})}
\]

\[
= \frac{n_{in,M}^L(M_{th}) s(M_{th})}{n(M_{th})}.
\]

We emphasize that such an estimation of the response bias does not rely on any assumption on the universality of halo mass function.

Note that measuring this quantity also defines the average bias in a finite mass bin

\[
\bar{b}_{th}^L(M_1, M_2) = \frac{\int_{M_{th}}^{M_2} \ln M dM \frac{\partial n_{in,M}^L}{\partial \delta_b}}{\int_{M_{th}}^{M_2} \ln M d\ln M}
\]

\[
= \frac{n_{in,M}^L(M_1) s(M_1) - n_{in,M}^L(M_2) s(M_2)}{n(M_1) - n(M_2)}.
\]

In the limit that \(M_2 \to M_1\) from above this quantity is simply the Lagrangian bias or mass function response itself \(b_{th}^L(M_1)\) and is equivalent to replacing the formal definition in terms of derivatives

\[
b_{th}^L(M) = -\frac{\partial s}{\partial \ln M} - s \frac{\partial \ln n_{in,M}^L}{\partial \ln M}.
\]

with a finite difference approximation. Since the clustering bias also must be explicitly estimated from finite mass binning it is in fact Eq. [16] that should be directly compared with it. As a shorthand convention we plot the average bias in a bin as

\[
\bar{b}_{th}^L(M) = \bar{b}_{th}^L(M_1; M_2)
\]

using the average mass of halos in the bin

\[
M \equiv \frac{\int_{M_{th}}^{M_2} \ln M d\ln M n_{in,M}^L}{\int_{M_{th}}^{M_2} \ln M d\ln M n_{in,M}^L}.
\]

Following our notational convention, we also take

\[
\bar{b}_{th}^L(M) = \tilde{b}_{th}^L(M; \infty)
\]

when no confusion will arise.

To measure these response bias quantities directly, we need the estimators of the cumulative mass function \(n(M)\), the threshold mass shift \(s(M)\) and the differential mass function \(n_{in,M}^L(M)\) in the Lagrangian volume. We consider their explicit construction in [III C].

### III. METHODOLOGY AND RESULTS

In this section we describe the methodology to calibrate the model ingredients needed to estimate response and clustering halo biases using suites of simulations in the fiducial cosmology and its separate universe pairs. We then show the main results that establish their consistency.

#### A. Simulations

We simulate the fiducial ΛCDM cosmology specified in Tab. [I]. Each pair of separate universe simulations have the same realizations of the initial Gaussian random density field, in order to reduce the sample variance in the change of the mass function.

| \(\Omega_m\) | \(\Omega_b\) | \(h\) | \(n_s\) | \(\sigma_s\) |
|--------|--------|-----|------|-------|
| 0.310  | 0.04508 | 0.703 | 0.964 | 0.785 |

**TABLE I. Parameters of baseline flat ΛCDM model [5].**

We set up the initial conditions using CAMB [44, 45], and 2LPTIC [40], with 1024\(^3\) particles at \(a_i = 0.02\). We then employ L-Gadget2 [47] with 2048\(^3\) TreePM grid to produce the simulations. For calibrating response bias we employ \(N_{sim} = 32\) simulations with \(V_c = (500\text{ Mpc}/0.703)^3\) for each of 3 \(\delta_b = 0, \pm 0.01\) at \(z = 0\). The separate universe variations all have the same comoving volume \(V_c\) in Mpc\(^3\) (see [II B]).

The \(\delta_b = \pm 0.01\) pairs are used in abundance matching and the \(\delta_b = 0\) simulations are used to calibrate the mass function (see [II B]). Since measuring clustering bias for rare high mass halos requires more numbers than response bias, we supplement these with \(N_{sim} = 25\) simulations with \(V_c = (1\text{ Gpc}/0.703)^3\) fiducial simulations at \(\delta_b = 0\). The particle masses for the two box sizes are \(1.4 \times 10^{10} M_{\odot}\) or \(1.1 \times 10^{11} M_{\odot}\) respectively which limits the minimum halo mass that we can robustly identify as we shall now discuss.

