Multi-Fidelity Emulation for the Matter Power Spectrum using Gaussian Processes

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ABSTRACT

We present methods for emulating the matter power spectrum by combining information from cosmological \textit{N}-body simulations at different resolutions. An emulator allows estimation of simulation output by interpolating across the parameter space of a limited number of simulations. We present the first implementation in cosmology of multi-fidelity emulation, where many low-resolution simulations are combined with a few high-resolution simulations to achieve an increased emulation accuracy. The power spectrum’s dependence on cosmology is learned from the low-resolution simulations, which are in turn calibrated using high-resolution simulations. We show that our multi-fidelity emulator predicts high-fidelity counterparts to percent-level relative accuracy when using only 3 high-fidelity simulations and outperforms a single-fidelity emulator that uses 11 simulations, although we do not attempt to produce a converged emulator with high absolute accuracy. With a fixed number of high-fidelity training simulations, we show that our multi-fidelity emulator is $\approx 100$ times better than a single-fidelity emulator at $k \leq 2 \, h \, \text{Mpc}^{-1}$, and $\approx 20$ times better at $3 \leq k < 6 \, h \, \text{Mpc}^{-1}$. Multi-fidelity emulation is fast to train, using only a simple modification to standard Gaussian processes. Our proposed emulator shows a new way to predict non-linear scales by fusing simulations from different fidelities.

Key words: cosmology: theory - cosmology: numerical - methods: statistical

1 INTRODUCTION

Current and next generation large scale structure surveys, such as \texttt{DES} (Abbott et al. 2020), \texttt{LSST} (Rubin Observatory, Tyson 2002), \texttt{EUCLID} (Amendola et al. 2018), \texttt{DESI} (DESI Collaboration et al. 2016), and the Roman Space Telescope \texttt{(WFIRST)} (Spergel et al. 2013) will probe gravitational clustering and galaxy formation at small scales with high accuracy. Thus, the future of cosmology relies on exploiting the information in non-linear structure formation at small scales, where numerical \textit{N}-body simulations must be used to give accurate theoretical predictions.

Cosmological linear perturbation theory provides accurate analytic predictions on the clustering of mass up to $k \sim 0.1 \, h \, \text{Mpc}^{-1}$. Despite the success of the standard model of cosmology, several fundamental physics puzzles are still unanswered: the accelerated expansion of the Universe (Caldwell & Kamionkowski 2009), the nature of dark matter (Feng 2010), and the sum of the neutrino masses (Wong 2011). To answer these questions and constrain cosmological parameters using future surveys, theoretical predictions from numerical simulations must be accurate on smaller scales than are accessible to linear theory. As a primary summary statistic, the matter power spectrum needs to be at percent-level precision for $k \lesssim 10 \, h \, \text{Mpc}^{-1}$ (Schneider et al. 2016).

Modelling non-linear gravitational clustering is done using \textit{N}-body simulations, where a dark matter fluid is sampled by macro-particles and evolved using a smoothed gravitational force. Each macro-particle is representative of an ensemble of microscopic dark matter particles. Generations of computational physicists have improved the accuracy of the gravitational evolution, and created quicker and more scalable algorithms to drive the mass resolution of the simulations ever higher (Hockney & Eastwood 1988, Barnes & Hut 1986, Couchman et al. 1995, Greengard & Rokhlin 1987, Dehnen 2002).

The mass resolution necessary to robustly predict the power spectrum at $k \sim 10 \, \text{Mpc}/h$ pushes the computational
limits of contemporary supercomputers. To adequately sample a high-dimensional input parameter space with Markov chain Monte Carlo (MCMC), millions of samples are needed, while a limited number (at best a few hundred to a few thousand) of high-fidelity simulations are computationally possible.

An efficient way to perform accurate cosmological inference with a limited number of simulations is to use emulators. Emulators are flexible statistical models, usually built with Gaussian processes, which learn the mapping from input cosmological parameters to summary statistics. This reduces the number of costly forward simulations by effectively interpolating the function outputs.

Emulators have been applied extensively in the field of cosmological inference. Heitmann et al. (2006); Habib et al. (2007) proposed a cosmic calibration project to make percent-level predictions on the matter power spectrum using a Bayesian emulator. Heitmann et al. (2009); Lawrence et al. (2010); Heitmann et al. (2014) implemented this cosmic emulator in their Coyote Universe suite using 37 high-resolution simulations. Heitmann et al. (2016). Lawrence et al. (2017) designed the Mira-Titan Universe suite to train emulators to make precise theoretical predictions using 36 simulations. The latest Euclid preparation (Euclid Collaboration et al. 2020) runs 256 simulations (3000^3 particles) to prepare their emulator for the matter power spectrum. Besides Gaussian processes, Agarwal et al. (2014) used a neural network to build a cosmic emulator from 6,380 N-body simulations spanning 580 cosmologies.

Beyond the matter power spectrum, emulators have been trained to predict the halo mass function (Bocquet et al. 2020), the concentration-mass relation for dark-matter haloes (Kwan et al. 2013), the galaxy power spectrum (Kwan et al. 2015), the galaxy correlation function (Zhai et al. 2019), the halo bias (McCintock et al. 2019), weak lensing peak counts (Liu et al. 2015), the cosmic shear covariance (Harnois-Déraps et al. 2019), weak lensing voids (Davies et al. 2020), the 21 cm signal (Kerr et al. 2017), and the Lyman-α 1D flux power spectrum (Bird et al. 2019). They also have been used for inferring beyond-ΛCDM cosmologies (Giblin et al. 2019; Pedersen et al. 2020) and f(R) gravity cosmologies (Ramachandra et al. 2020). While all these emulators successfully predict summary statistics using high-fidelity simulations, one question which remains is how to minimize the number of necessary training simulations to achieve a given accuracy. Here we demonstrate that building cosmological emulators from simulations can be improved with multi-fidelity models. Multi-fidelity models (Kennedy & O’Hagan 2000) minimize the computational cost by combining the predictive power of simulations at different resolutions. They fuse the expensive but accurate high-fidelity data with cheaply-obtained low-fidelity approximations. One standard model used by the multi-fidelity emulation is a multi-output Gaussian process (Bonilla et al. 2005). A multi-output Gaussian process (multi-output GP) generalizes a single-output GP to multiple outputs, while building a cross-covariance function to model the shared information between outputs. In this paper, low and high fidelity correspond to simulations at different resolutions. High-fidelity simulations have a finer mass resolution while low-fidelity simulations have a coarser mass resolution.

To train the multi-fidelity emulator using as few high-resolution simulations as possible, we also propose a method for selecting high-fidelity training samples, based on minimizing the loss computed among the low-fidelity simulations. By optimizing the low-fidelity emulator’s loss, we show that one can efficiently train a multi-fidelity emulator by avoiding worst-case combinations of the high-fidelity training samples.

Computational astrophysicists have used methods similar to multi-fidelity modelling to minimize the cost of performing high-resolution simulations (Lučić et al. 2015; Chartier et al. 2020). A notable example is Richardson extrapolation (Richardson 1911), a numerical method to improve a simulation’s accuracy by combining a sequence of simulations with varied spatial resolutions and fixed cosmologies. More recently, generative adversarial networks (GAN) have been used to produce high-resolution density fields (Kodi Ramanah et al. 2020) and particle displacements (Li et al. 2020) from low-resolution (but larger volume) input data. In principle, such ‘super-resolution’ simulations could be implemented as a multi-fidelity emulator’s high-fidelity training set, allowing an emulator to be built to a scale not directly accessible to simulations.

Rogers et al. (2019); Leclercq (2018) proposed using Bayesian optimization to improve emulator accuracy by a sequential choice of new simulation points designed to globally optimize the emulator function. Similar approaches to iterative selection of training data in a cosmological parameter space have been presented by Takhtaganov et al. (2019); Pellejero-Ibáñez et al. (2020). Computer scientists and engineers, including Huang et al. (2006); Forrester et al. (2007); Lam et al. (2015); Poloczek et al. (2016); McLeod et al. (2017), have extensively studied combining multi-fidelity methods with Bayesian optimization. Multi-fidelity Bayesian optimization arises when a cheaper approximation to the object function exists.

