The Mira-Titan Universe. II. Matter Power Spectrum Emulation

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Abstract

We introduce a new cosmic emulator for the matter power spectrum covering eight cosmological parameters. Targeted at optical surveys, the emulator provides accurate predictions out to a wavenumber $k \sim 5 \text{ Mpc}^{-1}$ and redshift $z \leq 2$. In addition to covering the standard set of $\Lambda$CDM parameters, massive neutrinos and a dynamical dark energy of state are included. The emulator is built on a sample set of 36 cosmological models, carefully chosen to provide accurate predictions over the wide and large parameter space. For each model, we have performed a high-resolution simulation, augmented with 16 medium-resolution simulations and TimeRG perturbation theory results to provide accurate coverage over a wide $k$-range; the data set generated as part of this project is more than 1.2Pbytes. With the current set of simulated models, we achieve an accuracy of approximately 4%. Because the sampling approach used here has established convergence and error-control properties, follow-up results with more than a hundred cosmological models will soon achieve $\sim 1\%$ accuracy. We compare our approach with other prediction schemes that are based on halo model ideas and remapping approaches. The new emulator code is publicly available.

Key words: dark energy – large-scale structure of universe

1. Introduction

The field of cosmology has undergone a remarkable transformation in the last two decades—from a somewhat qualitative picture of the makeup and evolution of the universe we have arrived at the “Standard Model” of cosmology with parameters constrained at the few percent level (Anderson et al. 2014; Antoja et al. 2016). Despite the phenomenological and descriptive success of the Standard Model, many foundational questions still remain unanswered. Our understanding of the fundamental physics is lacking in critical areas: we do not properly understand the cause of the accelerated expansion of the universe (Caldwell & Kamionkowski 2009), the nature of dark matter is unknown (Feng 2010), and our understanding of the physics of inflation remains incomplete, to mention three of the most prominent puzzles. Ongoing and upcoming cosmological surveys and experiments aim to address these and other questions by providing data sets with much smaller statistical errors and extended range in spatial scales and redshift. Analysis of these observations can uncover important clues by providing evidence against a cosmological constant, or even against general relativity as the preferred theory of gravity (Joyce et al. 2015). Some of the data will put added constraints on the properties of dark matter candidates, and also significantly tighten the current cosmological errors on determining the sum of neutrino masses. Because of the enhancement of data quality, it is therefore important—from a theoretical and modeling perspective—to open up new parameters beyond the standard set of $\theta = [\omega_{\text{cdm}}, \omega_{b}, \sigma_8, h, n_s]$ and also enter new uncharted areas with respect to length scales, exploring nonlinear regimes that might provide new insights into the dynamics of the universe.

In order to take full advantage of the new data, and not be theory/modeling-limited, prediction tools must be available at accuracy levels significantly better than those characteristic of the measurements. Since surveys increasingly probe the nonlinear regime of structure formation, theoretical predictions have to be derived from detailed and error-controlled simulations that are necessarily computationally expensive. While this may be a reasonable approach to studying individual models, it is not practical as a tool for exploring parameter space, nor does it help in solving the cosmological inverse problem of determining parameters based on observational knowledge of a set of summary statistics, where hundreds of thousands to millions of forward-model evaluations may be needed.

In order to address the above requirement, we have embarked on a program to create very fast oracles, or “cosmic emulators” for various cosmological probes. The aim of the approach is to achieve robustly accurate prediction schemes over a range of cosmological parameters, based on a relatively small number of underlying simulations. The complete framework not only provides predictions for specific cosmological statistics but also includes a self-contained Bayesian inference engine to constrain cosmological parameters by combining observational data and emulator predictions (“cosmic calibration”). We first introduced the concept in Heitmann et al. (2006) based on a set of lower-resolution gravity-only simulations and a simulated data set for the nonlinear matter power spectrum. In a second paper
(Habib et al. 2007), we extended the approach to include measurements for the cosmic microwave background (CMB). In a following set of four papers (Heitmann et al. 2009, 2010, 2014; Lawrence et al. 2010), the Coyote Universe series, we focused on providing a high-accuracy prediction tool for the matter power spectrum over a range of six cosmological parameters, adding \( w \) to the standard set of five. Later, we added other emulators to predict the halo concentration–mass relation (Kwan et al. 2013) and the galaxy power spectrum, using halo occupation distribution modeling (Kwan et al. 2015).

In this paper, we focus again on the matter power spectrum, while extending the range of cosmological parameters to eight, \( \theta = \{ \omega_m^c, \omega_b, \sigma_8, h, n_s, w_0, w_a, \omega_c \} \) and employing higher-quality simulations than in the original Coyote Universe, simultaneously improving on the mass resolution and the simulation volume. This work builds on the convergent sampling strategy described in Heitmann et al. (2016) to systematically improve emulation accuracy by adding new simulations to a previous sample, following Berger (2011). In the original work, the idea was demonstrated on a set of linear power spectra as well as for mass function predictions (assuming universality of the mass function across cosmologies, which is valid at the 5%–10% level)—we now release the first nonlinear emulator from the Mira-Titan Universe simulation suite. The inclusion of a dynamical dark energy component and massive neutrinos is nontrivial—the approach to the simulations is described in more detail in Heitmann et al. (2016). Several tests of the simulation methodology were carried out in Upadhye et al. (2014), where results on large scales were compared to TimeRG perturbation theory. Discussions of the range of validity and methods for adding baryonic corrections are provided in Section 3.1.

The eventual aim of the emulators constructed from the Mira-Titan Universe simulation suite is to reach simulation prediction accuracies at the 1% level, which requires results for more than a hundred cosmological models. The sampling strategy followed allows us to make emulators at intermediate accuracy levels before all the simulations are completed and to thereby check that the appropriate accuracies are in fact being achieved during this process. (This also includes demonstrating successful data filtering, data reduction with principal components, and finally, Gaussian process modeling to carry out the required interpolation.) Results presented in this paper demonstrate the success of this strategy.