#### B. Halo finding and catalog

While the choices made in halo finding can affect the mass function and bias results, for tests of the correspon-
C. Halo mass functions and mass shift

As discussed in §1C, we measure the response bias through an abundance matching technique to reduce the shot noise in its determination. This technique requires us to estimate the cumulative and differential mass function in the fiducial model as well as the mass shift from matching the ±δ_b pairs of SU simulations. We show here that these can be robustly estimated without binning the halo catalogs in mass. Coarse binning would miss the small changes in mass due to δ_b whereas fine binning would be subject to severe shot noise.

We start by combining the halo catalogs of all N_sim simulations of the same δ_b and V_c into a single halo catalog ordered from highest to lowest mass i > j for M_i < M_j with total number N_tot. We construct a table for the cumulative abundance above a given mass object in the catalog as

\[
\ln M = [\ln M_1, \ldots, \ln M_{N_{\text{tot}}}]^T, \\
\mathbf{n} = \left[\frac{1}{2}, \ldots, N_{\text{tot}} - 1\right]^{\frac{1}{2}}^T, \\
N_{\text{sim}}V_c
\]

which we will denote as the data vector \(\mathbf{n}(\ln M; \delta_b, V_c)\).

Here we count the halo with mass \(M_i\) as one half above and one half below \(M_i\) due to discreteness, and recall \(V_c\) is the comoving volume in \(\text{Mpc}^3\) and is fixed in the SU simulations when varying \(\delta_b\).

Next we construct a data vector of mass shifts by abundance matching. Since we have rank ordered the vector from highest to lowest mass, at a given \(i\), the abundances match by definition

\[
n_{i}(\ln M_i^+ + \delta_b, V_c) = n_{i}(\ln M_i^- - \delta_b, V_c),
\]

but relate to different masses. Note that the total length of the vectors can differ and so the matching stops at

\[
i = \min(N_{\text{tot}}^+, N_{\text{tot}}^-).
\]

We then form the elements of the mass shift data vector as

\[
s_i = \frac{\ln M_i^+ - \ln M_i^-}{2\delta_b}, \\
\ln M_i = \frac{\ln M_i^+ + \ln M_i^-}{2},
\]

which we denote as \(s(\ln M; V_c)\).
We then estimate the underlying smooth functions $\hat{n}(\ln M; \delta_b = 0, V_c)$ and $\hat{s}(\ln M; V_c)$ from these data vectors using the penalized spline technique described in detail in Appendix A with 2 spline knots per dex in mass

$$\ln \hat{n}(\ln M) = S\{ \ln n(\ln M) \},$$

$$\hat{s}(\ln M) = S\{ s(\ln M) \},$$

where $S\{\}$ denotes the smoothing operator. Finally we estimate the differential mass function as the derivative of $\hat{n}(\ln M)$

$$\hat{n}_{\ln M}(\ln M) = -\frac{d\hat{n}(\ln M)}{d\ln M}. \tag{27}$$

Using mock catalogs drawn from a known mass function, we demonstrate in Appendix A that the bias of estimators in Eqs. (25) and (27), if any, is better than sub-percent level and much smaller than the statistical error. To quantify the statistical error, we sample with replacement from the $N_{\text{sim}}$ simulations to make a bootstrap resampled construction of $\hat{n}$, $\ln \hat{n}_{\ln M}$ and $\hat{s}$. By repeating this procedure 100 times, we measure the bootstrap error as the standard deviation of the resamples.

We present the mass function measurement in Fig. 2 as well as the fitting function from Ref. 13, with the latter labeled as “T08” in this paper. Their difference is consistent with the stated precision of the fitting formula but is typically much larger than the bootstrap error. Fig. 3 shows mass shift estimate from all pairs of separate universe simulations. The bootstrap error is of order of a few percent or better over mass range $6 \times 10^{12} \sim 2 \times 10^{15} M_\odot$. Note the turn located between $10^{14} M_\odot$ and $10^{15} M_\odot$ corresponds to the transition between polynomial and exponential regions in halo mass function in Fig. 2.

