# Snowmass2021 Theory Frontier White Paper: Data-Driven Cosmology

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#### Abstract

Over the past few decades, astronomical and cosmological data sets firmly established the existence of physics beyond the Standard Model of particle physics by providing strong evidence for the existence of dark matter, dark energy, and non-zero neutrino mass. In addition, the generation of primordial perturbations most likely also relies on physics beyond the Standard Model of particle physics. Theory work, ranging from models of the early universe in string theory that that led to novel phenomenological predictions to the development of effective field theories to large-scale cosmological simulations that include the physics of galaxy evolution, has played a key role in analyzing and interpreting these data sets and in suggesting novel paths forward to isolate the origins of this new physics. Over the next decade, even more sensitive surveys are beginning to take data and are being planned. In this white paper, we describe key areas of the theory program that will be needed to optimize the physics return on investment from these new observational opportunities.

#### 1 Introduction

Cosmology is by now firmly established as a precision science. Different cosmological observations, ranging from observations of distant supernovae, to large scale structure (LSS) surveys, to measurements of the cosmic microwave background (CMB), have established a standard model of cosmology, referred to as  $\Lambda$ CDM. It describes the evolution of our universe from a time when it was only fractions of a second old until the present, and it does so with only six parameters. Four of the six parameters characterize the homogeneous solution, the remaining two characterize the power spectrum of primordial density

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perturbations. As a phenomenological model,  $\Lambda$ CDM has proven extremely successful and its parameters are now known at the percent level. However, the underlying microphysics behind these parameters remains completely unknown. How was the asymmetry between particles and anti-particles created? What is the nature of dark matter? Is dark energy just a cosmological constant or is it dynamical? When and how did the first stars form and how did reionization occur? What generated the primordial density perturbations that grew into the temperature anisotropies in the cosmic microwave background and eventually into the stars and galaxies?

Implicitly the model makes additional assumptions, like the existence of three species of neutrinos with the sum of their masses assumed to be the smallest mass consistent with neutrino oscillation experiments. But what really is the sum of their masses? Are there three species of relativistic degrees of freedom present at the time of recombination? Or does the number of relativistic degrees of freedom deviate from the standard model prediction, as expected in many extensions of the standard model?

Over the next decade, CMB experiments and LSS surveys are becoming powerful enough to begin to answer several of these questions. However, making full use of the upcoming data sets will require theoretical progress in several areas to ensure that our measurements are limited by the statistical power, not our theoretical understanding.

In this white paper we present an overview of the main areas where observational progress is expected as well as the theoretical challenges associated with each of these areas that have to be overcome to fully utilize the next-generation data sets to reveal the physics of the primordial universe (§2), dark matter (§3), neutrinos and other possible light relics (§4), dark energy (§5), and the nature of the Hubble tension (§6). Finally, in §7, we demonstrate the potential of theory to go beyond interpreting observations, but guiding new physics searches.

#### 2 Primordial Universe

One of the biggest open questions in cosmology is what generated the primordial perturbations that seeded the stars and galaxies around us. Observations have established that the primordial perturbations are dominated by density perturbations, and that, within observational uncertainties, these are adiabatic, Gaussian, nearly but not exactly scale-invariant, and well-described by a power law that is conventionally parameterized by the amplitude  $A_s$  and spectral index  $n_s$  [1].

All these properties of the primordial perturbations are consistent with inflation [2–5], the idea that the very early universe underwent a period of nearly exponential expansion driven by one or several scalar fields, and have ruled out various competing ideas, such as perturbations seeded by monopoles, strings, or textures [6–10]. Inflation is the most widely studied scenario for the early universe, but there are less explored alternative scenarios [11–14]. Future observations that constrain or detect the amplitude of primordial gravitational waves, measure the primordial power spectrum of density perturbations with higher precision, and further constrain departures from Gaussianity will provide stringent tests for any theory of the early universe.

In addition to a nearly scale invariant spectrum of primordial density perturbations,

inflation also predicts a nearly scale invariant spectrum of primordial gravitational waves. According to the simplest models of inflation, the expansion is driven by a single scalar field, the inflaton  $\phi$ , and the theory is specified by an a priori arbitrary function of the inflaton, the potential  $V(\phi)$ . In this context, the search for primordial gravitational waves will help answer several key questions, such as what the energy scale of inflation is, how far the inflaton traveled in field space, and over what range the scalar potential varies. A more detailed discussion of inflation and its predictions is available in [15].

A nearly scale-invariant background of gravitational waves is most easily detected through its imprint on the CMB, where the signal is characterized by a plateau on angular scales larger than a degree in the temperature anisotropies and a recombination peak on degree angular scales and a reionization bump on large angular scales in the polarization anisotropies. The primordial density perturbations generate temperature anisotropies and anisotropies in so-called *E*-mode polarization, primordial gravitational waves additionally generate so-called *B*-mode polarization. In the context of inflation, a detection of primordial *B* modes would provide evidence for quantum fluctuations in the spacetime metric itself, would imply that inflation took place at energy scales comparable to those associated with grand unified theories, and would imply a Planckian field range, just to mention some of the consequences. Because of these far-reaching implications, several CMB experiments are currently searching for this polarization pattern [16–21] and more will begin taking data soon.

One of these experiments, BICEP2, reported a detection of B-mode polarization on degree scales at 150 GHz and interpreted this detection as evidence for the existence of primordial gravitational waves [22]. Subsequent analyses demonstrated that the BICEP2 measurements are consistent with polarized emission from dust inside the Milky Way [23–25]. However, the measurement has both highlighted that experiments are reaching the sensitivities needed to detect the B modes expected if the simplest models of inflation describe the first fraction of our universe, and that accounting for astrophysical foregrounds is crucial for a convincing detection.

Over the next years the BICEP/*Keck* collaboration will continue to improve their measurements from the South Pole, and Simons Observatory will begin observations from Chile [26], both improving the sensitivity to the amplitude of power in primordial gravitational waves by an order of magnitude over current limits. By the end of the decade a larger NSF and DOE funded effort, CMB-S4, will further increase the reach by a factor of around five and either detect a primordial gravitational wave signal or exclude many of the best-motivated models of inflation [27–29]. Planning for space-based probes is also well-underway, for example, for the JAXA led LiteBIRD satellite [30] and for PICO [31].