We present a multi-fidelity emulator for the matter power spectrum, as output by the cosmological simulation code mp-gadget (Springel & Hernquist 2003; Feng et al. 2018a). In this paper, we target percent level relative accuracy: how well our emulators can reproduce the matter power spectra at our highest fidelity. We defer producing an emulator which allows percent level accurate reconstruction of observations or a hypothetical ideal simulation to future work. The main goal of this paper is to demonstrate that our multi-fidelity techniques can be used to reduce the computational budget required for an emulator.

We use two fidelities in a 256 Mpc/h box: a fast but low resolution version with 128^3 dark-matter particles and a slow but high resolution version with 512^3 particles. Even with only 3 high-fidelity simulations and 50 low-fidelity simulations, we show that we can predict the high-resolution matter power spectrum at percent-level accuracy on average at k ≤ 6.4 h Mpc^-1 at z = 0, with a total computational cost ≲ 4 high-fidelity simulations. Although we only show our application to the matter power spectrum, the methods presented in this paper could apply to other summary statistics, e.g., the halo mass function or the Lyman-α 1D flux power spectrum.

Frazier (2018) has a subsection that provides a short review on multi-fidelity Bayesian optimization.
van Daalen et al. (2011) showed that the lack of AGN feedback affects a dark matter-only simulation significantly (compared to the error requirements of upcoming surveys) at \( k > 0.1 \, \text{hMpc}^{-1} \). Furthermore, baryon cooling can alter the power spectrum at \( k \sim 10 \, \text{hMpc}^{-1} \) (White 2004). However, as techniques exist to model this effect in post-processing (Schneider et al. 2020), we defer extending our technique to hydrodynamical simulations including AGN feedback to future work. Here we validate that a multi-fidelity emulator is useful in the simplest case: dark matter-only \( N \)-body simulations.

We build two types of multi-fidelity emulators. One uses the linear autoregressive model of Kennedy & O'Hagan (2000) (first-order autoregressive model, AR1), which we will call the “linear multi-fidelity model.” The second multi-fidelity emulator uses the non-linear fusion model of Perdikaris et al. (2017) (nonlinear auto-regressive Gaussian process, NARGP), and which we call the “non-linear multi-fidelity emulator.” Kennedy & O'Hagan (2000) model the scaling factor between fidelities as a scalar, while Perdikaris et al. (2017) allow the scaling factor to depend on input parameters. Our implementation of AR1 and NARGP is based on emukit (Paleyes et al. 2019), an open-source package for emulation and decision making under uncertainty, with the modifications mentioned above.

In Section 2, we briefly describe the simulation code, mp-gadget, for training the emulator. We recap the general formalism of a single-fidelity Gaussian process emulator in Section 3. Section 4 describes the formalism of a multi-fidelity emulator. We explain our sampling strategy in Section 5. Section 6 shows the results, with comparisons between multi-fidelity emulation and single-fidelity emulation. We summarize the runtime for the mp-gadget simulations in Section 7. We conclude with a summary of key contributions and potential applications of our work in Section 8. Our code for multi-fidelity emulation in the matter power spectrum is publicly available at https://github.com/jibanCat/matter_multi_fidelity_emu

2 SIMULATIONS

We prepare our training set by running dark matter-only simulations using the massively parallel \( N \)-body code mp-gadget (Feng et al. 2018). MP-GADGET is a publicly available \( N \)-body+hydrocosmological simulation code derived from GADGET3 (Springel & Hernquist 2003). It is parallelized using a hybrid OpenMP/MPI strategy and has successfully performed a hydrodynamical simulation using all 8092 Frontera nodes, a total of 449,792 cores, demonstrating its good scalability properties. The gravitational forces are computed using a Fourier transform based particle-mesh algorithm on large scales and a Barnes-Hut tree on small scales.

We initialise our simulations from the linear power spectrum produced by class (Lesgourgues 2011) at \( z = 99 \) using the Zel’dovich approximation (Zel’Dovich 1970). The dark matter particles then evolve through gravitational dynamics. The matter power spectra are computed from the output snapshots of mp-gadget, and used as our emulation targets. In this paper, we fix the IC noise in the nodes and change only the cosmology for the emulator training. We do not use the “paired and fixed” technique (Angulo & Pontzen 2016), but it would be easy to do so using only low resolution simulations as these pairings are designed to remove variance on large scales.

The matter power spectrum, \( P(k) \), is a compressed summary statistic of the over-density field, \( \delta(x) \), evaluated as an angle average of the Fourier-transformed overdensity field:

\[
P(|k|) = \langle \hat{\delta}^* (k) \hat{\delta}(k) \rangle,
\]

where

\[
\hat{\delta}(k) = \int d^3\mathbf{r} \delta(\mathbf{r}) e^{-2\pi i \mathbf{k} \cdot \mathbf{r}}.
\]

We measure the power spectrum with a cloud-in-cell mass assignment, which is deconvolved. The Fourier transform is taken on a mesh the same as the PM grid of the simulation, which has a resolution of 2 times the mean inter-particle spacing.

For a multi-fidelity problem, our data are from simulations at different resolutions. Since low resolution simulations are cheaper to obtain (but are only approximations to the high resolution results), we typically have a limited number of high-fidelity data and many low-fidelity approximations.

To make the text of this section consistent with the following sections, we provide some notation to bridge the terminology, summarized in Table 1. We have data from \( s \) different fidelities (simulation resolutions). For each fidelity, we have pairs of inputs and outputs \( D_i = \{x_{i,t}, y_{i,t}\} = \{x_i, y_i\} \), where \( t = 1, \ldots, n_i \) denotes the fidelity level from low to high, and \( i = 1, \ldots, s \) where \( n_i \) is the number of data pairs at fidelity \( t \) and \( i \) indexes each individual simulation. The data pairs \( D_i = \{x_i, y_i\} \) for our emulation setup are the cosmological parameters of the simulations and the power spectrum outputs. Here we have \( s = 2 \) for two mass resolutions: 128\(^3\) and 512\(^3\) dark matter-only simulations. We will denote 128\(^3\) as low-resolution (LR, \( t = 1 \)) and 512\(^3\) as high-resolution (HR, \( t = 2 \)).

Each fidelity will have a different number of simulations, \( n_i \). Practically, the number of LR simulations will be much larger than the number of HR simulations, \( n_1 > n_2 \). The compute time for LR (\( n_{\text{ptl,side}} = 128 \)) is \( \sim 20 \) core hours

Table 1. Notations and definitions

| Notation | Description |
|----------|-------------|
| HR       | High-resolution simulation, 512\(^3\) particles |
| LR       | Low-resolution simulation, 128\(^3\) particles |
| \( x_{i,t} \) | Input cosmological parameters at ith simulation at fidelity \( t \) |
| \( y_{i,t} \) | Matter power spectrum at ith simulation at fidelity \( t \), at log scale |
| \( n_i \) | Number of simulations at fidelity \( t \) |
| \( N_{\text{ptl,side}} \) | Number of particles per box side |

MF Emulator 3

117 (2019)
and \( \sim 2000 \) core hours for HR (\( N_{\text{ptl\_side}} = 512 \)). We will empirically show we only need 3 HR and 50 LR to train a multi-fidelity emulator with an average emulator error per \( k \) smaller than 1%.

We do not emulate the matter power spectrum across redshifts, conditioning on a given redshift bin \( z_0 \). We generally focus on \( z_0 = 0 \), but will discuss multi-fidelity emulators at \( z_0 = 1 \) and \( z_0 = 2 \) in Section 6.4.2.

### 2.1 Latin hypercube sampling

As Heitmann et al. (2009) mentioned, a space-filling Latin hypercube design is well suited for GP emulators of the matter power spectrum. For a training set with \( d \)-dimensional inputs and \( N \) simulations, an \( N^d \) grid is created first, and simulations are placed on this grid so that only one simulation is present in any row or column. The Latin hypercube design improves on random uniform sampling by ensuring that the chosen points do not crowd together in any subspace.