D. Response vs. clustering bias

From the estimates of the mass functions and the shift of threshold mass, we construct the response bias cumulative from a threshold $b_1(M) = b_1(M; \infty)$ using Eq. (15) as shown in Fig. 4. We compare this result to the fitting formula for $b_1(M)$ from Ref. 22 integrated over the self-consistent mass function from Ref. 13. Our results are systematically low by $\sim 2\%$ at the low mass end and differ by up to $6\%$ at the high mass end.

In Fig. 5 we show the average bias in 5 logarithmically spaced mass bins per dex plotted as $b_1(M) = b_1(M_1, M_2)$ using Eqs. (16) and (18). We compare this to the un-binned $b_1(M)$ from Ref. 22 for reference.

To calibrate clustering bias, we follow Eq. (2), and measure the auto matter power spectrum $P_{b\delta}$ and the cross halo-matter power spectrum $P_{b\delta}$. We bin halos in either the same 5 logarithmic mass bins per dex or cumulative above threshold, and assign the particles or halos in each bin to a $256^3$ grid with the cloud-in-cell (CIC) scheme, and apply the FFT before deconvolving the CIC window.

For halos in a mass bin $[M_1, M_2]$ we can estimate the clustering bias following Eq. (2)

$$\hat{b}_1(M_1, M_2) = \frac{\sum_{|k|<k_{\text{max}}} (\delta_t^s(k)\delta_t(k))}{\sum_{|k|<k_{\text{max}}} (\delta^s(k)\delta(k))}, \tag{28}$$

where the average is over the $N_{\text{sim}}$ simulations of the same volume. This quantity matches its response bias analogue in Eq. (16) since linearity in $\delta_b$ implicitly weights the statistic by number density. We only use large-scale modes up to $k_{\text{max}} = 0.03 h/\text{Mpc}$, and show the scale dependence on $k_{\text{max}}$ in Appendix A. We conclude that $k_{\text{max}}$ is at most a source of systematic error that is comparable to our statistical error.

Given the lack of high mass halos in the $(500\text{Mpc}/h)^3$ simulation volumes, we combine these estimates with the $(1\text{Gpc}/h)^3$ simulations according to the expected inverse shot variance weight, i.e. 8 times higher weight for the larger volume simulations down to their 8 times higher minimum mass. In Appendix A2 we show results from the two sets separately to test for resolution and volume effects. To estimate the errors, we bootstrap resample with the $N_{\text{sim}}$ of each set.

We compare the clustering and response bias in Figs. 4 and 5. The agreement in the $1\lesssim b_1\lesssim 8$ region is an excellent 1–2%. For the higher bias of rarer halos the statistical errors for both quantities increase but the agreement is better than the 4–5% level for $b_1 \lesssim 8$. The bias in mass bins is slightly noisier but still consistent within the bootstrap errors for $1 \lesssim b_1 \lesssim 8$.

In addition to abundance matching, we also measure the response bias directly from the change of number counts in the same set of mass bins. We present the comparison between the two methods in Appendix A2 both to demonstrate the robustness of abundance matching and to show its statistical efficiency.
IV. DISCUSSION

Linear halo bias is the response of the halo number density to a change in the long-wavelength dark matter density as manifest in the cross correlation between the clustering of halos and the dark matter. In this paper we have used the separate universe (SU) simulation technique to calibrate the response bias of halos, by treating the long-wavelength density mode as a change in the background density in a separate universe. By using pairs of SU simulations with the same realizations of the initial Gaussian random seeds, we can reduce sample variance effects when comparing the mass functions in two separate universes.

Rather than comparing the mass functions at each mass bin in the SU simulations, we introduced an alternative method, the abundance matching method for the comparison, where we adjust the mass threshold so as to have the same cumulative abundance of halos above the mass threshold in the separate universes. We show how to calibrate the response bias from the mass threshold shift and the mass functions. The method can robustly extract the effect of subtle changes in the mass of individual halos, caused by the different merger and accretion histories in the paired SU simulations, thus outperform the direct method by a factor of 3 – 5 in statistical power.