These experiments will begin to cross critical thresholds in the search for primordial gravitational waves from inflation. For example, they will either detect gravitational waves or exclude one of the two classes of potentials that naturally predict a value of the spectral index  $n_s$  consistent with observations [27]. In this class of models the potential during the inflationary period is well approximated by a monomial potential  $V(\phi) \approx \mu^{4-2p} \phi^{2p}$ . The value of  $\mu$  is constrained by the observed amplitude of density perturbations  $A_s$ , and for plausible values of p the models predict an amplitude of the gravitational wave signal, measured in terms of the tensor-to-scalar ratio r, of r > 0.01. This class of models already appears in tension with observations [32]. However, the tension is predominantly based on

constraints on  $n_s$ , and the theoretical prediction is modified by the presence of additional degrees of freedom [33]. In addition, a detection of a primordial gravitational wave signal with an amplitude in excess of  $r \simeq 0.01$  are of interest because they imply that the distance in field space traveled by the inflaton during the inflationary period exceeds the Planck scale [34], which would have profound theoretical implications, like the existence of a symmetry that protects the inflaton potential in quantum gravity. See the Snowmass white paper [35] for more details.

An additional critical threshold that CMB experiments will begin to cross over the next decade is  $r \simeq 0.001$ . This threshold provides information about the structure of the inflationary potential rather than the field displacement. The second class of single-field models that naturally predict a value of the spectral index  $n_{\rm s}$  consistent with observations are hilltop and plateau models. Prominent examples in this class include Starobinsky's  $R^2$  inflation [2], models in which the Higgs boson takes on the additional role of the inflaton [36, 37],  $\alpha$ -attractors [38–40], fibre inflation [41], and Poincaré disk models [42, 43]. These potentials contain an additional parameter compared to the first class, the scale in field space over which the potential appreciably changes from its hilltop or plateau value. The absence of a detection by CMB-S4 and LiteBIRD would constrain the tensor-to-scalar ratio to be below  $r \simeq 0.001$ , and would exclude all models in this class in which this scale exceeds the Planck scale.

Primordial B modes generated by primordial gravitational waves are not the only source of B-mode polarization. As we already mentioned, astrophysical foregrounds also create B modes. In addition, the presence of matter along the line of sight between us and the so-called last-scattering surface at which the CMB is emitted deflects the CMB photons through weak gravitational lensing. This converts primordial E modes into a mixture of E modes and so-called lensing B modes [44, 45], which are brightest on angular scales around ten arcminutes.

Ground-based experiments will probe tensor-to-scalar ratios as small as  $r \simeq 0.001$  by searching for the recombination peak on a carefully selected part of the sky with minimal foreground contamination. To reduce the sample variance from lensing *B* modes, these experiments will rely on high-precision measurements of polarization on arcminute angular scales that will allow the removal of the lensing contribution on degree scales [46–49]. This process is referred to as delensing. Satellite missions measure primordial *B* modes over a large fraction of the sky. As a consequence, they are less dependent on delensing both because the sample variance of the lensing *B* modes is reduced, simply because more modes are observed, and because they also target the reionization bump on large angular scales where the ratio of primordial B-mode power to lensing B-mode power is largest. At the same time, because they observe the full sky, satellite missions must, on average, deal with significantly higher levels of foregrounds. As a consequence, the different approaches are highly complementary.

Contamination of the primordial B-mode signal by B modes of astrophysical origin remains one of the main challenges for both ground- and space-based observations. The two main sources of astrophysical B modes are polarized emission by dust grains that are aligned with the Galactic magnetic field, and synchroton radiation emitted by relativistic electrons in the Galactic magnetic field. The amplitude of the astrophysical signal exceeds the amplitude of the primordial signal at all frequencies and on all angular scales, even in the cleanest regions of the sky. As a consequence all experiments searching for primordial B modes necessarily rely on multifrequency observations that use together the different frequency dependence of the CMB and foreground signal. Ground-based observations can target the cleanest regions of the sky, but the atmosphere severely restricts the viable observing frequencies. All-sky observations from space are not subject to limitations imposed by the earth's atmosphere but must deal with higher levels of astrophysical B modes.<sup>1</sup> Independent of the observing platform, a better understanding of these astrophysical foregrounds is critical, both for the analysis and interpretation of current and upcoming data sets as well as for the design and planning of experiments. There has been recent progress both in the form of ab initio magnetohydrodynamic (MHD) simulations [50, 51], phenomenological models [52], and in the form of generative models [53, 54], but additional work in this direction, in particular a coordinated effort to make full use of the different approaches is needed.

While the frequency dependence of astrophysical foregrounds differs from that of the CMB signal, lensing B modes have the same frequency dependence as the primordial signal and cannot be reduced by multi-frequency observations. However, since the statistical properties of the CMB are well understood, high-precision measurements of the polarization on scales near the lensing peak can be used to reconstruct the lensing potential, and ultimately to remove the lensing B modes [46–49]. This has only recently been demonstrated on data [17, 55–60], and work is ongoing to develop techniques appropriate for the stringent requirements of future ground-based surveys [61–65]. A key aspect that remains to be better understood is the effect of foregrounds on delensing. Because delensing relies on the correlations between modes on arcminute and degree scales, this motivates higher resolution ab initio MHD simulations with a larger dynamic range than currently available.

Precision measurements of the polarization of the cosmic microwave background on small scales [26–29] will also lead to improved measurements of the power spectrum of primordial density perturbations that will provide interesting constraints on inflation and fundamental physics more generally. Over the next decade, constraints on the scalar spectral index  $n_s$  will improve by a factor of two. Similarly, constraints on its scale dependence, referred to as the running of the scalar spectral index, will improve by a factor of two to three [27–29]. In combination with the increased precision on r, this will significantly reduce the space of viable inflation models.