We apply a Latin hypercube design on the input parameter space, \( \{h, \Omega_0, \Omega_b, A_s, n_s\} \). We vary the LCDM cosmological parameters \( \{h, \Omega_0, \Omega_b, A_s, n_s\} \), which are the Hubble parameter \( h = H_0/(100 \text{ km s}^{-1} \text{ Mpc}^{-1}) \), the total matter density \( \Omega_0 \), the baryon density \( \Omega_b \), primordial amplitude of scalar fluctuations \( A_s \), and the scalar spectral index \( n_s \). We use the same set of LCDM cosmological parameters as Euclid Collaboration et al. (2020), allowing us to compute the relative errors of our simulations with respect to EuclidEmulator2.

We use bounded uniform priors for the input parameters:

\[
\begin{align*}
    h & \sim U(0.65, 0.75); \\
    \Omega_0 & \sim U(0.268, 0.308); \\
    A_s & \sim U[1.5 \times 10^{-5}, 2.8 \times 10^{-5}]; \\
    n_s & \sim U(0.9, 0.99); \\
    \Omega_b & \sim U(0.0452, 0.0492).
\end{align*}
\]

The dark energy density is \( \Omega_\Lambda = 1 - \Omega_0 \). The prior volume surrounds the WMAP 9-year cosmology (Hinshaw et al. 2013). The code to handle the simulation input files and Latin hypercube design is publicly available at [https://github.com/jiabanCat/SimulationRunnerDM](https://github.com/jiabanCat/SimulationRunnerDM).

### 2.2 Preprocessing of the simulated power spectrum

A numerical simulation is constrained by its box size and number of particles. The mass resolution limits the smallest scale (the highest \( k \)) of the power spectrum. Thus, high-fidelity simulations can model smaller scales, not fully resolved in low-fidelity simulations, as shown in Figure 1.

For \( k \) larger than the mean particle spacing, \( P(k) \) differs substantially from the resolved value, due to artifacts of the macro-particle sampling. The scale of the mean particle spacing is

\[
k_{\text{spacing}} = 2\pi N_{\text{ptl\_side}}/L_{\text{box}},
\]

where \( N_{\text{ptl\_side}} \) is the number of particles per side of the box. For instance, if we have \( 512^3 \) particles in the box, then

\[
N_{\text{ptl\_side}} = 512, L_{\text{box}} \text{ is the size of the simulation box in units of Mpc/h.}
\]

We use the same set of matter power spectrum \( k \) bins for all fidelities. The available information at small scales is sparse for the low-fidelity spectrum. To resolve the issue, we fix the \( k \) bins to high fidelity and linearly interpolate the low-fidelity power spectrum in a log scale, \( \log_{10}P(k) \), onto the high-fidelity \( k \) bins. The maximum \( k \) is set to be \( \simeq 6.4 \text{ Mpc}^{-1} \) when using \( N_{\text{ptl\_side}} = 128 \) as our low-fidelity training set. However, in practice we found that \( 128^3 \) and \( 512^3 \) simulations shared similar \( k \) bins with small offsets at small scales.

We do not model the high-fidelity spectrum with \( k \) larger than the maximum \( k \) of the low-fidelity spectrum:

\[
\max k_{t\_2} = \max k_{t\_1},
\]

where \( t \) indicates the fidelity level and \( t = 2 \) is the highest fidelity. If we do not have any data at a given \( k \) from low-fidelity, we cannot extract the correlations between fidelities without other more significant assumptions. In other words, the maximum \( k \) we can model is limited by the data available from the low-fidelity simulations, which always have a lower maximum \( k \) than high-fidelity simulations. We note that it is possible to get a higher maximum \( k \) by particle folding or by increasing the size of the PM grid size used for estimating the power spectrum, although we do not do that here.

We do model the low-fidelity \( P(k) \) even on scales smaller than the mean particle spacing, \( k > k_{\text{spacing}} \). We made this particular decision because we have a prior belief that even though \( P(k > k_{\text{spacing}}) \) is highly biased, it still captures some information about how \( P(k) \) depends on cosmological parameters. Thus, we should be able to exploit the correla-
tions between fidelities and improve the emulator accuracy at those scales.

To summarize, we:

(i) Use the same set of $k$ bins across different fidelities.
(ii) Preserve all available $P(k)$ from low-fidelity, even scales smaller than the simulation’s mean particle spacing.

3 SINGLE-FIDELITY EMULATORS

Here we briefly recap how we train a single-fidelity emulator. Readers familiar with this material may wish to skip to Section 4. The notation we use in this section follows those of Perdikaris et al. (2017); Cutajar et al. (2019). Consider a supervised learning problem, in which we wish to learn the mapping relation, $f$, between a set of input and output pairs $\mathcal{D} = \{x_i, y_i\} = \{x, y\}$, where $i = 1, \ldots, n$:

$$y = f(x), \text{ with } x \in \mathbb{R}^d,$$

where $d$ is the dimension of the input space. A Gaussian process (GP) [Rasmussen & Williams 2006] is a probabilistic framework modelling the observations, $y_i$, as drawn from a noisy realization of a single random function $f$ with a likelihood $p(y | f)$. It models the distribution over $f$

$$p(f) = \mathcal{GP}(f; \mu, K),$$

with $\mu$ the GP mean prior function, which is usually assumed to be a zero mean prior, and $K$ the covariance kernel function specified by a vector of hyperparameters, $\theta$. For a given set of inputs, $x_1, x_2, \ldots, x_n$, the kernel function evaluated on these points produces a symmetric, positive-definite covariance matrix $K_{ij} = K(x_i, x_j; \theta)$ with $K \in \mathbb{R}^{n \times n}$.

The choice of the covariance kernel depends on our prior knowledge about the data. The hyperparameters of a chosen kernel are optimized by maximizing the marginal log-likelihood:

$$\log p(y | x, \theta) = -\frac{1}{2} \log |K| - \frac{1}{2} y^\top K^{-1} y - n \frac{1}{2} \log 2\pi. \tag{8}$$

For an emulator, the main purpose is to predict an output $f_\ast = f(x_\ast)$ from a new input point $x_\ast$, given the provided data $\mathcal{D}$.

$$p(f_\ast | \mathcal{D}, x_\ast) = \mathcal{N}(f_\ast | \mu_\ast(x_\ast), \sigma_\ast^2(x_\ast)), \tag{9}$$

where $\mu_\ast$ is the posterior mean and $\sigma_\ast$ is the standard deviation of the uncertainty in the estimate of the predictions. The vector $\sigma_\ast \in \mathbb{R}^d$ is the covariance between the new point and trained data, $K_{\ast n} = [K(x_\ast, x_1), \ldots, K(x_\ast, x_n)]$.

3.1 Cosmological emulators

Consider we have a set of dark matter-only simulations with fixed box size and mass resolution. At each redshift bin $z_0$, we can compute the matter power spectrum, $P(k, z = z_0)$, given a set of input parameters. We will use the log power spectrum, $\log_{10} P(k, z = z_0)$, as our training data.

The training data, $\mathcal{D} = \{x_i, y_i\}$, are defined as

$$x_i = [h, \Omega_0, \Omega_m, A_s, n_s];$$

$$y_i = \log_{10} P(k, z = z_0),$$

where $i = 1, \ldots, n$ indicates the $i$th simulation we run with this specific set of input parameters.

The rest of the modelling is choosing an appropriate covariance function $K(x, x')$. We use a squared exponential kernel and use automatic relevance determination (ARD) weights for each input dimension. ARD assigns each input dimension, $x_i$, a separate hyperparameter, $w_i$:

$$K(x, x'; \theta) = \sigma^2 \exp \left( -\frac{1}{2} \sum_{i=1}^d w_i (x_i - x_i')^2 \right)$$

where $i = 1, \ldots, d$ indicates the dimension of the input space $x \in \mathbb{R}^d$, $\sigma^2$ is the variance parameter for the squared exponential kernel, $\{w_i\}_{i=1}^d$ are the ARD weights, $\{w_i\}_{i=1}^d$ are inverse length scales, which defines the degree of smoothness at a given input dimension. We note that we assign independent hyperparameters, $\theta = \{\sigma^2, w_1, \ldots, w_d\}$, for each $k$ mode.