Several other approaches have been suggested to provide predictions for the matter power spectrum going beyond \( \Lambda \)CDM. Agarwal et al. (2014) included neutrinos and constructed an emulator using machine learning techniques. Takahashi et al. (2012) used a set of simulations to improve the original HaloFit predictions and Bird et al. (2012) added a neutrino contribution to this model. Casarini et al. (2016) used an approximate approach to extend the Coyote Universe emulator to include \( w_a \) as a new parameter, in order to cover the model space of dynamical dark energy models. Finally, Mead et al. (2016) used a halo model approach to include effects of neutrinos, modified gravity, and dynamical dark energy. We will discuss these approaches and compare some of their results with the emulator presented here in Section 4.

The paper is organized as follows. In Section 2 we describe the cosmological parameter space covered and provide relevant details of the simulation suite used to build the emulator. In Section 3 we discuss emulator construction with a focus on error estimates. We compare our results to other approaches in Section 4, ending with a summary and outlook in Section 5. The emulator is publicly available via a github repository\(^{11} \) and is on our CosmicEmu webpage.\(^{12} \)

2. Parameter Ranges and Simulations

The parameter range now allows for dynamic dark energy and variation of the neutrino mass sum. The Mira-Titan Universe suite of simulations is well on its way to completion; below we describe the general characteristics of the simulations, including a separate discussion of how neutrinos are included.

2.1. Parameters

The choices for the parameter ranges covered in this paper are discussed in detail in Heitmann et al. (2016). In addition to the five standard parameters describing the \( \Lambda \)CDM model, we include a dynamical dark energy equation of state, parameterized by \( w_0, w_a \), and massive neutrinos. For the normalization of the primordial power spectrum, we choose \( \sigma_8 \) since the emulator mostly targets measurements in the nonlinear regime. In the Appendix we provide for each model the corresponding value of the CMB normalization, \( A_s \), in Table 3. Our models suitably cover the prior range for \( A_s \) picked by the Planck collaboration (see Table 1 in Planck Collaboration et al. 2014 listing the prior range of \([2.7, 4.0]\) for \( \ln(10^{10}A_s) \)). We fix the effective number of neutrino species to be \( N_{\text{eff}} = 3.04 \). The dark energy equation of state is parameterized in the standard form: \( w(a) = w_0 + w_a (1 - a) \) (Chevallier & Polarski 2001; Linder 2003). Our parameter ranges are informed by recent observations of the CMB and large-scale optical surveys. In addition, we aim to cover the relevant ranges for ongoing and upcoming surveys. With these considerations in mind, we choose the following ranges over the eight cosmological parameters (with a flat prior assumption):

\[
0.12 \leq \omega_m \leq 0.155, \quad (1) \\
0.0215 \leq \omega_b \leq 0.0235, \quad (2) \\
0.7 \leq \sigma_8 \leq 0.9, \quad (3) \\
0.55 \leq h \leq 0.85, \quad (4) \\
0.85 \leq n_s \leq 1.05, \quad (5) \\
-1.3 \leq w_0 \leq -0.7, \quad (6) \\
-1.73 \leq w_a \leq 1.28, \quad (7) \\
0.0 \leq \omega_c \leq 0.01. \quad (8)
\]

Note that \( w_a \) is actually jointly constrained with \( w_0 \) such that \( 0.3 \leq (-w_0 - w_a)^{1/4} \). See Heitmann et al. (2016) for a discussion. The cosmological models that have been used to build the emulator are listed in the Appendix in Table 3.

2.2. Simulations

The large-scale simulations described in this paper were carried out with the HACC (Hardware/Hybrid Cosmology Code) framework, a high-performance cosmology code, designed to take advantage of current and future supercomputer architectures; HACC is described in detail in Habib et al. (2016). HACC simulations were carried out on the Mira supercomputer at the Argonne Leadership Computing Facility (ALCF) and on the Titan hybrid supercomputer at the Oak

\(^{11} \text{https://github.com/lanl/CosmicEmu} \)

\(^{12} \text{http://www.hep.anl.gov/cosmology/CosmicEmu/emu.html} \)
Table 1
Additional Models for Testing

| Model | $\omega_M$ | $\omega_B$ | $\sigma_8$ | $\Omega$ | $n_s$ | $w_0$ | $w_a$ | $\omega_\nu$ |
|-------|------------|------------|-----------|--------|------|-------|-------|-----------|
| M038  | 0.1467     | 0.0227     | 0.7325    | 0.5902 | 0.9562 | −0.8019 | 0.3628 | 0.007077 |
| M039  | 0.1209     | 0.0223     | 0.8311    | 0.7327 | 0.9914 | −0.7731 | 0.4896 | 0.001973 |
| M040  | 0.1466     | 0.0229     | 0.8044    | 0.8015 | 0.9376 | −0.9561 | −0.0359 | 0.000893 |
| M041  | 0.1274     | 0.0218     | 0.7386    | 0.6752 | 0.9707 | −1.2903 | 1.0416 | 0.003045 |
| M042  | 0.1244     | 0.0230     | 0.7731    | 0.6159 | 0.8588 | −0.9043 | 0.8095 | 0.009194 |
| M043  | 0.1508     | 0.0233     | 0.7130    | 0.8259 | 0.9676 | −1.0551 | 0.3926 | 0.009998 |
| M044  | 0.1389     | 0.0224     | 0.8758    | 0.6801 | 0.9976 | −0.8861 | −0.1804 | 0.008018 |

Ridge Leadership Computing Facility (OLCF). Mira belongs to the family of IBM’s Blue Gene Q systems (BG/Q) and has 786, 432 compute cores, while Titan achieves its high performance due to the NVIDIA K20 Graphics Processing Units (GPUs) attached to each of its ~18,000 compute nodes. The simulations described in this paper are modest in size compared to the capabilities of these machines, but the sheer number of simulations needed for our full program (~100) makes this work computationally expensive. We note that HACC uses different algorithms on the above systems but the results for the power spectrum agree to within small fractions of a percent (Habib et al. 2016), much smaller than the final target error of the emulator.