In addition, the improved measurements of  $n_s$  have implications for the aftermath of inflation. As inflation ends, the potential energy density stored in the inflaton is transferred into kinetic energy and eventually into the energy density of a thermal plasma of standard-model particles. This process is referred to as 'reheating' [66–68]. How reheating occurs in detail remains unknown, but at least for the simplest models of inflation the observational predictions related to inflationary physics only depend weakly on these details of reheating [69–71]. The dependence only arises because observables depend on the relation between physical scales today and physical scales during inflation, which depends on the amount by which the Universe expands during reheating. More quantitatively, the

<sup>&</sup>lt;sup>1</sup>Of course, this also provides an opportunity to those interested in a better understanding of the processes that produce the foreground emission.

details of the reheating process lead to small changes of the spectral index  $n_s$ . With the increase in precision on  $n_s$ , observations will begin to distinguish between different reheating histories for a given model of inflation [72–74]. The physics that is probed in this way is very rich. For example, the expansion history and the duration to radiation domination after inflation can depend on the self-interactions of the inflaton [75, 76], inflaton couplings to other fields and the efficiency of the energy transfer between the inflaton and daughter fields [77, 78]. Constraints on the expansion history can also impact predictions for dark sector abundances [79–85], provide insights into the possibility of producing primordial black holes [86, 87] and additional small scale structure in the early universe [88–90]. For a recent review, see [74].

There are several well-motivated classes of inflationary models that predict departures from a power law in the form of oscillatory or sharp features in the primordial power spectrum. For example, as we mentioned earlier, a detection of primordial gravitational waves with an amplitude above  $r \simeq 0.01$  would imply the existence of a symmetry that protects the inflaton potential. In this case axions are natural inflaton candidates because they enjoy a shift symmetry to all orders in perturbation theory. Non-perturbatively, the inflaton acquires a potential that may contain both a non-periodic contribution suitable to drive inflation and a subdominant periodic contribution. The small periodic contribution leads to features in the primordial power spectrum [91]. These contributions have been searched for and have been constrained using CMB data [91–95] and more recently using the BOSS data, which currently provides the strongest constraints on these models for a significant part of parameter space [96]. Constraints from LSS data will improve further as new data from DESI [97] and Euclid [98] becomes available [96].

If the inflaton is the only light degree of freedom during inflation, the primordial density perturbations are adiabatic [71]. The improved measurements of the power spectrum of primordial density perturbations will tightly constrain departures from adiabaticity, referred to as isocurvature modes, that would be expected in theories with additional light degrees of freedom like axions [99–101], or in the curvaton scenario [102–106]. Just like the inflaton, light degrees of freedom present during inflation experience quantum fluctuations and contribute to the density perturbations. Since the two fields fluctuate independently, their contributions are uncorrelated. If the density perturbations are predominantly sourced by the inflaton and departures from adiabaticity are associated with additional light fields, the adiabatic and isocurvature modes are uncorrelated. Over the next decade limits on this type of departures from adiabaticity will improve by a factor five [27]. The curvaton scenario is an alternative to single-field models of inflation in which the observed density perturbations are dominated by the vacuum fluctuations in a second field, the curvaton, that subsequently decays. Depending on the details of the decay process, this scenario allows for a wide variety of departures from adiabaticity. Since the density perturbations are dominated by the curvaton and the departures from adabaticity are set by the curvaton as well, in this scenario the adiabatic and isocurvature components are fully correlated (or anti-correlated). Constraints on these departures from adiabaticity will improve by as much as an order of magnitude [27].

The upcoming precision measurements of CMB polarization will also tighten constraints on departures from Gaussianity. The constraints are most commonly presented as constraints on amplitudes of different functional forms, typically referred to as shapes, of low-order correlation functions. Constraints on the amplitudes of the most widely studied shapes of the 3-point function will improve by a factor of two to three compared to existing constraints [27, 28]. These constraints can, for example, help answer the questions how strongly the inflaton interacts with itself, and more generally whether there was a single light degree of freedom or several. The constraints achievable with CMB observations alone just fall short of key theoretical targets [107], and further improvements will require measurements of higher order correlation functions from galaxy surveys or intensity mapping [108, 109].

Nominally, LSS data provides access to orders of magnitude more Fourier modes than the CMB. However, as already briefly mentioned, the analysis of LSS data is more challenging because of nonlinear effects of matter clustering, galaxy formation physics, and redshift space distortions. On sufficiently large scales (larger than 1 Mpc), these effects can be systematically described within the Effective Field Theory (EFT) of Large Scale Structure [110–112], and there has recently been significant progress in deriving constraints on departures from non-Gaussianity from large scale structure [113–116].

The EFT framework provides robust first-principle theoretical models for the late-time non-Gaussian patterns in the galaxy distribution, which act like a background noise that complicates the extraction of the primordial non-Gaussian signal. The other important ingredients necessary for the analysis of primordial non-Gaussianity (PNG) in galaxy surveys are optimal estimators of summary statistics [117, 118], efficient data compression and covariance matrix estimation techniques [119, 120], and codes for EFT calculations [121–123]. The recent application of these tools to the galaxy power spectrum and bispectrum data from the BOSS [124] is a proof of principle that measurements of PNG from galaxy surveys are feasible, and there is a systematic program that aims to reach the level of precision necessary to answer key questions about inflation.

Over the next few years the upcoming surveys like DESI [97] and Euclid [98] will create a detailed map of our Universe up to redshift of  $z \approx 2$ , which will permit the improvement of the current limits on PNG from galaxy surveys at least by a factor of four [125]. An even more impressive improvement will become possible with future surveys like MegaMapper [125–127], which will map our Universe up to  $z \approx 5$  and will reach unprecedented precision in measuring PNG. In addition, the local type of non-Gaussianity will soon be probed with the SPHEREx mission [128].

To make full use of the data, it will be important to improve the accuracy of the EFT calculations (higher order *n*-point functions and high loop orders), and to obtain inputs from high fidelity hydrodynamical simulations. These simulations will yield tight priors on the Wilson coefficients of the EFT (nuisance parameters) that capture the details of galaxy formation on large scales. This will break the degeneracy between PNG and galaxy formation physics, and hence reduce the error bars on the potential PNG signal [115, 119]. On the experimental side, the biggest challenge will be imaging systematics. This issue can be addressed, e.g. with recently developed network-based techniques [129].