A larger $w_i$ corresponds to a smaller length scale, reflecting that the learned function varies more in the $i$th dimension. On the other hand, a smaller $w_i$ implies a larger length scale, indicating that the learned function is smoother along the $i$th dimension. ARD allows each dimension of the learned function to have a different degree of smoothness.

We do not decompose the power spectrum into principle components for training the emulators, as described by Heinemann et al. (2000), Habib et al. (2007) because we want to compare single-fidelity emulators to the multi-fidelity emulators, and an MFEmulator only has a limited number of high-resolution simulations available. In our default case, we only have 3 high-resolution simulations for an MFEmulator, and it is not sensible to perform dimension reduction on three power spectra.

To ensure that our single-fidelity emulator is not unfairly disadvantaged in the comparison with our multi-fidelity emulator by poorly constrained hyperparameters, we built a single-fidelity emulator which shared kernel parameters across all $k$ modes and empirically verified that it had similar performance.

4 MULTI-FIDELITY EMULATOR

In this section, we describe how we train a multi-fidelity emulator. We outline the modelling assumptions in Section 4.4. Section 4.2 describes the formalism of the linear multi-fidelity emulator proposed by Kennedy & O'Hagan (2000), a multi-output GP with a linear correlation between fidelities. Section 4.3 outlines the non-linear multi-fidelity emulator of Perdikaris et al. (2017), which models the correlation between fidelities as a function of cosmological parameters. We follow the notation and formalism of Kennedy & O'Hagan (2000); Perdikaris et al. (2017); Cutajar et al. (2019).
(i) Correlations between the code fidelities: For an $N$-body simulation, the simulation cost depends on the mass resolution. We assume a simulation with a low mass resolution can approximate a simulation with a high mass resolution. The matter power spectrum from different fidelities is strongly correlated at large scales since all fidelities are resolved and the mass resolution has negligible effects. At small scales, however, we expect different fidelities are only weakly correlated.

(ii) Smoothness: For an emulation problem, we assume that neighbouring inputs give similar outputs. For example, suppose two sets of input parameters to MP-GADGET are close to each other. In that case, we assume that an $N$-body simulation will provide a similar outcome.

(iii) The prior belief on each fidelity is a Gaussian process: We assume a prior belief that the mapping from code input to output is a Gaussian process for each fidelity.

The first assumption is the core assumption of a multi-fidelity emulator. Different levels of the same code are simulating the same physical reality: It is thus reasonable to assume different code fidelities should correlate at some level. However, a naive simulation, for example, $N_{ptl_{side}} = 16$ could only barely approximate a HR with $N_{ptl_{side}} = 512$. Therefore, we should also assume the correlation between fidelities depends on the distance between two fidelities in the dimension of mass resolution.

There is thus a trade-off between the strength of correlation and the computational expense: for example, a simulation with $N_{ptl_{side}} = 256$ provides more information about a HR ($N_{ptl_{side}} = 512$), but running a 256$^3$ simulation is 8 times most expensive than running a LR ($N_{ptl_{side}} = 128$).

One can select an optimal choice of simulation cost by balancing the computational time and the emulation accuracy. Here we choose $N_{ptl_{side}} = 128$ for our low-fidelity simulations because:

(i) The maximum $k$ is $\approx 6.4$ hMpc$^{-1}$, which includes enough non-linear scales to test the emulation accuracy;

(ii) A 128$^3$ simulation is 64 times cheaper than a HR, and thus the resolution difference between $N_{ptl_{side}} = 128$ and $N_{ptl_{side}} = 512$ is large enough to demonstrate whether simulations with lower costs can accelerate the training of an emulator.

In Section 6.4.1 we will show our method is applicable to simulations with different resolutions, $N_{ptl_{side}} = 64$ and 256. Empirically, we found that using $N_{ptl_{side}} = 256$ as low-fidelity is similar to $N_{ptl_{side}} = 128$, while $N_{ptl_{side}} = 64$ gives a worse emulation accuracy.

The second assumption, the smoothness assumption, is the general assumption of a GP emulator. A GP emulator will have poor accuracy if the code does not behave similarly with similar input. The smoothness assumption is also the assumption behind the Latin hypercube sampling scheme (for a detailed discussion, see Heitmann et al. 2009).

A multi-fidelity emulation could in principle be implemented using other models (see Pecherstorfer et al. 2018 for different data-fit models for surrogates). We chose to use GPs simply because their Bayesian approach supports uncertainty quantification and there is a well-developed community around GP emulation.

4.2 Linear multi-fidelity emulator (AR1)

We have multi-fidelity data $D_t$ as described in Section 2. A multi-fidelity emulator is essentially inferencing the highest fidelity model conditioned on data from all model fidelities. The final goal of a multi-fidelity emulator is to find a mapping relation $f$ such that, from an arbitrary input vector $x$, we can always find the highest fidelity code output:

$$ y_* = f(x_*). $$

As described by Kennedy & O’Hagan (2000), a linear autoregressive model can be applied in a multi-fidelity setting by assuming a hierarchical order between fidelities:

$$ f_t(x) = \rho_1 f_{t-1}(x) + \delta_t(x), $$

where $f_t$ is the function emulated at the previous fidelity level and $f_{t-1}$ is the function emulated at the previous fidelity level $(t-1)$. The linear component of Eq 12 is $\rho_1$, which models the correlation between fidelities as a linear relation, $\delta_t$ is a GP modelling the bias term:

$$ \delta_t \sim \mathcal{GP}(\mu_t, K_t). $$

We modify Eq 12 so inference is performed on each $k$ bin independently. For $k = k_1$, we have independent kernel and scaling parameters for each $k = k_1$ mode. For simplicity, we will drop the $k = k_1$ notation in the rest of the paper:

$$ f_t(x) = \mu_t - \mu_{t-1} + \delta_t(x). $$

The mean of the bias term, $\mu_t$, is assumed to be the zero function. For the low-fidelity part, we subtract the sample mean of the logarithm training power spectra, log$_{10} P(k)$, and model the low fidelity part of the power spectra as a zero mean GP:

$$ (f_t(x) - \mu_t) \sim \mathcal{GP}(0, K_t(x, x'; \theta_t)). $$

As shown in Figure 1 the low-fidelity power spectrum is biased high. We pass variations of the low-fidelity power spectrum around its mean to the next fidelity to avoid passing biased outputs. In practice, we found this slightly improves emulation accuracy for multi-fidelity models.

For the highest fidelity bias function, $\delta_t(x)$, we model the power spectrum using a zero mean GP without subtracting the sample mean. We do not have enough points at the highest fidelity for the sample mean to be a good estimate of the true mean. Since for $t = 1$, $f_t(x)$ is completely determined by $f_{t-1}(x), \delta_t(x)$, and $\rho_t$.

As mentioned by Kennedy & O’Hagan (2000), there is a Markovian property implied in the covariance structure of Eq 12

$$ \text{cov}(f_t(x), f_{t-1}(x')) = 0, $$

which is true for all $x \neq x’$. Eq 16 indicates that if we have $f_{t-1}(x)$, then other input parameters $f_{t-1}(x')$ do not contribute to training $f_t(x)$.

The Markovian property also suggests that an efficient training set $\{D_1, D_2, \ldots, D_s\}$ for a multi-fidelity GP is a nested structure:

$$ x_1 \subseteq x_2 \subseteq \cdots \subseteq x_s. $$

The above notation says that, given an input point $x$ at fidelity $t$, there must be an input $x$ in its lower fidelity $u$, where $u < t$ and $t, u \in \{1, 2, \ldots, s\}$. The reason for using a
nested experimental design is that since we have \( x_{t-1} \subseteq x_t \), we can immediately get an accurate posterior \( f_{t-1}(x) \) at the \( x \) location without interpolating at the \( t-1 \) level. However, in practice we found our multi-fidelity emulators performed well even without a nested design in the input space.\(^\text{11}\)

At a given fidelity \( t \), the posterior at a test input \( x_* \) could be written as

\[
p(x_* | D, x_*) = N(f_{*t}; \mu_{*t}(x_*), \sigma^2_{*t}(x_*)),
\]

where we denote predictions from new inputs as subscript \( * \).