The results for each sampled cosmological model were obtained as follows. We first evaluate the power spectrum using the TimeRG perturbative approach (introduced in Pietroni 2008), as described in Upadhye et al. (2014). This provides a smooth and very accurate prediction of the power spectrum on large scales (small $k$), out to $k \sim 0.04$ Mpc$^{-1}$ for $0 \leq z \leq 1$ and $k \sim 0.14$ Mpc$^{-1}$ for $z \leq 2$. Several N-body simulations were carried out next. In order to cover the intermediate scales (out to $k \sim 0.25$ Mpc$^{-1}$), we used 16 realizations of particle mesh (PM) simulations carried out with HACC. These simulations evolve $512^3$ particles on a $1024^3$ grid and cover a volume of $(1300$ Mpc$)^3$ each. For the small-scale (high $k$) regime we carry out one high-resolution simulation with HACC per cosmology. These simulations evolve $3200^3$ particles starting at $z_0 = 200$ using the Zel’dovich approximation, each in a $(2100$ Mpc$)^3$ volume, leading to a mass resolution of approximately $\sim 10^{10} M_\odot$, depending on the detailed cosmological parameters. The force resolution of these simulations is $\sim 6.6$ kpc. For each of the high-resolution runs we store a range of outputs:

1. Particle outputs (full and randomly down-sampled to 1%) at the following redshifts: $z = \{4.00, 3.04, 2.48, 2.02, 1.78, 1.61, 1.38, 1.21, 1.01, 0.78, 0.74, 0.70, 0.66, 0.62, 0.58, 0.54, 0.50, 0.47, 0.43, 0.40, 0.36, 0.30, 0.24, 0.21, 0.15, 0.10, 0.0\};$
2. Halo information at the same redshifts for friends-of-friends halos with a linking length of $b = 0.168$, with at least 20 particles per halo; halo centers are based on a potential minimum evaluation;
3. Halo information at eight redshifts for friends-of-friends halos with a linking length of $b = 0.2$, with at least 20 particles per halo; halo centers are based on a potential minimum evaluation;
4. Halo information at the same redshifts for spherical overdensity halos with $M_{200}$, with at least 1000 particles per halo;
5. Halo information at eight redshifts for spherical overdensity halos with $M_{500}$, $M_{500}$, with at least 1000 particles per halo;
6. All particles that reside in halos with at least 1000 particles, 1% of particles in smaller halos, randomly selected, at least 5 particles per halo;
7. Particle and halo tags for all particles in halos;
8. Power spectra at the same redshifts, though only the following are used for building the emulator: $z = \{2.02, 1.61, 1.01, 0.66, 0.43, 0.24, 0.10, 0.0\}$. Keeping this data leads to an uncompressed data set size of approximately 38 TB per model, and more than 1 PB for the simulation suite discussed in this paper. Storing the relatively large number of time slices allows the creation of light cones from the outputs, following the approach presented in Sunayama et al. (2016). For the power spectrum emulator, generation of a subset of the power spectrum measurements is sufficient due to the smooth evolution of $P(k)$. In addition, many more emulators can be created from this data set, for quantities such as the mass function, galaxy correlation function, etc. While it is difficult to make the full data set publicly available (the raw particle outputs will reside on tape for long-term storage and retrieval is currently slow), we are planning to make the processed data, such as the halo catalogs, publicly available in the near future.

2.2.1. Treatment of Neutrinos

The treatment of neutrino effects in cosmological simulations is nontrivial. This is mainly due to two issues: (1) the very high neutrino thermal velocities early on in the simulation, and (2) the very large mass ratio between the dark matter tracer particles and the neutrino tracer particles. Many solutions to these problems have been discussed in the literature, from adding the neutrinos only at late times, when the thermal velocities are much smaller (helping with the first but not the second problem), to introducing coarser force resolution for the neutrinos to avoid the second problem, to treating the neutrinos perturbatively (for more details, see, e.g., Klypin et al. 1993; Gardini et al. 1999; Brandbyge et al. 2008; Brandbyge & Hannestad 2009, 2010; Viel et al. 2010; Agarwal & Feldman 2011; Bird et al. 2012; Inman et al. 2015; Banerjee & Dalal 2016 and references therein).

We follow the approach discussed in detail in Heitmann et al. (2016), applying a small correction to account for the scale dependence of the growth function as discussed in Upadhye et al. (2014). We provide a short summary of our neutrino treatment here and show comparisons to results found by other groups in Section 4. Since we consider the case of relatively small neutrino masses, the most conservative treatment of
neutrinos suffices. In this treatment, the neutrinos are not evolved as a separate species, but the linearly evolved neutrino component is added at each redshift separately. At \( z = 0 \), the simulation is normalized to the full linear neutrino-baryon-CDM power spectrum as given by CAMB (Lewis et al. 2000). The baryon-CDM component is taken to the starting redshift with a scale-independent growth function and evolved forward with the \( N \)-body code, including the neutrino component in the background equations. This is done for consistency, since the forward evolution does not have the scale-dependent growth characteristic of massive neutrinos. At each redshift of interest, we add the linear neutrino power spectrum to the nonlinear baryon-CDM component. This approach is valid as long as the neutrino density fraction \( f_\nu \equiv \Omega_\nu/\Omega_m \) is sufficiently small.