Given the leaps in sensitivity and data quality for both CMB experiments and LSS surveys, cross-correlations between the data sets are an important additional avenue to constrain PNG and cosmological parameters more generally. For example, upcoming CMB experiments like Simons Observatory and CMB-S4 will provide exquisite measurements of the lensing convergence that contains information about the projection of matter along the

line of sight. Correlations between the CMB lensing maps and deep LSS surveys can provide complementary and highly competitive constraints on PNG [130]. Secondary CMB anisotropies, caused by interactions of CMB photons with electrons in non-linear structures along the line of sight similarly correlate with LSS surveys and provide yet another route to constrain PNG [131, 132].

Most theoretical work and analyses have focused on scale-invariant shapes of the 3point correlation function. However, the inflationary models mentioned earlier that predict oscillatory or sharp features in the primordial power spectrum also predict corresponding features in higher order correlation functions [91, 133]. Since searches for these shapes are computationally more challenging than the searches for the scale-invariant shapes, at present only constraints from the CMB exist [134–139], and the information available in LSS data remains to be extracted.

Finally, there are several examples of physical processes for which departures from Gaussianity are not well described by the first few moments of the probability distribution function [140–145]. Signatures associated with these processes might be missed in traditional searches. For the example of reference [141] the optimal estimator has been found and is naturally formulated in real space [146]. This raises the more general question of how to systematically and optimally extract the information stored in the data beyond the power spectrum and low-order correlation functions [147]. See [35] for additional discussion.

### 3 Dark matter

The discovery of dark matter in galaxy clusters [148] and individual galaxies [149, 150] was one of the first signs of physics beyond what we now know as the Standard Model [151–153]. By the 1980's it was clear from astronomical observations what dark matter could NOT be, namely neutrinos [154, 155, 155–157]. *Simulations* showed that the clustering of halos in a neutrino-dominated universe could not be reconciled with observations for masses consistent with matching the relic abundance of neutrinos. Instead, simulations suggested that another, colder form of dark matter could be consistent with both the cosmological abundance of dark matter and its small-scale clustering [158, 159]. Since then, it has been recognized that the physics of dark matter shapes the homogeneous evolution of the Universe and the evolution of perturbations. Particle theorists have drawn inspiration for dark matter model building from astronomical observations (e.g., [160]), and the community is using observations paired with high-resolution simulations to illuminate dark-matter particle properties.

In fact, dark matter astrophysics is becoming a precision science [161–164]. On the observational side, there are many different probes of dark matter on a variety of scale, from the expansion history to LSS to dark-matter halos so small that they may not contain luminous matter. Importantly, new wide-field surveys, from radio to optical to gamma-ray, are enabling the discovery of new targets for dark-matter searches, with well-quantified statistical and systematic uncertainties (e.g., [165–169]). When these observations are paired with a commensurate cosmological simulation and theory program (e.g., [170–183]), we as a community are obtaining stringent constraints on the WIMP annihilation

cross section, the momentum distribution of dark matter at its production era, dark matter self-interactions and interactions with Standard Model particles, and the dark matter particle mass (e.g., [184–194]). The constraints inform dark matter model builders and complement dark matter searches in the lab.

As detailed in other Snowmass contributions, the observational facilities of the next decade or two can provide tremendous insight into the nature of dark matter (e.g., [195-203]). However, this opportunity can only be realized with a strong theory and simulation program. The opportunities and challenges are detailed in Ref. [199] (see also Ref. [203]), which we summarize here. In brief, collaboration between particle theorists and simulators is desirable to translate from the Lagrangian model level to phenomenological cosmologically relevant parameter space (e.g., as in the ETHOS framework [204, 205]). Part of this process is figuring out how best to map specific physics into simulation algorithms. For example, for self-interactions, what matters is simulating the transfer of momentum and energy in dark-matter halos, and so careful thought must go into determining which cross section is relevant for the coarse-graining of the transfer [206]. Simulations must include the physics of galaxy formation, and the simulation outputs need to be rendered in the space of real astronomical observations (see Ref. [207] for an application to dwarf HI single-dish observations). Because simulations are slow, we will use simulations to train emulators and semi-analytic models (e.g., [208-211]). Thus, likelihood function approaches to constraining dark-matter parameter space will become possible in finite compute time, and we will have a unified theoretical framework to consider all astronomical probes of dark matter together (e.g., [188, 212, 213]). Simulations can also point to completely new types of observables [190, 214, 215], including ones that affect lab dark matter searches [216-218]. This mapping between dark matter particle models and astronomical observables, including the effects of galaxy evolution physics, enables sharp tests of dark matter microphysics with telescopes, and a connection to terrestrial experiments.

There is an enormous discovery potential for dark matter physics with the next generation of experiments on telescopes and in the lab. Revealing the particle nature of dark matter from these experiments requires a theoretical and simulations program to unite all probes of dark matter into a consistent interpretation framework.

#### 4 Neutrinos and other light relics

Standard cosmology predicts that the Universe is filled with a sea of relic neutrinos produced during the Hot Big Bang. As the Universe expands and cools, the neutrino momenta redshift along with photons and other particles leaving a relic background characterized by a temperature  $T_{\nu} \propto 1/a \approx 10^{-4}$  eV today. In the early Universe, when  $T_{\nu}(a) \gg m_{\nu i}$ , these particles were relativistic and contributed to the radiation energy budget. Today, we expect that at least two of the three neutrino mass eigenstates have masses  $m_{\nu} \gg T_{\nu}$ . Cosmology therefore probes neutrinos across a range of epochs from the era of decoupling  $(T \sim 10 \text{ MeV})$  through the non-relativistic transition and to today. Measurements of the radiation density in the early universe provide constraints on the number of neutrino states and the energy density carried by each. Measurements of the Universe at late times characterizing the matter budget and amplitude of large-scale structures provide constraints on the neutrino energy density at late times, and therefore the sum of the neutrino masses. Both provide powerful constraints on the thermal history of the Universe and new physics beyond the Standard Model. For a thorough discussion of the science of light relics, see these Snowmass papers [219, 220].