We found agreement between the response and clustering biases at the 1 – 2% level for average biases $1 \lesssim \bar{b}_1 \lesssim 4$ and no significant deviations at the 4 – 5% level out to $\bar{b}_1 \sim 8$. This excellent agreement provides a precise test of the consistency relation between the changes in a one-point function, the halo mass function, and a two-point function, the halo-matter cross-correlation in the large-scale limit that can in principle test for new physics in the dark matter, dark energy or primordial non-Gaussianity sectors. Our results are systematically lower than the bias given by the T10 fitting formula [22] by 2% and differs by up to 6% at high mass end.

Our method can be easily extended to including other effects in halo bias beyond the flat ΛCDM cosmology. It would be straightforward to apply SU techniques in cosmological hydro-simulations for studying effects of baryonic physics on large-scale halo bias. Further, massive neutrinos and/or dark energy change the growth of long-wavelength dark matter perturbation, and will in turn cause changes in the response of halo mass function. Primordial non-Gaussianity causes additional mode-coupling between the long- and short-wavelength modes, inducing a characteristic scale-dependent effect on halo bias at large scales [2]. Different halos of the same mass can have different large-scale bias if the halos experience different assembly histories – the so-called assembly bias [39, 49]. A generalization of SU simulation technique can give a better handle on calibrating these modifications in halo bias by reducing the sample variance effects for both the long wavelength and short wavelength modes.

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Appendix A: Robustness of techniques

In this appendix we describe our smoothing procedure, and demonstrate its robustness when applied as a mass function estimator in §A2. Appendix A shows the robustness and statistical power of the abundance matching technique compared with the direct measurement of abundance changes in fixed mass bins. We test the dependence of clustering bias on $h_{\text{max}}$, resolution and volume in §A3.

1. Spline smoothing robustness

The halo abundance and mass shift measured from a simulation is defined at a discrete set of masses of its constituent halos. Instead of the commonly adopted method that bins the noisy data in mass, we smooth the cumulative mass function and mass shift, and demonstrate its advantage and robustness below.

Among all the twice differentiable functions that model our discrete observations $(x_i, y_i), i = 1, \ldots, n$, we look for the $f(x) = \hat{f}(x)$ that minimizes

$$\sum_{i=1}^{n} [y_i - \hat{f}(x_i)]^2 + \lambda \int_{x_1}^{x_n} f''(x)^2 \, dx. \quad (A1)$$

The first term is the residual sum of squares which encourages $\hat{f}(x)$ to fit the data well, while the second one is a penalty term that suppresses variability. The non-negative smoothing parameter $\lambda$ controls the trade-off between fidelity and smoothness, or bias and variance. When $\lambda = 0$ the resulting $f(x)$ becomes the interpolating spline, while $\lambda \to \infty$ it converges to the linear least squares.

It can be shown that the solution that minimizes Eq. (A1) is a natural cubic spline with knots at $x_i$ (see e.g. [50]), known as a smoothing spline. This procedure is nonparametric, but is computationally intense for a large number of data points. In practice we can greatly improve the performance and avoid overfitting by using a smaller number of knots. This latter approach is sometimes referred to as penalized spline.

Consider the function estimates of the form

$$f(x) = \beta^T b(x) \equiv \sum_{j=1}^{m} \beta_j b_j(x), \quad (A2)$$

where $b^T(x) \equiv [b_1(x), \ldots, b_m(x)]$ are the basis functions for natural cubic splines with $m$ knots. So we can write Eq. (A1) in terms of the bases

$$|y - B\beta|^2 + \lambda \beta^T \Omega \beta, \quad (A3)$$

where $B_{ij} \equiv b_j(x_i)$ and $\Omega_{jk} \equiv \int b'_j(x)b'_k(x) \, dx$. with $i = 1, \ldots, n$, and $j,k = 1, \ldots, m$. The coefficients $\beta^T \equiv [\beta_1, \ldots, \beta_m]$ that minimize Eq. (A3) are