The result of the procedure outlined above is a low-redshift power spectrum that accurately includes nonlinearity in the CDM + baryon sector as well as neutrinos treated linearly. Castorina et al. (2015) have found this assumption to be accurate at the 1\% level for neutrino masses satisfying current bounds, when compared with \( N \)-body simulations that include massive neutrinos as separate particles. Meanwhile, at higher redshifts \( z \geq 1 \), our use of the scale-independent CDM + baryon growth factor leads to an error at large scales where neutrinos cannot be neglected. Fortunately, these scales are linear, and Upadhye et al. (2014) showed that the resulting error can be removed by multiplying the \( N \)-body power spectrum by the \( k \)-dependent correction factor

\[
D_{b+CDM+\nu}(k,z)^2/D_{b+CDM}(z)^2. 
\]

Here \( D_{b+CDM+\nu} \) and \( D_{b+CDM} \) are, respectively, the linear growth factors for baryons + CDM + \( \nu \) and baryons + CDM. The corrected \( N \)-body power spectrum is consistent with perturbation theory at large scales to within the simulation error bars. This procedure can be interpreted in the separate universe sense where it has been shown that the scale-dependent clustering of an extra field (quintessence or neutrinos) can be neglected (up to some level of approximation) when the simulation box size is smaller than the Jeans length of that field (Chiang et al. 2016; Hu et al. 2016). Our neutrino treatment is reasonable below the Jeans (neutrino free-streaming) scale, and we correct it on super-Jeans-scales.

3. Emulator Construction and Testing

In this section we discuss the range and validity of the emulator, including the possibility of adding baryonic corrections in post-processing, the smoothing procedure applied to the power spectrum from the set of individual simulations to produce the mean spectrum, and the final process of constructing the emulator. In the latter two cases we discuss the associated errors and how they are estimated and checked.

3.1. Range of Validity

Upcoming surveys require accurate predictions of the matter power spectrum at levels of a fraction of a percent. The error budget is complicated because many interacting sources of uncertainty are present. First, the numerical accuracy of the underlying cosmological simulations induces an irreducible error. We follow here the discussions in Heitmann et al. (2010) in setting the starting redshift and force and mass resolution. Given our simulation specifications, the numerical accuracy at the redshifts \( z \lesssim 2 \) and scales \( k \lesssim 5 \text{ Mpc}^{-1} \) of interest is at the percent level. Second, there are errors due to the simulation scheme; we discuss these and estimate their values below. The main source for inaccuracy is the limited number of models that we consider here. As stated earlier, this error will reduce significantly as more models are added. As in our previous work on emulators, we have chosen flat priors for the cosmology parameters covered. With this design, the error due to the emulation scheme should be more or less the same throughout the sampling hypercube, although they will be naturally worse if several of the parameters are chosen close to the hypercube boundaries. This is simply due to fact that using edge points in the design leads to less accurate interpolation compared to using points well in the interior of the hypercube. The emulator does not return results outside of the parameter ranges defined in Equations (1)–(8). It is therefore up to the user to ensure that the analysis of their data sets does not require results outside of the preset prior ranges. Finally, the largest systematic uncertainty is due to the modeling of neutrinos and incomplete knowledge of baryonic effects.

Strictly quantifying the error of the neutrino treatment is difficult since no error-controlled, fully self-consistent, neutrino simulation exists currently. As explained in Section 2.2.1, we treat the neutrinos not as a separate species but evolve them only in the background, and we add the linear neutrino power spectrum to the \( P_{\nu+b} \)-component obtained from the simulation rather than compute the nonlinear neutrino power spectrum. The validity of the first assumption was tested in Upadhye et al. (2014) using TimeRG perturbation theory. In the regime in which the perturbative approach is valid, the agreement was excellent. The second assumption, investigated in detail in Castorina et al. (2015), holds at the 1\% level.

A similar situation holds for the uncertainty due to the lack of a baryonic treatment. In our simulation, the baryons are only included in the initial transfer function and gas dynamics and star formation and feedback effects are not modeled. Baryonic effects on the power spectrum remain inconclusive due to uncertainties in the modeling of several effects, such as feedback from active galactic nuclei (AGN) and supernovae (SNe). Attaining predictive control at the percent level at smaller length scales \( k > 1 \text{ Mpc}^{-1} \) is difficult due to these uncertainties.

An alternative approach to carrying out a large number of expensive hydrodynamics simulations was put forward in Mead et al. (2015), where the authors incorporated baryonic effects into a halo model approach and were able to reproduce results from full hydrodynamics simulations at the 5\% level of accuracy. In the same spirit, one could model baryonic effects with emulator predictions, if reliable results from hydrodynamics simulations are available. Zentner et al. (2013) followed a similar path targeting the convergence power spectrum in modeling baryonic effects by varying the halo concentration. Approaches where the baryonic physics is modeled top of the matter power spectrum informed by a small number of hydrodynamics simulations will be the only viable option for the foreseeable future. Eifler et al. (2015) proposed using a PCA decomposition of the OWLs suite of simulations to parameterize the effect of baryons on the matter power spectrum, which can then be included in cosmological model fitting and subsequently marginalized. Kitching et al. (2014) and MacCann et al. (2015) introduced another method to account for the impact of baryons in the dark matter power spectrum by multiplying the Halofit power spectrum by the ratio of the OWLs dark matter and baryonic power spectrum over the OWLs dark only power spectrum. Typically, the most extreme OWLs simulation is chosen, the AGN feedback scenario, such that the impact of
baryonic effects is maximized to provide an upper bound. This technique was applied by the The Dark Energy Survey Collaboration et al. (2016) and Kwan et al. (2017) to estimate the effect of baryonic physics on the power spectrum of cosmic shear and tangential shear for galaxy–galaxy lensing respectively.

With increasing computing power, a better understanding of uncertainties in sub-grid modeling, and more observational data for cross-calibration, the situation will likely improve over time. Given current uncertainties, it is nevertheless difficult to state an absolute error on the full matter power spectrum over the range of scales considered in this paper.

3.2. Smoothing

Our overall approach uses ideas described in the Coyote Universe series of papers (Heitmann et al. 2009, 2010, 2014; Lawrence et al. 2010). In this subsection and the next, we briefly describe the approach, referring the reader to earlier work for further details.

The first task is to smooth the noisy power spectra generated from the N-body simulations. We use the process convolution algorithm described in Lawrence et al. (2010). A process convolution is a mechanism for producing realizations of a smooth function as a weighted average of a simple stochastic process. Figure 3 in Lawrence et al. (2010) shows a simple example with Gaussian variates (the stochastic process) averaged with a Gaussian smoothing kernel (the weighting scheme).