The radiation energy budget is conventionally parameterized by  $N_{\text{eff}} \equiv (\rho_{radiation}/\rho_{\gamma} - 1)/(\frac{7}{8}(\frac{4}{11})^{4/3})$ , where  $\rho_{\gamma}$  is the CMB photon energy density and  $\frac{7}{8}(\frac{4}{11})^{4/3}\rho_{\gamma}$  is the expected energy density of a single species of neutrino and anti-neutrino that decouples instantaneously. The standard model prediction of three light neutrino and anti-neutrino states translates into a prediction of  $N_{\text{eff}} = 3.044$ , where the additional digits after the decimal are due to residual heating of neutrinos due to electron-positron annihilation [221–225]. Current constraints on  $N_{\text{eff}}$  from CMB and BAO data are  $N_{\text{eff}} = 2.99 \pm 0.17$  [226], in remarkable agreement with the Standard Model expectation. CMB data is expected to continue to provide evermore stringent constraints on  $N_{\text{eff}}$ , large-scale structure is an emerging probe of  $N_{\text{eff}}$  [227, 228] that can also produce interesting limits on neutrinos.

A variety of well-motivated beyond-the-Standard-Model scenarios predict additional light degrees of freedom such as axions, gravitinos, gravitational waves, or other dark radiation ([219]) that, at some point in the early Universe, would have been in thermal equilibrium with the rest of the Standard Model particles. These very same measurements of neutrinos in the early and late Universe can be used to infer the presence of these new particles. There are firm theoretical predictions for the additional contribution to  $N_{\rm eff}$  from any light ( $\leq$ eV) thermal relic particle that was ever in equilibrium with the primordial plasma, specifically  $\Delta N_{\rm eff} = 0.027, 0.047, 0.054$  for a single scalar, Weyl fermion, or vector Boson that decoupled at epochs when all Standard Model degrees of freedom were in equilibrium. Remarkably, experiments in the next decade are approaching these thresholds of detection [26–28, 219, 229, 230]. For particles that decoupled at later epochs, the contribution to  $N_{\rm eff}$  is larger because those particles would have experienced the same heating as the photon bath when heaver particles fell out of equilibrium.

Simple counting of particles and spins gives a prediction for  $\Delta N_{\text{eff}}(T_{\text{freeze-out}})$ , the function specifying the contribution to  $N_{\text{eff}}$  from a species that freezes out at  $T_{\text{freeze-out}}$ , that is accurate to the %-level at epochs when the relativistic degrees of freedom are not changing. For particles that decouple during the QCD or electroweak phase transitions, for instance, computing  $\Delta N_{\text{eff}}$  is considerably more complicated. During this epochs perturbative techniques and lattice gauge theory are required (for a summary, see, e.g. [27, 231]) and theoretical uncertainties are currently present at the 10%-level. Reaching sub-percent-level accuracy for the neutrino contribution to the energy density requires detailed computations including non-instantaneous decoupling and, to a lesser extent, neutrino oscillations [221–225].

CMB and LSS datasets sensitive to  $N_{\rm eff}$ , a measure of the total energy density in relativistic particles, are also able to infer properties of the perturbations in relativistic particles. This allows these experiments to set limits on the existence of non-standard neutrino self interactions [232–239] and interactions among other new contributions to the relativistic energy budget [80, 240] such as self-interacting dark radiation [241] or dark radiation that is tightly coupled to other dark sector particles [242].

At present the strongest constraints on  $N_{\text{eff}}$  come from CMB temperature and polarization anisotropies. The physical effects can be understood as follows: the radiation density

in the early Universe dictates the Hubble rate, which characterizes lengths and timescales that impact features in the CMB power spectra (for a review see, e.g. [27, 243]). For free-streaming contributions to  $N_{\rm eff}$ , there is an additional change to the power spectra, a phase shift in the peaks, due to the different propagation speeds of perturbations in free-streaming particles (c) and perturbations in the photon-baryon fluid ( $c_s = c/\sqrt{3}$ ) [244]. These signatures on CMB primary power spectra are well-understood and straightforward to model, for instance using publicly available Boltzmann codes CLASS and CAMB [245, 246]. On the other hand, reaching target constraints on  $N_{\rm eff}$  will require removing the changes to the CMB power spectra induced by gravitational lensing from matter along the line of sight [60, 247] as well as cleanly separating out any foreground emission contaminating the measured power spectra. While galactic and extragalactic foregrounds are not expected to be a limiting factor for CMB polarization data at  $\ell \lesssim 5000$ , future experiments will be measuring CMB polarization anisotropies on those scales for the first time. Quantifying the impact of foregrounds, and delensing in the presence of foregrounds, on measurements of  $N_{\rm eff}$  is an active area of research that requires accurate simulations of high-resolution maps of galactic and extragalactic foreground emission, as well as nonlinear CDM and baryon structure.

Neutrino oscillation data specifies the splitting of the square of the neutrino masses to be  $\Delta m_{12}^2 = 7.42^{+0.21}_{-0.20} \times 10^{-5} \text{ eV}^2$  and  $\Delta m_{13}^2 = |2.51 \pm 0.027 \times 10^{-3}| \text{ eV}^2$  [248]. As the relic neutrino temperature is  $T_{\nu} \sim 10^{-4}$  eV today, at least two of the three mass eigenstates are non-relativistic. These particles then contribute to the matter budget of the Universe today, with  $\Omega_{\nu}h^2 \approx \sum_i m_{\nu i}/94 eV$  (e.g. [249]). This contribution has yet to be detected, but remains the only unknown parameter in the simplest  $\Lambda$ CDM cosmology. As the mass splittings are known, a cosmological measurement of  $\Omega_{\nu}$  translates into a constraint on the lightest of the neutrino mass states<sup>2</sup>. Detecting the neutrino mass scale, and finding consistency with laboratory experiments, would be a triumph of cosmology and particle physics. Determining the neutrino mass scale would also set a benchmark for neutrinoless double- $\beta$  decay experiments: if the neutrino mass sum is detected at  $\gtrsim 0.1$  eV via cosmology and that process is not observed, the simplest interpretation is that neutrinos are Dirac particles (see, e.g. [27, 220]). In the event that neutrinoless double beta decay is detected, a cosmological measurement of the neutrino mass sum can help to constrain the Majorana phases. Pinning down the neutrino mass scale is also important for studies of new physics. Dark energy constraints, for example, can be affected by degeneracies with the neutrino mass.