$$\hat{\beta} = (B^T B + \lambda \Omega)^{-1} B^T y, \quad (A4)$$

and thus our function estimate

$$\hat{f}(x) = b^T(x)(B^T B + \lambda \Omega)^{-1} B^T y \equiv S(y(x)), \quad (A5)$$

where $S\{}$ denotes the smoothing operator that maps discrete data to the estimate of a continuous function. The fitted values at $x^T \equiv [x_1, \ldots, x_n]$ are

$$\hat{y} \equiv \hat{f}(x) = S y, \quad (A6)$$

where matrix $S \equiv B(B^T B + \lambda \Omega)^{-1} B^T$ acts linearly on the data $y^T \equiv [y_1, \ldots, y_n]$.

To avoid either overfitting or over-smoothing, we choose the smoothing parameter $\lambda$ by cross-validation. Specifically, the criterion of the leave-one-out cross-validation (LOOCV) is widely used [50]. In LOOCV, we successively take each data point $i$ as a validation point for the smoothing operation trained on the remaining $n - 1$ data points. We choose the value of $\lambda$ that minimizes the sum over the squared residuals for these points,

$$\sum_{i=1}^{n} [y_i - \hat{f}_\lambda^{(-i)}(x_i)]^2 = \sum_{i=1}^{n} \left[ \frac{y_i - \hat{f}_\lambda^{(-i)}(x_i)}{1 - |S|_{ii}} \right]^2, \quad (A7)$$

where the superscript $^{(-i)}$ indicates the fit leaving the $i$th observation $(x_i, y_i)$ out, and the subscript $\lambda$ makes the $\lambda$-dependence explicit. The equality in Eq. (A7) [50] allows this procedure to be performed without explicitly obtaining $\hat{f}_\lambda^{(-i)}$ for each point.

In this paper, we utilize this penalized spline method to smooth discrete data sets, including halo catalogs in fiducial simulations and shift of threshold mass when matching the abundance between paired separate universe simulations. This procedure avoids problems with binning halos in mass as well as taking derivatives of noisy data.

To verify the robustness, we test our smoothing estimator on mock data, drawn from a known distribution.
mass functions \( [\text{Gpc}^{-3}] \)

\( T_{08} \)  

\( n \)  

\( T_{08} \)  

\( n \)  

\( \ln M \)  

\( n_{\text{smooth}} \)  

\( \ln M \)  

\( n_{\text{smooth}} \)  

\( \ln M \)  

\( M \) \([\text{M}_\odot]\)

-5%  

0  

5%  

rel. diff.

**FIG. 6.** Robustness of smoothing procedure verified by comparing smoothed abundance estimates from 1000 mocks drawn from the fitting mass function \( T_{08} \) [48] to the function itself (solid). We generate each mock catalog for halos between \( 1.4 \times 10^{12} \text{M}_\odot \) and \( 10^{16} \text{M}_\odot \), in an volume of 4 Gpc/\( h \)^3 same as that of all fiducial (500Mpc/\( h \))^3 simulations combined. Lines and shaded regions show mean and scatter of the estimated cumulative (thick green) and differential (thin blue) mass functions.

For this purpose, we use the fitting formula for halo mass function in [48] to generate 1000 mock catalogs. The minimum mass in the catalogs is \( 1.4 \times 10^{12} \text{M}_\odot \), corresponding to the smallest halos that our halo finder keeps (100 particles). We also introduce a maximum mass \( 10^{16} \text{M}_\odot \) since there is a negligible probability of obtaining even one such halo in the \( \Lambda \text{CDM} \) cosmology. We populate catalogs with total number \( \hat{N}_{\text{halo}} \) drawn from a Poisson distribution, with mean as the mean number of halos in a volume of 4 Gpc/\( h \)^3, same as that of all fiducial simulations combined. For each halo in the catalog, we use the inverse cumulative distribution function algorithm to draw its mass and form a realization of the cumulative number density \( n_i(\ln M_i) \).