As in our previous work, we assume that the unobservable smooth power spectrum is the result of a two-layer process convolution. The top layer describes the transformed power spectrum as a process convolution where Brownian motion realized on a grid is smoothed with a Gaussian kernel whose kernel width changes over the domain. The kernel width is described by the second-layer process convolution, which is simply Gaussian variates on a grid smoothed with a Gaussian kernel. The spectrum computed from each N-body simulation is modeled as a multivariate Gaussian variable with a mean given by the two-layer process convolution and known diagonal covariance. The unknown smooth spectrum and a number of nuisance parameters are estimated using a Markov Chain Monte Carlo (MCMC) based approach. Details of the procedure are provided in Lawrence et al. (2010).

The current results are obtained by making a slightly different assumption compared to our previous work. Earlier we assumed, and it appeared to be the case, that different resolutions had about the same variance for any given value of $k$ for which a given resolution was unbiased. It now appears that our current high-resolution spectra have smaller variance about the true spectrum than the low-resolution runs. For now, we have used the larger variance associated with the lower-resolution runs in every case—as shown below this does not adversely affect the results. In future iterations, however, we will take this change in variance into account.

As one example, Figure 1 shows the data from the M012 runs that are used in the estimation procedure for the smooth power spectra. The dashed gray lines show the TimeRG perturbation theory results used up to $k = 0.04$ Mpc$^{-1}$ for $z < 1$ and up to $k = 0.14$ Mpc$^{-1}$ for $z > 1$. The gray dotted lines show the lower-resolution runs that go from the TimeRG perturbation theory results up to $k = 0.25$ Mpc$^{-1}$. The solid black line shows the high-resolution run used from the TimeRG perturbation theory results up to the maximum value of $k = 5$ Mpc$^{-1}$. Figure 2 shows the estimated smooth spectra for this simulation. M012 is representative of the results for all parameter settings (the Appendix provides a complete list of the sampling design space).

Figures 3 and 4 show some diagnostics for the process convolution fit. Both of these plots consider the standardized residuals for the high-resolution run for cosmology M012 (the other cosmologies and resolutions lead to similar conclusions). The standardized residuals are computed in the following:

\[
\frac{\hat{P}(k) - \mu_{\hat{P}}}{\sigma_{\hat{P}}}
\]
manner. First, the smoothed process convolution estimate is subtracted off across \( k \). If the process convolution process has provided a good estimate for the mean, the residuals should now have zero mean across \( k \), that is, the mean taken across \( k \) should be close to zero. Next, each residual is divided by the standard deviation, the square root of the variance, of the raw data at each \( k \). This variance changes over \( k \) in a log-linear fashion, i.e., the log of the variance decreases linearly with the logarithm of \( k \). This behavior is used as part of the process convolution procedure (see Lawrence et al. 2010 for details.) If this variance prediction is correct, the resulting standardized residual should have a variance of one. If there is little correlation, the collection of standardized residuals should resemble an independent sample from the standard normal distribution.

Figure 3 presents evidence that the process convolution works well for capturing the mean structure. The residuals are centered on zero across \( k \) and there are no major trends in the data, supporting the unbiased nature of the mean estimate. (There is some evidence of oscillatory behavior at high \( k \), which might indicate that our process convolution mean is not flexible enough or might arise for some other cause; either way, it is not quantitatively significant.) Here, we see some confirmation of the aforementioned fact that the high-resolution runs have smaller variance than the low-resolution runs. Most of these residuals are between \(-1 \) and \( 1 \), which is too small to match our assumption that these residuals should resemble draws from a standard normal (which would produce numbers mostly between \(-3 \) and \( 3 \)). Figure 4 tests our distribution of Gaussianity. Here, the empirical quantiles of the standardized residuals (basically the sorted residuals) are plotted against the theoretical quantiles of the standard normal distribution. The colors match Figure 3. The straight lines indicate that the residuals do appear to be Gaussian and are relatively uncorrelated. The slope of the lines is related to the variance. The fact that these are less than unity is another indication that the variance of these residuals is smaller than expected. This conclusion about the variance is not detrimental, as every indication is that we are estimating the smooth spectra well and the errors are fairly Gaussian.

### 3.3. Emulation

The follow-up task is to construct the emulator from smooth estimates of the matter power spectra. As in the extension of the original Cosmic Emulator in Heitmann et al. (2014), we also have a number of partial power spectra using the TimeRG perturbation theory approach. In fact, we have results from TimeRG perturbation theory for the complete design (111 models). To build the emulator, we follow a version of the basic plan from Heitmann et al. (2014). Our goal is to predict the multivariate power spectrum from an \( N \)-body simulation as a function of the eight input parameters. As detailed in Lawrence et al. (2010), the first step is to standardize the simulation outputs by centering and scaling, and then projecting them onto an empirical basis computed via SVD (i.e., principal components or empirical orthogonal functions). This process discovers the directions of greatest variation in the high-dimensional outputs and reduces the modeling to these dimensions. The basis weights are then modeled as functions of the simulation inputs using Gaussian processes.

In this case, we have TimeRG perturbation theory results for the entire 111 run design and complete, smoothed spectra from \( N \)-body results over the first 36 runs in the design. The 36 complete runs are used to compute the mean vector, the scaling factor, and 35 basis vectors. The complete spectra are centered, scaled, and projected onto the basis to obtain their weights. The partial TimeRG perturbation theory power spectra (up to the \( k \) values described in the description of the smoothing) are
centered using the relevant portion of the mean vectors, scaled, and then projected onto the relevant part of the basis vectors to obtain their weights. However, the partial power spectra are only projected onto the first seven basis vectors. This number was chosen by comparing the weights from the partial and complete runs. Beyond seven basis vectors, the weights from the partial runs begin to differ visually from the weights from the complete runs when plotted against the eight input parameters. As a result, using the partial run weights will actually begin to degrade the performance of the emulator. All of the weights, from both complete and partial spectra, are put together to estimate the Gaussian process emulator. See Lawrence et al. (2010) and Heitmann et al. (2014) for details on the estimation via an MCMC based approach.