Neutrinos were relativistic for much of the history of the Universe and therefore kinematically forbidden from participating in gravitational clustering until late times. This manifests as a strong suppression in the amplitude of neutrino perturbations on scales smaller than the neutrino free-streaming scale, a length scale characterizing the typical distance neutrinos travel in a Hubble time. The absence of neutrinos on these scales weakens the gravitational potentials and slows the overall growth of cold dark matter and baryon structures. The net result is a suppression in the amplitude of structures, which

<sup>&</sup>lt;sup>2</sup>Unless  $m_{\nu \text{lightest}}$  is sufficiently large (e.g.  $\gtrsim$  few meV), next generation cosmological detections of the neutrino mass sum will only provide an upper bound on  $m_{\nu \text{lightest}}$ . Detecting the value of  $m_{\nu \text{lightest}}$  directly would require  $\sigma_{\Sigma m_{\nu}} \lesssim m_{\nu \text{lightest}}$ .

can be parameterized by  $\sigma_8$ . The suppression in structure is detectable via a variety of methods, from gravitational lensing of galaxies or CMB [226, 250–253], to redshift space distortions to galaxy clustering [97, 253, 254], and galaxy cluster counts (for a summary, see [220]). The transition of relic neutrinos from relativistic to non-relativistic also alters the evolution of the neutrino energy density, and therefore the Hubble rate, but this signature is expected to be too small to detect [243]. The physical processes and observables described here will also occur for other light relic species. Consequently, constraints on neutrino mass and  $N_{\text{eff}}$  can be generalized to constrain the mass of other light relic species [255].

If neutrino masses are described by the minimal mass normal or inverted orderings,  $\sum m_{\nu} \approx 0.06$  eV or  $\approx 0.1$  eV. In these scenarios the primary observable for neutrino mass – a suppression in the matter power spectrum, relative to what would be seen from CMB predictions for the amplitude of structure in a universe with massless neutrinos – is a small effect ( $\sim 3 - 6\%$ ). To robustly detect the neutrino signal and confidently limit the masses of any other new light relic particles, will require exquisite control over theoretical and observational systematics. Achieving that control will require strong efforts in the theory and simulations of structure formation, astrophysical processes, and survey data. There are also opportunities to identify observables or techniques that may help isolate a signature of neutrino or other light relic particle masses.

Current constraints on the neutrino masses from primary CMB, CMB lensing, and LSS power spectrum measurements combined are  $\sum m_{\nu} < 0.16$  eV at 95% confidence [256]. This bound on the mass puts the neutrino free-streaming scales well into the linear regime of structure formation. Yet, datasets probing the suppression in structure due to neutrinos receive contributions from quasilinear and nonlinear scales where simulations, or advanced techniques such as EFT [110–112], are typically used to model nonlinear gravitational evolution. Neutrinos are fast-moving particles that travel over cosmological distances and have a significant velocity dispersion, accurately incorporating them into studies of gravitational evolution can therefore pose challenges. A number of different approaches exist in the literature.

On the simulations side, a popular technique consists in including neutrinos as particles, while adding a thermal component to their initial velocities [257–265]. This method naturally takes into account neutrino nonlinearities, which can be important in some scenarios [266–269]. However, it also suffers from a few challenges that are associated to the large thermal velocities of neutrinos, such as the need for a special relativistic description [270] and shot noise. Shot noise arises as a problem when treating neutrinos as *N*-body particles because the neutrino density field lacks intrinsic power on small scales so shot noise due to finite sampling of the density field quickly dominates. The shot noise can be reduced by increasing the number of neutrino particles, at the expense of significantly increasing the use of computational resources. Alternative approaches have been developed to mitigate this problem [271–274]. To achieve robust constraints with future survey, simulations will also need to accurately account for baryonic feedback processes [275].

Another simulations-based approach consists in treating the neutrinos in linear theory, while coupling to the non-linear gravitational potential of the cold dark matter [276–281]. This can make simulations with massive neutrinos only as computationally expensive as in the case of cold dark matter alone, while also accounting for all relativistic correc-

tions [282–284]. This approach of treating neutrinos in linear theory, while accounting for nonlinear evolution of CDM, is also adopted in separate universe simulations, which allow for precise calculations of a subset of nonlinear statistics such as halo bias and the squeezed-limit bispectrum [285]. However, in all of these approaches the effects of nonlinear clustering of neutrinos are neglected. While neglecting nonlinear clustering of massive neutrinos should be adequate for  $\sum m_{\nu} \leq 0.3$  eV and studies of structure on large scales [268], for heavier neutrinos or observables on halo scales one should account for them. There are also some hybrid schemes that aim to combine the advantages in both methods [286–288].

Finally, there continues to be rapid progress in the development of analytic or hybrid methods for large-scale structure. For example, multi-component perturbation theories to compute the power spectra and bispectra of matter fields [289–296], spherical collapse models to compute halo formation [297, 298], and peak-background split / separate universe approaches to halo clustering statistics [285, 299]. At this stage there continues to be a strong interplay between simulations and analytic approaches to modeling large-scale structure in the presence of massive neutrinos, and therefore observables sensitive to neutrino mass.

# 5 Dark energy

Discovering the mechanism that drives cosmic acceleration, whether it is a cosmological constant  $\Lambda$ , a time-dependent scalar field, or modifications of the laws of gravity, is a core science goal of ongoing and future DOE experiments and NASA missions. Dark energy as a term describes our lack of understanding of the physical concepts that underlie cosmic acceleration. As such it encompasses a wide variety of fundamental physics topics including modified gravity, neutrino physics, dark matter-dark energy coupling, early dark energy, and more. A joint analysis of multiple cosmological probes across multiple experiments is required to control the systematics budget and to increase the constraining power such that the community can discriminate between the different physical concepts that explain cosmic acceleration.