The predictive mean and variance are

\[
\mu_{*t} = \mu_{*t-1}(x_*) + \mu_{t} + \mathbf{k}_{\rho_{t}} \mathbf{K}^{-1}_{t} [y_t - \mu_{*t-1}(x_t) - \mu_{t}],
\]

\[
\sigma^2_{*t} = \sigma^2_{*t-1}(x_*) + \mathbf{K}(x_*, x_*) - \mathbf{k}_{\rho_{t}} \mathbf{K}^{-1}_{t} \mathbf{k}_{\rho_{t}}^\top,
\]

where \( \mathbf{k}_{\rho_{t}} = \{K_t(x_*, x_1), \ldots, K_t(x_*, x_n)\} \) is a vector of covariance between the new location and the training locations at fidelity \( t \). \( K_t = K_t(x_*, x_1) \) is the covariance matrix of training locations at fidelity \( t \).

### 4.2.1 Covariance kernel

For a linear multi-fidelity emulator, we place an independent squared exponential kernel on each \( K_t \). The mathematical form of the kernel is the same as Eq. [10].

Having ARD weights means we assign different length scales to each dimension so that the kernel can be trained anisotropically. We found that using ARD in the highest fidelity did not improve the model’s accuracy. Thus, we decided to assign an isotropic kernel for \( \delta_s \). For a two-fidelity emulator \( (s = 2) \), we have 6 hyperparameters in low-fidelity for each \( k \) bin; 5 of them are the length scale parameters and 1 is the variance parameter. We have 3 hyperparameters for each \( k \) bin in high fidelity, with one scale factor \( \rho_{t} \) between fidelities, one variance parameter, and one length scale parameter. We have 49 bins in \( k \), so the total number of trainable hyperparameters is 441.

Figure 2 shows the learned scale factor, \( \rho_{t} \), \( \rho \) is roughly unity at large scales \( k \ll 2 h \text{Mpc}^{-1} \), but its value increases dramatically after \( k > 2 h \text{Mpc}^{-1} \). Non-linear physics becomes important and the low-fidelity simulations become less reliable at small scales, making the relationship between fidelities non-trivial. We want to emphasize that the scale factor, \( \rho \), is learned from the multi-fidelity emulator. We did not enforce \( \rho \) to be a specific shape during the training. Because we learn the mapping from LR to HR using the training data, it is expected that LR runs deviate from HR power spectra. The purpose of multi-fidelity emulation is to correct these deviations.

### 4.3 Non-linear multi-fidelity emulator (NARGP)

The linear multi-fidelity model in Eq. [12] assumes the scale factor \( \rho_{t} \) is independent of input parameters, \( x \), and so does not model the cosmological dependence of the scale factor \( \rho_{t} \). The non-linear multi-fidelity model proposed by [Perdikaris et al. 2017] drops this assumption, allowing the scale factor, \( \rho_{t} \), to be a function of both input cosmology and output from the previous fidelity. As for the linear multi-fidelity model, we model the non-linear multi-fidelity GP independently for each \( k \):

\[
f_t(x) = \rho_{t}(x, f_{t-1}(x) - \mu_{t-1}) + \delta_t(x),
\]

where \( \rho_{t}(\cdot) \) is a function of both input parameters \( x \) and the previous fidelity’s output, \( \rho_{t}(\cdot) \) is modelled as a GP. Eq. [20] results in a more complicated distribution over \( f_t \), a deep Gaussian process [Damianou & Lawrence 2013]. To avoid added computational and statistical complexity, we follow the same approximation as [Perdikaris et al. 2017] and replace \( f_{t-1} \) in Eq. [20] with its posterior, \( f_{t-1} \). The result is a regular Gaussian process,

\[
f_t \sim \mathcal{N}(0, K_t),
\]

whose kernel can be furthermore decomposed:

\[
K_t(x, x') = K_{t_0}(x, x'; \theta_{t_0}) \cdot K_{t_1}(f_{t-1}(x), f_{t-1}(x'; \theta_{t_1})) + K_{t_2}(x, x'; \theta_{t_2}),
\]

where \( f_{t-1} \equiv f_{t-1}(x) - \mu_{t-1} \) for simplicity. The first kernel \( K_{t_0} \) models the cosmological dependence of the scale factor \( \rho \). Next, \( K_{t_1} \) models the covariance of the output passing from the previous fidelity to the current level. The final term \( K_{t_2} \) models the model discrepancy between fidelities. For the lowest fidelity, the matter power spectrum is only modelled with \( K_{t_0} \).

Each kernel in Eq. [22] \( (K_{t_0}, K_{t_1}, K_{t_2}) \), is modelled as a squared exponential kernel. Suppose we assign a different length scale parameter for each \( x \) dimension, \( K_{t_0} \) will have \( d + 1 \) hyperparameters, \( K_{t_1} \) will have \( 2 \) hyperparameters, and \( K_{t_2} \) will have \( d + 1 \) hyperparameters. As for the linear emulator, we found no improvement in accuracy in practice by using ARD for the high-fidelity model. Thus, we have 2 hyperparameters for each kernel in high fidelity and \( d + 1 \) hyperparameters in low fidelity.
hyperparameters for low-fidelity. To be explicit, in the high-fidelity model, \( K_{\text{hr}} \) has 2 hyperparameters, \( K_{\text{lf}} \) has 2 hyperparameters, and \( K_{\text{hp}} \) has 2 hyperparameters. For \( d = 5 \), we have 6 hyperparameters for low-fidelity and 6 for high-fidelity models at each \( k \) bin.

4.3.1 Halo Model Interpretation

The formulation of our multi-fidelity emulator bears a marked resemblance to the equations which form the basis of HALOFIT (Smith et al. 2003), and are themselves motivated by the halo model (Peacock & Smith 2000; Seljak 2000). This correspondence allows us to provide a physical interpretation of our results. In the halo model, matter clustering is schematically divided into two components: a two-halo term and a one-halo term. The two-halo term arises from correlations between halos on large scales, while the one-halo term, which has a weaker dependence on cosmology, is sensitive to the density profile inside each halo. We can model this by splitting the non-linear power spectrum

\[
P_{\text{NL}}(k) = P_2(k) + P_1(k).
\]

The quasi-linear term \( P_2(k) \) is a two-halo term, while \( P_1(k) \) is a one-halo term. The two-halo term can be modelled by the linear theory power spectrum filtered by a window function \( W(M, k) \):

\[
P_2(k) = P_L(k) \left( \int W(M, k) dM \right)^2.
\]

The window function depends on the halo mass function and halo bias, encodes how virialisation displaces the linear matter field, and tends to unity on large scales.

There is a clear connection between this model and the form of our multi-fidelity emulator. Eq 12 (AR1) and Eq 20 (NARGP) move between fidelities via two terms: a scaling factor \( \rho \) and an additive factor \( \delta_t \). The correlations between fidelities are strong on large scales, and so \( \rho \to 1 \) as \( k \to 0 \). \( \rho \) is analogous to the quasi-linear window function, except that it filters not the linear theory power spectrum \( P_L \), but the low-fidelity N-body model \( f_\text{\textbf{}}(x) \). In the context of the halo model, it extrapolates the existing quasi-linear halo filtering to include lower mass halos not included in the low-fidelity simulation.

The additive factor \( \delta_t \), which is important on small scales, is analogous to the one-halo term. It models the difference in halo shot noise and internal halo profiles between resolutions. Notice that \( \delta_t \), like the one-halo term, depends only weakly on cosmology, as evidenced by it requiring only one length-scale hyperparameter.