Figure 5 shows test results of the emulator fit for the total matter power spectrum emulator, \( P_{\text{tot}} = (P_{\text{dm}}^2 + P_{\text{b}}^2)^{1/2} \). The dashed lines show the results for spectra from design points M038–M044, which are completed runs from the next stage of the emulator lattice design. The tests are done by holding out the partial TimeRG perturbation theory results for these runs and predicting the complete spectra. The maximum error is about 3% and most are below 2%. The solid lines are the results for the best-fit cosmology M000. This is a true out-of-sample test. At low \( k \) the error reaches its maximum, with one redshift showing about a 2.5% error. Figure 6 shows the results from predicting the training set. Typically, emulators are expected to interpolate the training set, but that is not true in the current case. It seems likely that the emulator has difficulty interpolating the weights from the TimeRG perturbation theory-only results. The resulting fit becomes more like standard regression where the data is not interpolated, but errors are minimized. This issue shows up most prominently at high \( k \), where the TimeRG perturbation theory-only runs provide no direct information. Still, the worst-case error is only 5%, with the vast majority of errors under 2%. (These numbers are consistent with the linear theory tests carried out in Heitmann et al. 2016.) As the number of complete runs continues to increase in later releases, we anticipate that this issue will disappear; tests using the linear theory results from Heitmann et al. (2016) are consistent with this expectation. Overall, the emulator performs very well despite only 36 complete sets of spectra in 8 dimensions. We also measured the errors in just the the baryon-dark-matter component, \( P_{\text{ch}}(k) \), finding very similar results.

4. Comparison with Other Approaches

In this section we provide some comparisons with alternative approximate prediction methods. Since most other groups have addressed either neutrinos or a dynamical dark energy equation of state but not both (as done here), we divide our tests accordingly. In each of the following subsections we compare the alternative approaches to our full simulations, if an appropriate model is available. In addition, we use a set of new models that are not in the simulation design to compare the emulator with the other prediction schemes if those schemes do allow variation of all eight parameters. We carry out our comparisons for the two extreme redshifts, \( z = 0 \) and \( z = 2.02 \).

4.1. Neutrino Predictions

For the case of power spectrum predictions including neutrinos, we study the Halofit approach by Takahashi et al. 2012, which was augmented with a neutrino term by Bird et al. (2012). Takahashi et al. (2012) improved the Halofit model originally developed by Smith et al. (2003) around the \( \Lambda \)CDM model by adding a set of 16 high-quality gravity-only simulations. Six of those models were chosen around the best-fit WMAP results from different years. The other 10 were at the same design points as the first 10 models from the original Coyote Emulator (Lawrence et al. 2010; the simulation results agreed with those run for the Coyote Emulator mostly within 3%). These additional simulations allowed them to include a constant equation of state parameter \( w \) as a new cosmological parameter. Next, they refitted their parametric
model (adding additional parameters) to achieve an accuracy at the 5%–10% level out to \( k \leq 10 h \text{ Mpc}^{-1} \). Based on this work, Bird et al. (2012) added a neutrino component to Halofit with a new set of simulations covering neutrino masses between 0.15 ≤ \( \sum m_\nu \) ≤ 0.6 eV. Their neutrino treatment is particle-based, with the neutrinos modeled as a separate species, albeit at lower force resolution than the dark matter particles. In order to avoid problems due to large neutrino velocities, they started the simulations as late as \( z_\text{in} = 24 \) for the lightest neutrinos, using the Zel’dovich approximation. This leads to systematic inaccuracies in the power spectrum at the few percent level, as shown in Heitmann et al. (2010) and Schneider et al. (2016). (In both papers effects at the 2%–3% level were shown with a starting redshift \( z_\text{in} = 50 \) at \( k \approx 1 h \text{ Mpc}^{-1} \), extrapolating these results would suggest a 5% error due to the late start alone, and even more at higher \( k \).) In addition, the small volumes and limited mass resolution (\( 512^3 \) particles) further degrade the accuracy of the simulations. All these effects combined will lead to systematic errors and scatter in the power spectrum, particularly on small length scales. The above-discussed neutrino-augmented results are available in the latest CAMB release and have been updated over time (Lewis et al. 2000).

Figure 7 shows a comparison of our new emulator with the Takahashi et al. (2012) implementation. The ΛCDM model (M000, brown line) agrees with our emulator at the 5% level at \( z = 0 \), which is in agreement with our previous findings in Heitmann et al. (2014) for the same model (see Figure 11 in that paper). Note that in the extended emulator paper the ratio is taken with respect to the simulation, meaning that the y-axis in that paper is the inverse from what we show in Figure 7 here). Our finding of very similar agreement with Takahashi et al. (2012) with the new emulator for M000 stresses the excellent agreement between GADGET-2 and HACC (the original Coyote Emulator papers were based on GADGET-2 simulations, while the new simulations have been carried out with HACC; agreements are well within the sub-percent level). Similar results comparing GADGET-2 and HACC were also reported in the HACC code paper by Habib et al. (2016).

For all models, the agreement on large scales (small \( k \), \( k < 0.02 \text{ Mpc}^{-1} \)) is at the 1%–2% level at both redshifts, \( z = 0 \) and \( z = 2.02 \), demonstrating that our use of a \( k \)-dependent correction factor for the growth function works very well. In the quasi-linear to nonlinear regime the agreement between the Halofit approach and the new emulator varies between 5% up to 20%. This is again consistent with our previous findings in Heitmann et al. (2014), Figure 12, where for some cosmological models, the differences for the power spectrum prediction between Halofit and the extended emulator were as large as 15% over a similar \( k \)-range (0.1 Mpc\(^{-1} \) < \( k \) < 1 Mpc\(^{-1} \)). Contemplating this level of error in Halofit is disconcerting in the context of using the matter power spectrum to obtain cosmological constraints, since these deviations of around 10%–15% occur in the range of scales typically accessed by measurements of the cosmic shear power spectrum.