Two complementary avenues emerge in order to constrain the underlying physics model driving cosmic acceleration: 1) Measuring tensions between different experiments within the same underlying model and 2) combining the constraining power of different experiments that are not in tension in order to compare different models.

Major progress on this topic is made by the current (Stage 3) generation of photometric surveys, such as Kilo-Degree Survey (KiDS) [300], the Hyper Suprime Cam (HSC) [301], the Dark Energy Survey (DES) [302] and spectroscopic surveys, such as the Baryon Oscillation Spectroscopic Survey (BOSS) [303]. These low-redshift constraints of the  $\Lambda$ CDM model can be contrasted with CMB measurements from the early Universe made e.g., by the Planck satellite [1], the Atacama Cosmology Telescope (ACT) [304, 305], and the South Pole Telescope (SPT) [17].

These initial results will become more exciting in the near future with the decreasing statistical uncertainty and better systematics control. With the advent of so-called Stage 4 surveys, e.g., the Dark Energy Spectroscopic Instrument (DESI) [97], the Prime Focus Spectrograph (PFS) [306], the Vera C. Rubin Observatory [307], Euclid [98], the Spectro-Photometer for the History of the Universe, Epoch of Reionization, and Ices Explorer (SPHEREx) [128], and the Nancy Grace Roman Space Telescope [308] the science community can expect an abundance of data to study the late-time Universe at increased precision. Similarly, the next generation of CMB surveys, such as the Simons Observatory (SO) [26] and CMB-S4 [27] will enable us to contrast high and low redshift at increased precision and to combine information from both eras to increase the constraining power on cosmological models.

Below we list the main focus areas in theory and numerical modeling that need to be addressed in order to fully extract the cosmological information from multi-probe, multi-survey analyses (see e.g. [309, 310] and the Snowmass Computational Frontier white paper [311] for more details):

**Observational modeling uncertainties:** For example, photo-z errors, shear calibration, depth variations need to be parameterized consistently across the different probes and surveys if the datasets are combined.

**Astrophysical modeling uncertainties:** For example, nonlinear modeling of the density field, baryonic physics, intrinisic alignment, galaxy bias and Halo Occupation Distribution models are key astrophysical uncertainties that need to be modeled through a combination of numerical simulations, analytical models and combinations thereof. Consistent parameterizations and coordination of priors is important if datasets or probes are to be combined.

**Statistical uncertainties:** For example, the functional form of the likelihood and, if a multivariate Gaussian is assumed, the computation of data covariances are key uncertainties in a joint CMB-LSS analysis.

**Simulated likelihood analyses:** Simulated likelihood analyses are important early on to design survey strategy, and at later stages to inform costly numerical simulation campaigns, and to optimize the final analyses on the measured survey data. These simulated mock analyses need to be run to quantify the error budget as a function of the analysis choices (scales, redshifts, galaxy samples, summary statistics) for the different probe and experiment combinations. At later stages, mock analyses are required to quantify tensions between different probes and/or experiments and to do model comparison.

**Numerical simulations:** Nonlinear modeling of the density field and exploring the statistical uncertainties mentioned above requires numerical simulations. The initial conditions of these simulations should be coordinated across all survey collaborations to enable a better comparison.

**Hydrodynamic simulations:** Baryonic physics, intrinsic alignment, galaxy bias and Halo Occupation Distribution models require a hydrodynamic simulation campaign that is computationally extremely expensive. In order to utilize the available computing resources most effectively this simulation campaign must be informed by the composition of the error budget of a joint analysis. In other words, the requirements for a simulation campaign will be different when analyzing data from a single survey as opposed to data from multiple surveys. Simulated cosmological likelihood analyses of multi-survey data can identify the main contributors to the overall error budget and can inform a corresponding simulation campaign. A close connection between the simulated analyses and the simulation effort is required.

#### 6 Expansion rate of the universe

A current cosmological mystery that could have significant implications for our understanding of the Universe in the near future is the observed large discrepancy between different inferences of the Hubble constant  $H_0$ . Indeed, measurements of the luminosity distance of Cepheid-calibrated Type Ia supernovae [312] differ at  $\sim 5\sigma$  from the predictions of our current standard ACDM cosmological model once its parameters are fitted to observations of the temperature and polarization anisotropies of the CMB [226, 313, 314]. This inconsistency is known as the " $H_0$  tension" since distances in cosmology are inherently linked to the Hubble constant. At the moment, there is a strong case that this discrepancy is not caused by systematics in CMB data [315–317]. The situation is more ambiguous for distance-ladder-based inferences, for which different calibration techniques yield somewhat conflicting distance-redshift relations. Of particular note, a distance-ladder calibration based on the Tip of the Red Giant Branch (TRGB) [318-327] find important inconsistencies with the Cepheid-based SH<sub>0</sub>ES team [328–331] in estimates of luminosity distances to neighboring supernovae. Nonetheless, several independent attempts to determine  $H_0$ from distance and redshift measurements from a suite of different observations [332–343] also find higher values than inferred from the CMB, albeit with larger uncertainties [344]. To shed new light on this observational puzzle, several new ideas for probing the recent expansion history of our Universe have been proposed (see e.g. Ref. [345]). Turning these ideas into actual observational realities is a key priority in the coming decade to help provide more clues into the fundamental nature of the tension.

While this discrepancy is commonly referred to as the  $H_0$  tension, it is important to realize that what is actually in "tension" is cosmological distance measurements [346–348]. For instance, one could rephrase the current tension by saying that a  $\Lambda$ CDM model fit to Planck CMB data [226] places the Hubble-flow Type Ia supernovae further away from us than the Cepheid-calibrated distance ladder does. Turning the problem around, we could also phrase the issue by saying that a  $\Lambda$ CDM model fitt to Cepheid-calibrated Type Ia supernovae places the CMB last-scattering surface closer to us than what is required by CMB observations. This emphasis on distances is important to identity physics-based solutions that can actually address the root cause of the problem. In other words, simply finding a cosmological model that has a value of  $H_0$  compatible with that quoted in Ref. [312] is not sufficient [349, 350]; the model must instead provide a good fit to all distance measurements available (including supernovae, BAO, time-delay strong lenses, etc.), in addition to CMB data. Therefore, a better characterization of the current situation would be that we have a cosmological "distance crisis" on our hands.