5 SAMPLING STRATEGY FOR HIGH-FIDELITY SIMULATIONS

In this section, we will describe how we select the training simulations for our multi-fidelity emulators. We will first describe the nested structure implemented in multi-fidelity emulators in Section 5.1. Section 5.2 explains how we find the optimal choice of high-fidelity training simulations.

5.1 Nested training sets

The proposed sampling scheme for training and testing is shown in Figure 3. The corresponding output power spectra are shown in Figure 4. In Figure 3, the sampling is done using two different Latin hypercubes:

(i) Training simulations: a Latin hypercube with 50 points. HR points are a subset of LR points.

(ii) Testing simulations: another Latin hypercube with 10 points.

(iii) We use the notation “X LR-Y HR emulator” to represent a multi-fidelity emulator trained on \( X \) number of low resolution simulations and \( Y \) number of high resolution simulations.

The first hypercube with 50 points ensures that we will have a nested experimental design. The second hypercube is to ensure we will not test on the training simulations during the validation phase. In practice, we found that the emulation accuracy roughly converged with \( \sim \) 30 LR points.

5.2 Optimizing the loss of low-fidelity simulations

For a multi-fidelity problem, we want to minimize the required high-fidelity training simulations to achieve a given accuracy. We search for the optimal subset of LR points to simulate at HR by picking the subset that would minimize the low fidelity training set’s single-fidelity emulator errors. In our experiments with two fidelities, \( s = 2 \), there are \( \binom{n_2}{1} \) possible combinations for \( x_2 \), which are input parameters for the high-fidelity data, \( D_2 = \{ x_2, y_2 \} \).

Retraining low-fidelity only emulators on all possible subsets of the low-fidelity grid is computationally intensive. For example, selecting two samples out of 50 points means that we have to train \( \binom{50}{2} = 1,225 \) low-fidelity emulators. To save computational cost, we employed a greedy optimization strategy. Instead of exploring all possible subsets, we grew the subset one point at a time, fixing the previously chosen points. As a further optimisation, we used the same set of kernel hyperparameters for all \( k \) bins.

Consider \( S \), a potential \( D_2 \) with \( x_2 \subset x_1 \). We train a low-fidelity only emulator based on Eq 8 using the \( n_2 \) low-fidelity points in \( S \) and get a GP:

\[
p(f_\star \mid \mathcal{S}, x_\star) = \mathcal{N}(f_\star \mid \mu_i(x_\star), \sigma_i^2(x_\star)^2),
\]

which is the posterior as described in Eq 9.

With the trained low-fidelity only emulator in Eq 23 we can test this single-fidelity emulator’s performance by predicting the rest of the data in the low-fidelity Hypercubc. To evaluate the accuracy, we compute the mean squared error by averaging over the test data:

\[
\text{MSE} = \mathbb{E}[(y_\star - \mu_i(x_\star))^2],
\]

where \( \{x_\star, y_\star\} \) are the low-fidelity data pairs from the rest of the Latin hypercube,

\[
\{x_\star, y_\star\} \in \{D_1 - S\}.
\]

This simply means that we test the single-fidelity emulator on the available data not included in the training subset.

Suppose we repeat the training of single-fidelity emulators until we train all possible subsets in the low-fidelity
We will now have \( n_1 \) trained single-fidelity emulators. Each single-fidelity emulator will provide a mean squared error, which is the test error that the emulator generates against the low-fidelity hypercube test data. To select the optimally trained emulator, we compute

\[
S^* = \arg \min_{S} \mathbb{E}[(y_s - \mu^1(x_s))^2]
\]

where we find the subset \( S^* \) which minimizes the mean squared errors on the test set. We use \( S^* \) as our high-fidelity training set \( D_2 \) under the nested experimental design. To be explicit:

\[
x_2 = x_{S^*} \subset x_1,
\]

where \( x_2 \) are the selected high-fidelity input points, \( x_{S^*} \) are the input points from the selected subset \( S^* \) (which minimize the low-fidelity emulator mean squared error), and \( x_1 \) are the low-fidelity input points.

This strategy assumes that the effect of a sampling scheme on a low-fidelity emulator is the same as that on a corresponding multi-fidelity emulator. For example, suppose \( \Delta \Omega \) is crucial for learning how the low-fidelity power spectrum \( y_1 \) changes for inputs \( x_1 \). In that case, we expect that information about \( \Delta \Omega \) can also effectively change the high-fidelity spectrum \( y_2 \).

The above assumption could be violated if the power spectra at small scales, which are not included in the low-fidelity data, behave very differently from those at large scales. This could happen if the smoothness length scale acts very differently between low-fidelity and high-fidelity data for a given input dimension. For example, imagine that a parameter, \( \theta \), has a small effect on the outcomes of low-
fidelity simulations, but a large effect on the outcomes of high-fidelity simulations.

Figure 5 shows the mean squared errors computed from $64^3$ single-fidelity emulators and $256^3$ single-fidelity emulators. First, note that the selection of the training simulations affects the emulator accuracy. Second, the low-fidelity emulator errors are correlated with their higher fidelity counterparts. This suggests that a low-fidelity emulator can serve as a guide for placing high-fidelity training simulations. The HR parameter choices used in Section 6 were selected with an earlier version of our model using $64^3$ particle simulations. We checked that using either $64^3$ or $128^3$ for selection gave almost the same emulation accuracy for a non-linear 50LR-3HR emulator, though one of the selected samples is different.

In practice, we find the procedure above can prevent us from selecting the HR combination that will give us the worst multi-fidelity emulation result. Although we have tested that our procedure works for the matter power spectrum, we would suggest that when emulating a new summary statistic (e.g., the halo mass function), the reader investigates the effectiveness of this method using small test cases. We may in future work investigate using Bayesian optimization (e.g., Forrester et al. 2007; Lam et al. 2015; Poloczek et al. 2016) to select the optimal HR samples for multi-fidelity training.

6 RESULTS

This section shows the interpolation accuracy of multi-fidelity methods and compares our multi-fidelity emulators to single-fidelity emulators. Section 6.1 compares test set emulator errors for the linear multi-fidelity emulator (AR1) and non-linear multi-fidelity emulator (NARGP). Section 6.3 shows the multi-fidelity emulator uncertainty with more training simulations, Section 6.3 shows the emulator errors with more LR or HR training simulations. Finally, Section 6.4 checks the performance of the multi-fidelity method for other emulation settings. To test how much a multi-fidelity emulator can improve with more training simulations, Section 6.3 shows the emulator errors with more LR or HR training simulations. Finally, Section 6.3 checks the performance of the multi-fidelity method for other emulation settings.

6.1 Comparison of Linear and Non-Linear Emulators

Figure 6 and Figure 7 show the predicted power spectrum divided by the exact power spectrum. Both emulators, linear (AR1) and non-linear (NARGP), are trained with 50 low-fidelity simulations and 3 high-fidelity simulations. We will call these emulators “50LR-3HR emulators” for simplicity. A non-linear (linear) multi-fidelity emulator requires at least 3 (2) HR simulations for training and has $\pm 2\%$ ($\pm 5\%$) worst-case accuracy per $k$ bin. For a linear multi-fidelity emulator, the minimum re-

Figure 5. Emulator mean squared errors evaluated from $64^3$ emulators and $256^3$ emulators. We compute all subsets of 3 samples from a 50 samples Latin hypercube, $\binom{50}{3} = 19,600$ subsets in total. Colorbar is in log scale. The blue dashed line represents a perfect linear relationship.

Figure 6. Predicted divided by exact power spectrum from a 50LR-3HR emulator using a linear multi-fidelity method (AR1). Different colours correspond to 10 test simulations spanning a 5-D Latin hypercube. The shaded area indicates the worst-case $1 - \sigma$ emulator uncertainty. There is one test simulation driving the larger error compared to the non-linear one in Figure 7.

Figure 7. Predicted divided by exact power spectrum from a 50LR-3HR emulator using a non-linear multi-fidelity method (NARGP). Different colours correspond to 10 test simulations spanning a 5-D Latin hypercube. The shaded area indicates the worst-case $1 - \sigma$ emulator uncertainty. Note that the y-scale in this plot is the same as Figure 6.
required number of HR simulations is 2, reflecting the lower number of hyperparameters in the kernel.