We employ the smoothing algorithm described above to provide an estimate of the underlying smooth function \( \hat{n}(\ln M) \) from the discrete data. The smoothing function needs to handle both the polynomial and exponential regions of the mass function. To achieve this, we take the natural logarithm of the cumulative number density \( n_i \) and the mass \( M_i \), \( i = 1, \ldots, \hat{N}_{\text{halo}} \), before applying the smoothing operation in Eq. (A5) with 2 knots per dex in mass

\[
\ln \hat{n}(\ln M) = S\{ \ln n(\ln M) \}, \quad (A8)
\]

where \( \hat{n}(\ln M) \) is the function estimate. Thus we can estimate the mass function by taking derivative of the smooth cumulative mass function estimator

\[
\hat{n}_{\ln M}(\ln M) = -\frac{d\hat{n}(\ln M)}{d(\ln M)}. \quad (A9)
\]

Note that we include halos with \( 100 - 400 \) particles for smoothing, to avoid the enhanced error near the edge, but only trust and present results for halos with \( \geq 400 \) particles.

We set up the robustness test to exactly parallel to our estimation of halo mass functions. Fig. 6 shows that the bias of the smoothing estimator, if any, is at sub-percent level, much smaller than the statistical error per catalog.

**FIG. 7.** Abundance matching robustness and efficiency. Blue + points show the response bias with bootstrap errors centered on average masses (Eq. 19) by abundance matching, and grey • points show the same by direct measurement of abundance changes within fixed mass bins. The two methods give consistent results, while the former has much reduced errors by a factor of 3 – 5. Dotted line shows the fitting formula of clustering bias from T10 [22].

2. Abundance matching robustness and performance

In [11C] we demonstrate the abundance matching technique for response bias calibration from separate universe simulations, and show the results in [11C]. Abundance matching efficiently makes use of the mass information of almost all the halos, whereas in a direct measurement of abundance changes within a set of fixed mass bins, only halos near bin edges are shifted into neighboring bins and counted. Here we compare the bias measured with both methods, from the same set of simulations, both as a test of robustness of abundance matching and as a demonstration of its statistical power.
Let’s denote the number counts of halos with mass in \([M_1, M_2]\) in all separate universe realizations of the same \(\delta_b\) and \(V_c\) by \(\Delta N(\delta_b, V_c)\) and \(\Delta N(-\delta_b, V_c)\). Following Eq. (8) the average bias in this mass bin is

\[
\bar{b}_1(M_1, M_2) = \frac{\ln(\Delta N(\delta_b, V_c)/\Delta N(-\delta_b, V_c))}{2\delta_b}.
\]

We show the response bias by both methods in Fig. 7 where the statistical consistency verifies the robustness of the abundance matching technique. Its advantage over the direct calibration is obvious with the greatly reduced errors by a factor of 3 - 5.

### 3. Clustering bias robustness

The calibration of clustering bias depends on the \(k_{\text{max}}\) cut on the large scale modes as well as the resolution and volume of the simulations. Repeating the bias estimation in Eq. (28) with different \(k_{\text{max}}\), we present the scale dependence in Fig. 8 for \(V_c = (500\text{Mpc}/h)^3\) and \(V_c = (1\text{Gpc}/h)^3\) separately. As \(k_{\text{max}}\) approaches the nonlinear scale the bias increases with \(k_{\text{max}}\) for the most massive halos, and slightly decreases for \(\lesssim 10^{13} M_\odot\) halos, similar to the trend demonstrated in Fig. 2 of Ref. [21]. These trends are also stable between the two volumes which have different mass resolutions.