Finally, we emphasize that as shown in our previous work by Upadhye et al. (2014), the agreement of our simulations including neutrinos with a TimeRG-based perturbative approach was better than 2% at \( \sim 0.2 \text{ Mpc}^{-1} \) at \( z = 2 \) and \( \sim 0.1 \text{ Mpc}^{-1} \) at \( z = 0 \), for values of \( \omega_\nu \) as high as 0.01. Given these results, in combination with the findings in Castorina et al. (2015) discussed in Section 2.2.1, the differences in Halofit and the new emulator are apparently due to the general inaccuracy of Halofit away from ΛCDM models rather than due to the different neutrino treatment applied.

4.2. Dynamical Dark Energy Equation of State Predictions

Next, we compare our results with the work of Casarini et al. (2016). Based on our earlier emulator work in Heitmann et al. (2014), these authors developed a prediction for \( (w_0, \omega_\Lambda) \) cosmologies by introducing an effective constant equation of state that captures the influence of a time-varying dark energy equation of state to sub-percent accuracy. This idea was introduced in Francis et al. (2007) and is based on the assumption that cosmologies beyond ΛCDM can be mapped back to wCDM models by requiring both models to have the same distance to last scattering and the same values of \( H_0 \) and energy densities, \( \Omega_{m,r,b,0} \) at \( z = 0 \). This has the effect of tuning the growth in constant \( w_0 \) models to match the \( (w_0, \omega_\Lambda) \) models of interest for some new value of \( \omega_\Lambda \). The new value of \( \omega_\Lambda \) is constrained by the chosen values of \( (w_0, \omega_\Lambda) \) and within the context of the Coyote emulator, this limits the space of allowable models because of the parameter range of the design.

Based on the above general idea and the results from Heitmann et al. (2014) for wCDM models, Casarini et al. (2016) delivered predictions for the nonlinear power spectrum for dynamical dark energy models for scales of \( 0.1 h \text{ Mpc}^{-1} \ll k < 2 h \text{ Mpc}^{-1} \) and between redshift 0 ≤ \( z \) ≤ 3 at high accuracy.

Before we show a comparison of the Casarini et al. (2016) approach with the emulator, we compare two of our smoothed power spectra from the simulations for M005 and M007 directly with their prediction in Figure 8. By testing against the smoothed input power spectra as well, we are able to distinguish between various sources of error in Figure 8, that is, whether the discrepancy, should there be any, is due to the assumptions of the Casarini et al. model or the predictive power of the Gaussian Process modeling. The solid line shows results at \( z = 2 \), while the dashed lines show results at \( z = 0 \). The results for \( z = 0 \) are in agreement at a level better than 5%, for M005 at both redshifts. For M007 at \( z = 0 \) the agreement is also excellent (below 5%), and for \( z = 2 \) it degrades slightly but
stays well under 10%. Next, Figure 9 shows a comparison of the emulator with Casarini et al. (2016) for M005 and M007. We compare at $z = 2$ (solid line) and $z = 0$ (dashed line). For M007 we have $w_\text{N} = -1.0$ and for M008 we have $w_\text{N} = 0.4333$. The values for $\omega_\text{m}$ and $\sigma_8$ are higher for M007, leading to stronger nonlinear effects. The Casarini et al. (2016) approach leads to <5% inaccuracy for M005 and <10% for M007.

4.3. Eight-parameter Model Predictions

In their work, Mead et al. (2016) provided new power spectrum predictions, covering not only neutrinos but also dynamical dark energy and modified gravity models. Their approach is based on re-deriving the different contributions to the halo model. In an earlier paper, Mead et al. (2015) used results from the “Coyote Extended” emulator (Heitmann et al. 2014) to optimize the halo model approach for $\Lambda$CDM models. They ran the emulator at the exact design points...
(37 cosmological models) to obtain predictions as close to the original simulations employed to build the emulator as possible. These “on-node” predictions have a very small error by design compared to the direct simulation, i.e., they suffer very little from the interpolation error. While it might seem that the comparison of Mead et al. (2016) to our new emulator therefore might be biased toward emulator results, this is in fact not the case, since the current emulator is built on an entirely different sampling scheme; so there is no notion of nearness in the Coyote sampling points and the ones used here. Additionally, the Coyote emulators were built with GADGET-2 runs, while the new Mira-Titan suite of simulations has been carried out with HACC with somewhat different simulation parameters (although, since Gadget-2 and HACC give very close results, this is unlikely to be an issue).

The new prediction scheme introduced in Mead et al. (2016) is supposed to be valid for $k < 10 h \, \text{Mpc}^{-1}$ at the few percent level accuracy for most models. They arrive at this conclusion by comparing their results to a range of simulations. This is the only approach for which we can compare our full emulator and our simulation results directly. We use the seven additional models for this comparison that were also employed to investigate the accuracy of our emulator, as given in Table 1.

We show the comparison of the Mead et al. (2016) fit with our smoothed simulations directly in Figure 10 for M000 and M038–M044, given in Table 1. We show models with lower and higher neutrino mass separately. The agreement for the ΛCDM cosmology is excellent, basically perfect on large scales up to $k \sim 0.04 \, \text{Mpc}^{-1}$ and at the 2%–3% level in the nonlinear regime. The models with a varying dark energy equation of state show some disagreement on the very largest scales, which is most likely due to our different implementation of $(w_0, w_a)$ cosmologies in CAMB than in the version that was used by Mead et al. (2016). For relevant details the reader is referred to our previous work (Upadhye et al. 2014), where we provide a description of our implementation and a publicly available CAMB version. In the quasi-linear regime, the agreement is around the 5% level for the low-mass neutrino models and up to 10% for the high-mass neutrino models. At $k \sim 1 \, \text{Mpc}^{-1}$ and beyond, the low-mass neutrino models still agree at the 5% level, while some of the high-mass neutrino models show differences at the 10%–15% level.