Figure 8 shows a comparison between a linear multi-fidelity emulator and a non-linear multi-fidelity emulator in relative emulator error. We include linear and non-linear 50 LR-3 HR emulators. We define the relative emulator error:

$$\text{Emulator Error} = \frac{P_{\text{pred}}}{P_{\text{true}}} - 1.$$  \hfill (30)

$P_{\text{pred}}$ is the predicted power spectrum from the multi-fidelity emulator, and $P_{\text{true}}$ is the power spectrum from the high-fidelity test simulation.

Figure 8 shows that the linear 50 LR-3 HR emulator predicts an average error $< 1\%$ per $k$ bin for $k \leq 4 \text{ hMpc}^{-1}$ and $< 2\%$ per $k$ bin for $4 < k \leq 6.4 \text{ hMpc}^{-1}$. The non-linear multi-fidelity emulator predicts an average error $\lesssim 1\%$ per $k$ bin, which implies we only need 3 HR to achieve a percent-level accurate emulator using the non-linear multi-fidelity method. At $k \leq 3 \text{ hMpc}^{-1}$, both emulators predict mostly the same accuracy, but the non-linear one performs better at smaller scales $k > 3 \text{ hMpc}^{-1}$.

We found that the non-linear multi-fidelity emulator outperforms the linear one in all aspects. For simplicity, we will only show the non-linear multi-fidelity models in the following sections, but we note that a linear multi-fidelity model is still useful when only two HR simulations are available. We also found that, for the linear model, changing from 50 LR-3 HR emulator to 50 LR-2 HR emulator only slightly degrades the overall accuracy.

### 6.2 Comparison to single-fidelity emulators

#### 6.2.1 Comparison to high-fidelity only emulators

Figure 9 shows a comparison between a non-linear 50 LR-3 HR emulator and high-fidelity only emulators. The high-fidelity only emulators are single-fidelity emulators trained solely on HR simulations. The non-linear multi-fidelity emulator outperforms the single-fidelity emulator with 11 HR at all $k$ modes. It also predicts a worst-case error smaller than the worst-case error from the 11 HR single-fidelity emulator. At $k \leq 2 \text{ hMpc}^{-1}$, the multi-fidelity emulator performs much better than the single-fidelity emulators. Since LR simulations can predict accurate power spectrum at large scales $k \leq 2 \text{ hMpc}^{-1}$, we expect a single-fidelity emulator requires $\sim 50$ HR to compete with the 50 LR-3 HR emulator on large scales. A HR is $\sim 64$ times more expensive than a LR, thus the core time for a 50 LR-3 HR emulator is $\sim 4$ HR. The non-linear multi-fidelity outperforms a single-fidelity 11 HR emulator with $\sim 3$ times lower computational cost.

The error reduction rate is the relative error of a single-fidelity emulator divided by the error of a multi-fidelity emulator. Both linear and non-linear 50 LR-3 HR emulator show an error reduction rate of $\approx 100$ for $k \leq 0.5 \text{ hMpc}^{-1}$, $\approx 100$ times better than the single-fidelity counterpart using 3 HR. At smaller scales $k > 3 \text{ hMpc}^{-1}$, the multi-fidelity emulators are $\approx 20$ times (non-linear), and $\approx 10$ times (linear) better than their single-fidelity counterpart.
6.2.2 Comparison to low-fidelity only emulators

Figure 10 shows a single-fidelity emulator trained on 50 LR simulations, compared to a non-linear 50LR-3HR emulator. Figure 10 demonstrates how multi-fidelity modelling improves the emulator accuracy at each $k$ scale. At $k \lesssim 3 \, \text{hMpc}^{-1}$, multi-fidelity modelling uses 3 HR to correct the resolution and reduce the average emulator error from $\lesssim 5\%$ to $\lesssim 1\%$. A low-fidelity emulator predicts a biased power spectrum beyond $k = 3 \, \text{hMpc}^{-1}$. However, the multi-fidelity method can moderately correct the bias and reduce the error to $\lesssim 1\%$. Again, the multi-fidelity technique can use a few HR simulations to calibrate the resolution difference.

6.2.3 Core hours versus emulator errors

Figure 11 shows the average relative emulator error as a function of core hours for performing the training simulations. The emulator errors shown in Figure 11 are averaged over all $k$ modes, so each emulator corresponds to a single point in the plot. An ideal emulator will be on the left bottom corner, implying both low cost and high accuracy. The slope of a given emulator in the plot indicates how easily we can improve the emulator with more training data. A steeper (more negative) slope means we can increase the emulator accuracy with a lower cost.

We notice three types of emulators are clustered in separate regions in the plot. The low-fidelity only emulator (LF-only) has the lowest cost and shows no noticeable improvement from increasing training simulations from 50 to 400 LR. The high-fidelity only emulator (HF-only) shows an accuracy improvement with more HR simulations from 3 HR to 11 HR. However, performing one HR requires $\sim 2000$ core hours, making the HF-only emulator much more expensive than the other two emulators in the plot.

6.3 Varying the number of training simulations

6.3.1 Effects of more low-resolution training simulations

The benefit of using a multi-fidelity emulator is that we can improve the emulator accuracy using extra low-fidelity simulations. Figure 12 shows the emulator error colour coded by the number of LR training simulations. With more LR training data, the emulator performance improves at both large and small scales. We only show the non-linear emulator here for simplicity, but we observe a similar trend in the linear emulator. For NLR-3HR with $N \in \{10, 20, 30, 40, 50\}$ emulators, the last $k$ bin gives $3.77\%$, $1.16\%$, $1.15\%$, $0.97\%$, and $1.04%$ emulator errors, indicating an increase of accuracy with more LR training simulations. Dividing the errors into large and small scales at $k = 1 \, \text{hMpc}^{-1}$, the average emulator errors are $0.65\%$, $0.22\%$, $0.10\%$, $0.09\%$, and $0.09\%$ for $k \leq 1 \, \text{hMpc}^{-1}$ and $1.60\%$, $1.04\%$, $0.60\%$, $0.61\%$, and $0.56\%$.
for $k > 1 \, h\text{Mpc}^{-1}$. The decrease in error is nearly saturated with $\sim 40$ LR simulations.

6.3.2 Effects of more high-resolution training simulations

In Figure 13, we add more HR training simulations to our multi-fidelity emulator. The 50 LR-N HR emulator with $N \in \{3, 5, 7, 9\}$ shows no improvement in average error with more HR, although the worst case error improves noticeably for the 50 LR-9 HR emulator. One reason may be stochasticity in the training set due to simulation modelling error, which is around 1%, and limits the prediction accuracy. In particular, MP-GADGET simulations with 512$^3$ particles may not be fully converged on small scales, and this limits the emulator’s learning. Another possibility is that the prior from 50 low-fidelity simulations may be too hard to overcome with only 9 HR simulations.

To improve multi-fidelity emulator accuracy further, one could build a more complicated model than the one proposed in this paper. The improvement from the linear to the non-linear model shows that different decisions about the scaling factor $p$ could better predict the non-linear structure. However, those complicated models will require more high-fidelity training simulations. We will leave more complex modelling structures to future work.

6.4 Effect of other emulation parameters

6.4.1 The resolution of low-fidelity simulations

We have so far tested multi-fidelity emulators using 128$^3$ simulations (LR) as low-fidelity and 512$^3$ simulations (HR) as high-fidelity. Figure 14 shows non-linear 50 LR-3 HR emulators using different mass resolutions, 64$^3$ and 256$^3$ simulations, as low-fidelity.

A 64$^3$ simulation is $\simeq 512$ times cheaper than a HR but has a smaller maximum $k$ with max $(k) \simeq 3 \, h\text{Mpc}^{-1}$. It produces percent level accuracy for $k \leq 1 \, h\text{Mpc}^{-1}$ and has worst-case errors $< 5\%$ at small scales $k \geq 1 \, h\text{Mpc}^{-1}$. A 256$^3$ simulation is $\simeq 8$ times cheaper than a HR simulation, so the computational cost for a 50 LR-3 HR emulator is $\simeq 9$ HR simulations. This emulator mildly outperforms the emulator where LR is 128$^3$, with an average percent-level emulation until $k \simeq 12 \, h\text{Mpc}^{-1}$, but at a substantially increased computational cost.