In the main text, we compromise between losing modes, increasing the statistical errors, and using more modes but increasing the systematic bias by choosing \(k_{\text{max}} = 0.021\text{Mpc}^{-1}\). Taking the measurement with this choice as the fiducial values, we can quantify the possible systematic bias of using a different \(k_{\text{max}}\) by the deviation averaged over mass bins

\[
\frac{1}{N_{\text{bin}}} \sum_i \frac{[b_1(M_i; k_{\text{max}}) - b_1(M_i; k_{\text{max,fid}})]^2}{\sigma_i(M_i; k_{\text{max,fid}})^2}.
\]

For \(V_c = (500\text{Mpc}/h)^3\), the \(k\)-range where this average variance is below 1 is from 0.013\text{Mpc}^{-1} to 0.03\text{Mpc}^{-1}; for \(V_c = (1\text{Gpc}/h)^3\), a very similar range from 0.015\text{Mpc}^{-1} to 0.035\text{Mpc}^{-1}. Given the substantial range in the linear regime over which results are stable, we conclude that systematic error due to \(k_{\text{max}}\) is at most comparable to our statistical error.

With the fiducial \(k_{\text{max,fid}} = 0.021\text{Mpc}^{-1}\) we show in Fig. 9 the results for \(b_1(M)\) of the two volume types separately. In the main text we combined the volumes (cf. Fig. 7). For most of the mass bins, the clustering bias measured from the large (1 Gpc/h)^3 volume simulations agrees well with that from the small (500 Mpc/h)^3 ones, confirming that 400 particles are enough to resolve halos for estimating clustering bias. The small volume estimates fluctuate substantially at the high mass end due to having very few high mass halos in such volumes. In fact the high point at \(\sim 8 \times 10^{14} M_\odot\) can be traced back to Fig. 8 as a statistical fluctuation of the \(k_{\text{max,fid}} = 0.021\text{Mpc}^{-1}\) modes that is not present at higher \(k_{\text{max}}\).
Appendix B: Universal mass function

As explained in §II A, response bias is often approximated by assuming a universal mass function (UMF) rather than the more exact separate universe approach introduced in the main text. In addition to the universality assumption, the mass function is typically fit to a specific functional form motivated by spherical collapse and the excursion set approach (e.g. [22, 27]). To separate the roles of these assumptions we calibrate the universal form nonparametrically and compare the results to the clustering bias, both measured from the same halo catalog.

1. UMF response bias

The universality assumption restricts the halo mass function in the following form

$$n_{\ln M}(M) = \frac{\bar{\rho}_m}{M} \nu f(\nu) \frac{\partial \ln \nu}{\partial \ln M},$$  \hspace{1cm} (B1)

where the multiplicity function $\nu f(\nu)$ captures the mass fraction (per ln$\nu$) contained in halos of peak height $\nu \equiv \delta_c/\sigma(M)$. Here $\delta_c$ is the linear threshold of spherical collapse and is usually taken as the Einstein-deSitter value $\delta_c = 1.686$ due to its weak cosmology dependence. The rms of the linear density fluctuation is computed as usual

$$\sigma^2(M) = \int \frac{d^3k}{(2\pi)^3} P_{\text{lin}}(k) |W(kR)|^2,$$  \hspace{1cm} (B2)

where $M = 4\pi \bar{\rho}_m R^3/3$ is the enclosed mass, $P_{\text{lin}}(k)$ is the linear power spectrum, and the top-hat window function is

$$W(x) = \frac{3}{x^3} (\sin x - x \cos x).$$  \hspace{1cm} (B3)

In the UMF response bias approach, the shift in the background density is viewed as an effective change in the collapse threshold $\delta_c \rightarrow \delta_c - \delta_b$, or in the peak height

$$\nu = \frac{\delta_c - \delta_b}{\sigma}.$$  \hspace{1cm} (B4)

Thus the linear bias becomes

$$n_{\ln M}^{-1} = \frac{\bar{\rho}_m}{M} \frac{\partial}{\partial \delta_b \ln M} \left( \nu f(\nu) \frac{\partial \ln \nu}{\partial \ln M} \right)$$

$$= \frac{\bar{\rho}_m}{M} \frac{1}{\delta_c} \frac{\partial \ln \nu}{\partial \ln M} - \mu n_{\ln M}^{-1},$$  \hspace{1cm} (B5)

where we have introduced a shorthand

$$\mu = \frac{1}{\delta_c} \left( \frac{\partial \ln \nu}{\partial \ln M} \right)^{-1}.$$  \hspace{1cm} (B6)
and the average UMF bias above $M_{th}$ becomes

$$\bar{b}_1(M_{th}) = \frac{1}{n(M_{th})} \int_{M_{th}}^{\infty} \frac{dM}{M} \bar{b}_1 n_{inM}$$

$$= \frac{\mu(M_{th}) n_{inM}(M_{th})}{n(M_{th})} - \bar{\mu}(M_{th}),$$

$$\bar{\mu}(M_{th}) = \frac{1}{n(M_{th})} \int_{M_{th}}^{\infty} \frac{dM}{M} \mu n_{inM}. \quad (B7)$$