Figure 11 shows the ratio of the new emulator with respect to the Mead et al. (2016) fit for the same models. The results are very similar to the comparison to the smoothed simulations, which is to be expected from Figure 5 (obviously, taking the ratio of Figures 10 and 11 would lead back to the results of Figure 5). On large scales, we see slightly poorer agreement compared to the comparison to the smoothed simulations, but still at the 2% level. On small scales, the agreement is very similar to the direct comparison with the simulations to 15%.

### Table 2

| Model | $\omega_m$ | $\omega_b$ | $\sigma_8$ | $h$ | $n_s$ | $w_0$ | $w_a$ | $\omega_\nu$ |
|-------|------------|------------|------------|-----|-------|-------|-------|-------------|
| FC1   | 0.15110    | 0.02217    | 0.81110    | 0.8167 | 1.0280 | −1.09038 | 0 | 0 |
| FC2   | 0.15110    | 0.02217    | 0.82813    | 0.8167 | 1.0280 | −1.19484 | 0 | 0 |
| FC3   | 0.12000    | 0.02306    | 0.70000    | 0.6833 | 1.0060 | −0.74838 | 0 | 0 |
| FC4   | 0.12000    | 0.02306    | 0.68981    | 1.0060 | 0.6727 | 0.9645 | 0 | 0 |
| FC5   | 0.14205    | 0.02225    | 0.83000    | 0.6727 | 0.9645 | −0.84095 | 0 | 0 |
| FC6   | 0.14205    | 0.02225    | 0.81830    | 0.6727 | 0.9645 | −0.78951 | 0 | 0 |
| FC7   | 0.14205    | 0.02225    | 0.83000    | 0.6727 | 0.9645 | −1.12210 | 0 | 0 |
| FC8   | 0.14205    | 0.02225    | 0.83757    | 0.6727 | 0.9645 | −1.18190 | 0 | 0 |
1.0 0.0 0.0 2.1405
0.0 0.0 0.0 3.8937
0.0 0.0 0.0 3.8820
0.0 0.0 0.0 2.0913
0.0 0.0 0.0 4.1559
0.0 0.0 0.0 1.2767
0.0 0.0 0.0 1.5076
0.0 0.0 0.0 1.9293
0.0 0.0 0.0 1.5058
0.000345 3.7807
0.001204 1.8433
0.003770 3.0120
0.001752 3.7941
0.002789 3.8417
0.002734 3.3265
0.000168 1.7313
0.000649 7.4406
0.004673 3.1484
0.000977 2.5171
0.000067 1.9998
0.008829 5.1152
0.003733 2.5108
0.003063 5.3500
0.0007024 5.0573
0.0002082 4.6830
0.0002902 5.5056
0.0009086 10.442
0.0006588 11.909
0.0008126 3.7051
0.000650 4.0408
0.0009095 2.1376
0.0007968 2.9679
0.0003620 2.1504
0.0004440 2.6644
0.0001082 7.3825

4.4. Comparison with the Extended Emulator

Finally, as a last check, we compare our earlier, “Coyote Extended” emulator, developed in Heitmann et al. (2014), with our new emulator, keeping \( w_0 = \omega_m = 0 \). We list the models used for this test in Table 2. Several of the values used are close to the edge of our parameter design, making this test rather stringent. Figure 12 shows the ratio of the new emulator over the extended emulator from our previous work. We show results for eight models at redshift \( z = 0 \). The agreement for most models is at 2%, with two instances showing disagreement up to 4%. Given the estimated accuracy of our current emulator at approximately 4% and of the previous emulator at the \( \sim 5\% \) level, this agreement is within the expected limits.

5. Summary and Outlook

We introduce a new cosmic emulator for the matter power spectrum that covers eight cosmological parameters, and spans a redshift range from \( 0 \leq z \leq 2 \) and wavenumbers out to \( k \sim 5 \text{ Mpc}^{-1} \). We achieve an accuracy at the 4% level (better for most models) over the full \( k \)-range and all eight parameters, using a sampling space of just 36 cosmological models.

The parameter sampling approach for designing the simulation suite is described in Heitmann et al. (2016). Because this scheme has demonstrated convergence properties, the accuracy of the emulator can be systematically improved by adding more simulations at well-defined points, reaching close to 1% with about 100 evaluation points in the eight-dimensional space; the next set of 26 simulations is currently being analyzed. The internal accuracy tests presented in this paper are consistent with the estimates from the linear theory-based test presented in Heitmann et al. (2016) and with the error estimates of a previously constructed emulator that relied on a different set of simulations (Heitmann et al. 2014). These positive results are an important consistency check for our planned further improvement of the error bounds.

We have compared our results to other predictions for the nonlinear power spectrum by a number of authors. The agreement in the linear regime is excellent, as expected. The agreement degrades for models away from \( \Lambda \text{CDM} \) in the quasilinear to nonlinear regime and we find differences at the
5%–10% level for most models, but up to 15%–20% depending on the model and redshift investigated and prediction scheme used (only Mead et al. 2016 provide predictions over the eight cosmological parameters that we investigate here; all other approaches only treat a subset of the parameters). The agreement we find between different methods is consistent with our evaluation in the extended Coyote emulator, presented in Heitmann et al. (2014), where we found differences between the emulator predictions and, e.g., Halofit at the 20% level for some models. The Mead et al. (2016) predictions are the closest to our results and for low neutrino masses they match the emulator at around 5%, while showing larger differences at higher neutrino masses.

The simulation suite presented here lends itself to many more investigations. We are currently building a large set of emulators for quantities such as the halo mass function, redshift space distortions, and halo correlation and galaxy correlation functions and bias functions. As emulation accuracies continue to improve, the addition of “post-processing” modules for, e.g., baryonic effects and galaxy modeling, will also become easier to implement in a robust fashion.

In the future, we expect emulators and observations to co-evolve. There will likely be a greater emphasis on cross-correlation-based probes; also, as measurements squeeze the parameter space priors, the quality of emulation will improve significantly.

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Appendix

In this appendix we list all the cosmological models that have been used in the paper to construct the new emulator in Table 3.

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