Figure 15 demonstrates that one can fuse various qualities of LR with HR simulations to build a multi-fidelity emulator. Figure 14 also shows that the multi-fidelity emulator’s accuracy depends on the correlation between LR and HR. A 64$^3$ simulation is only a rough approximation to its 512$^3$ counterpart, so the emulator that uses 64$^3$ simulations as low-fidelity is less accurate than the others in Figure 14.

6.4.2 Emulation at $z = 1$ and $z = 2$

This section examines the performance of a non-linear emulator at higher redshifts, $z = 1$ and $z = 2$. Figure 15 shows the emulator error of a non-linear 50 LR-3 HR emulator at $z = 0, 1, 2$. The mean error at $z = 1$ is smaller than the $z = 0$ error at $k \leq 2 \, h\text{Mpc}^{-1}$ while it is larger for $k > 2 \, h\text{Mpc}^{-1}$.
This result shows that it is easier to train the correlation between fidelities at large scales, $k > 2 \, h \, \text{Mpc}^{-1}$, while harder to train at small scales, $k > 2 \, h \, \text{Mpc}^{-1}$. The emulator at $z = 2$ also shows a better performance than $z = 0$ at large scales, $k < 2 \, h \, \text{Mpc}^{-1}$, but the error diverges to $\sim 10\%$ on smaller scales, $k > 2 \, h \, \text{Mpc}^{-1}$. The improved performance on large scales may be because at higher redshifts the matter power spectrum is closer to linear theory and so the correlation between fidelities is easier to learn.

Figure 16 shows the matter power spectrum at $z = 2$, with the same cosmological parameters as Figure 1 and indicates a potential explanation. At $z = 2$, the low-fidelity simulation contains a systematic at the scale of the mean interparticle spacing, related to the initial spacing of particles on a regular grid. This systematic is a transient and disappears by $z = 0$. However, at redshifts where it is present it implies that the low fidelity simulations contain very little cosmological information on scales near their mean interparticle spacing, $k \approx 3 \, h \, \text{Mpc}^{-1}$ and thus cannot significantly improve the emulation accuracy. It may be possible to improve performance at high redshift with the use of other pre-initial conditions such as a Lagrangian glass (White 1994).

8 CONCLUSIONS

We have presented multi-fidelity emulators for the matter power spectrum. Multi-fidelity methods fuse together N-body simulations from different mass resolutions to improve interpolation accuracy. Multi-fidelity emulators use many low-fidelity simulations to learn the power spectrum’s dependence on cosmology, correcting for their low resolution by adding a few high-fidelity simulations. The result is equivalent in accuracy to a single-fidelity emulator performed entirely with much more costly high-fidelity simulations. A multi-fidelity emulator’s physical motivation can be understood using the halo model: low-fidelity simulations capture the two-halo term at large scales, while a few high-fidelity simulations are used to learn the (almost cosmology independent) one-halo term at small scales.

We have also proposed a new sampling strategy which uses low-fidelity simulations as a prior to place high-fidelity training simulations. We choose our high-fidelity training sample and 512 high-fidelity one at large scales, while the non-linear one has a better accuracy at small scales. However, the low-fidelity power spectra are less reliable beyond the mean particle spacing at higher redshifts, inducing some difficulty modelling small scales with $k > 2 \, h \, \text{Mpc}^{-1}$.

Our multi-fidelity emulators could provide percent-level accuracy using only 3 hr simulations and 50 lr simulations, with a total computational cost $\lesssim 4$ hr simulations. We showed it outperforms a single-fidelity emulator with 11 hr simulations. We expect that a single-fidelity emulator would require $\sim 50$ hr simulations to compete with the multi-fidelity one at large scales, $k \lesssim 2 \, h \, \text{Mpc}^{-1}$.

In this paper, we used 128$^3$ simulations as our low-fidelity training sample and 512$^3$ simulations as high-fidelity, with a fixed 256 Mpc/h box. However, Figure 16 indicates our method still has a good performance when extended to other resolutions. We tested our emulator with a series of 10 hr simulations in a Latin hypercube. Two types of multi-fidelity emulators, linear (AR1) and non-linear (NARGP), are used. We showed that both emulators perform similarly at large scales, while the non-linear one has a better accuracy at small scales.

We focussed on $z = 0$, but also investigated higher redshifts. Higher redshift power spectra behave more linearly than at $z = 0$, so it is easier to learn the large-scale correlation between fidelities. However, the low-fidelity power spectra are less reliable beyond the mean particle spacing at higher redshifts, inducing some difficulty modelling small scales with $k > 2 \, h \, \text{Mpc}^{-1}$.

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predictions for future space- and ground-based surveys at a minimum computational cost. All current emulators are single-fidelity, training only on expensive high-fidelity simulations. A single-fidelity emulator requires at least ~ 40 simulations to give percent-level accuracy in an ΛCDM Universe. For example, [14] use 37 simulations to emulate a 5-dimensional ΛCDM model. Euclid Collaboration et al. (2020) use ~ 200 high-fidelity simulations (3003 dark matter particles) to achieve the upcoming Euclid mission’s desired accuracy in an 8-dimensional parameter space.

Our multi-fidelity methods can also be used to improve the existing single-fidelity emulators. For example, suppose we have run 50 high-resolution simulations to build an emulator. We can perform 3 additional super-resolution simulations and combine them to build a super-resolution multi-fidelity emulator. The choice of these 3 simulations could be selected via the optimization strategy proposed in this paper. Instead of performing super high-resolution simulations, one could use generative adversarial network techniques (see [15] et al. 2020) to generate super-resolution simulations and combine them with a multi-fidelity emulator.

Besides increasing the resolution, multi-fidelity methods could also be used to decrease the emulation uncertainty of an existing emulator by extending it with many lowresolution simulations. This indicates a low-cost way to enhance current emulators. Multi-fidelity emulators may make possible efficient expansion of the prior parameter volume. Since high-fidelity simulations are only used to calibrate the resolution, they might not need to span the whole parameter space, implying we can expand the sampling range of an existing emulator by extending the low-fidelity sampling range. We will leave this technique to future work.

In this work, we have tested our multi-fidelity emulators with 512 resolution and a relatively small box 256 Mpc/h. In future we will apply the framework developed here to create a production quality emulator using higher particle load simulations (e.g., 20485 particles) in larger boxes. Other summary statistics, including the halo mass function and the cosmic shear power spectrum, could also be emulated using the same framework.

The multi-fidelity framework may also be extended to hydrodynamical simulations, which are much more costly than their dark matter-only counterparts. No production hydrodynamical emulators including galaxy formation effects such as AGN feedback yet exist. However, AGN feedback significantly affects the matter power spectrum at k > 0.1 hMpc−1 (van Daalen et al. 2011) and pressure forces can affect the power spectrum at k ∼ 10 hMpc−1 (White 2004). Thus practical exploitation of the small-scale information from future surveys will require the development of hydrodynamical emulators. By decreasing the computational cost of an emulator by a factor of 3 and still outperforming a single-fidelity emulator, the work presented here makes emulation development substantially more practical.

SOFTWARE

We used the GPy (GPy 2012) package for Gaussian processes. For multi-fidelity kernels, we moderately modified the multi-fidelity submodule from emukit (Paleyes et al. 2019). We used the mp-gadget (Feng et al. 2018a) software for simulations. We generated customized dark matter-only simulations using astin hypercubes a modified version of SimulationRunner.

DATA AVAILABILITY

The code to reproduce a 50 LR-3 HR emulator is available at https://github.com/jibanCat/matter_multi_fidelity_emulator alongside the power spectrum data.

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14 Aricò et al. (2020) has an emulator using baryonization methods for BACCO simulations.

15 https://github.com/EmuKit/emukit
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17 https://github.com/sbird/SimulationRunner

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