Given $\bar{b}_1(M_{th})$ we can difference to get the average bias in a finite mass bin

$$\bar{b}_1(M_1, M_2) = \int_{M_1}^{M_2} d\ln M \frac{d\bar{b}_1 n_{inM}}{d\ln M}$$

$$= \frac{\bar{b}_1(M_1) n(M_1) - \bar{b}_1(M_2) n(M_2)}{n(M_1) - n(M_2)}. \quad (B8)$$

We should emphasize that Eq. (B7) and (B8) describe a non-parametric procedure to calibrate the UMF response bias quantities. In deriving them we do not assume any functional form for the multiplicity function $\nu f(\nu)$ (cf. $[22, 27]$), as such assumptions can introduce systematic bias into the measurement. On the other hand, by doing so we can no longer make the connection to excursion set methods based on either a fixed or moving barrier $[19]$.

Similar to the SU response bias calibration, here we also need the cumulative and differential mass functions. In addition, we need to estimate the number density weighted $\bar{\mu}$ above threshold mass $M_{th}$ to quantify the UMF response bias.

### 2. Bias comparisons

In $[11C]$ we have explained how to make continuous estimates of $n_{inM}$ and $n$ from discrete halo catalog measured from simulations. Following the same reasoning, we can construct the estimator for $\bar{\mu}(M_{th})$. Similar to Eq. (22), we start from a halo catalog and arrange the cumulative sum in descending order in mass

$$\ln M = [\ln M_1, \ldots, \ln M_{N_{tot}}]^T,$$

$$\bar{\mu} = \left[ \frac{\mu(M_1)/2}{1/2}, \ldots, \frac{\sum_{i=1}^{N_{tot}} \mu(M_i)}{N_{tot} - 1/2} \right]^T. \quad (B9)$$

Recall that the factor of $1/2$ arises from partitioning discrete points. From these data vectors we can obtain a smooth estimate of $\ln \bar{\mu}$ using a penalized spline (see $[A1]$ with 2 spline knots per dex in mass

$$\ln \bar{\mu}(\ln M) = S\{ \ln \bar{\mu}(\ln M) \}, \quad (B10)$$

where $S\{ \}$ is the smoothing operator.

From these estimates of the mass functions and $\bar{\mu}$, we construct the UMF response biases from Eq. (B7) and (B8). To verify our estimator for the UMF response bias, we test it on 1000 mocks from the Sheth-Tormen mass function $[19]$, drawn in the same way as explained in $[A1]$ and compare the result to that analytically derived assuming universality. We show this comparison in Fig. 10, and find that our estimator is accurate to sub-percent level, well below the statistical scatter of each catalog.

Using simulations from the same set of $V_c = (500\text{Mpc}/h)^3$, we compare the UMF response biases to the clustering bias ($[11D]$) in Fig. 11 and 12. The UMF response bias is systematically lower than the clustering $b_1$ by $5 - 10\%$ for $1 \leq b_1 \leq 7$, or lower by $\geq 6\%$ than the clustering $b_1$ for most of the measured mass range.

The fitting function for clustering bias from T08 and T10 are also added as references. For both $\bar{b}_1$ and $b_1$, the UMF response biases are systematically lower than the fitting functions by $\sim 8\%$.

We conclude that the UMF response bias is statistically inconsistent with the clustering bias, at least for halos identified at $\Delta = 200$. Given the excellent agreement between clustering bias and the SU response bias, the UMF response bias is also inconsistent as an approximation of the latter.