For theoretical physics, this apparent discrepancy presents an opportunity to carefully reexamine all the different assumptions that go into our current cosmological model. As a starting point, one could ask how well we understand the late-time expansion history of our Universe. Observations of the *relative* luminosity distances to Type Ia supernovae at  $0.02 \leq z \leq 2$  [351, 352] strongly constrain deviations from the standard  $\Lambda$ CDM expansion history at those redshifts, giving us confidence that our understanding of the Universe is on solid ground at these epochs. Given these constraints, one might be tempted to instead change the expansion history at very late times (z < 0.02). Such models, while technically able to accommodate large value of  $H_0$  (typically at the price of a phantom dark energy

equation of state), do not provide good fits the actual measured *distances* to low-redshift supernovae and therefore do not address the root cause of the tension [348–350]. Given the variety of low-redshift distance measurements available, such "late solutions" do seem to face an uphill battle in resolving the current discrepancy. Future measurements of low-redshift cosmological distances, such as those from multi-messenger astronomy, will play an important in determining whether late solutions are at all viable.

Another possibility is that we are missing some important physics in the early Universe. Since the CMB is fundamentally observed in angular space, making it compatible with a larger value of  $H_0$  (which brings the last-scattering surface closer to us) requires shrinking all physical length scales present near photon decoupling to leave the observed angles invariant. In particular, the angular size of the baryon-photon sound horizon  $\theta_*$  is one of the most precisely measured quantities in all of cosmology. Since  $\theta_* \propto r_s H_0$ , where  $r_s$  is the physical size of the sound horizon, keeping this angle constant with a larger  $H_0$  value requires a smaller  $r_s$ . Not too surprisingly, most proposed "early times" solutions (see e.g. Refs. [49, 353–357]) to the current tension effectively work by reducing the size of the baryon-photon sound horizon. As  $r_s$  is mathematically given by an integral over the sound speed  $c_s$ ,

$$r_{\rm s} = \int_{z_{\star}}^{\infty} \frac{c_{\rm s} dz}{H(z)},\tag{1}$$

several models shrink the sound horizon by *increasing* H(z) in the pre-recombination universe, which suppresses the integrand. Others do so by changing  $z_*$  (the photon decoupling redshift) to an earlier epoch (see e.g. Refs. [358–360]). Whichever mechanism is used, the difficulty lies in doing so without ruining the detailed fit to the temperature and polarization power spectra of the CMB. Indeed, another important length scale to the CMB is the photon diffusion length (also called the photon mean free path). Shrinking the baryon-photon sound horizon without also reducing the photon diffusion length by *the same factor* nearly guarantees either a poor fit to CMB data, or the introduction of new tensions with other data sets, especially those from large-scale structure, or both. Thus, any successful "early solution" needs to include a mechanism to properly adjust this diffusion length.

The centrality of the photon diffusion length (or its inverse, the photon scattering rate) to the Hubble tension as a whole was recognized in Ref. [361]. Modifying this quantity is highly non-trivial as it involves low-energy Standard Model physics, which is well understood. While this represents a significant model-building challenge, it also provides a clear target for future studies on which kind of new physics is required. One possibility that has been explored is a variation of the fine-structure constant and of the electron mass between the epoch of last scattering and today [362, 363]. Such an approach has had significant phenomenological success in a fair model-to-model comparison [364, 365]. However, significant model-building is required to explain the required percent-level changes in these quantities (see e.g. Refs. [366, 367]). Another possibility is modify the helium abundance near the epoch of recombination, which would affect the free-electron fraction in the cosmic plasma and thus change the photon diffusion length. Such an approach would require modifying Big Bang Nucleosynthesis predictions of the helium and deuterium abundances, which is challenging given their current consistency with direct light-element abundance measurements [368]. Whichever physical mechanism is proposed to adjust the photon

diffusion length to make the CMB compatible with a larger Hubble constant, it will leave subtle signatures in the data that could be detected in future observations, such as those from CMB-S4 [29].

Whether it is the result of unknown systematics or new physics, the Hubble tension presents a golden opportunity to scrutinize both our theoretical beliefs and our data analysis techniques with the hope that they can be reconciled. As more high-precision data become available, our leading cosmological model might have to be amended, ushering in a new era of fundamental physics understanding.

## 7 Theory as guide for the development of future experiments

As we consider future opportunities, it is useful to consider past successes at the intersection of particle theory, particle experiment, astronomical observations, and simulations as a guide for what might be possible.

The simplest models of inflation predicted a universe with primordial perturbations that are dominated by adiabatic, Gaussian, and nearly but not exactly scale-invariant density perturbations with a spectral index  $n_{\rm s} \lesssim 1$  at a time when measurements with a precision that could test these predictions were a distant dream. These predictions have now all been confirmed to high precision [1]. In addition to the density perturbations, many of the simplest models of inflation predict primordial gravitational waves within reach of the next generation of experiments [26, 27]. The detection of this characteristic signature of inflation is one of the main science goals for upcoming CMB experiments, and both the planning and design relies on close collaboration between theorists and experimentalists.

While this example was one about inflation, other examples exist for the other fundamental physics topics in this work. Theorists can guide the development of new experiments (e.g., SPHEREX).

As another example of fruitful interplay that leads to the development of a novel class of experiments, consider the case of dark matter with a hidden-sector Yukawa coupling (see Ref. [206] for a comprehensive review). In the early 2000's, the "missing satellites problem" [369, 370]—the apparent mismatch between the number of luminous satellite galaxies in the Milky Way relative to simulated dark matter subhalos, now recognized to not, in fact, be a problem [193, 371, 372]—motivated physicists to consider that dark matter may have a strong self-interaction cross section [373]. As direct-detection and collider experiments continued to search for WIMP and axion dark matter without success<sup>3</sup>, attention turned to the anomalous ratio of cosmic-ray positrons to electrons as observed with the ATIC [376] and PAMELA [377] experiments. Many particle theorists suggested that such an excess could arise via enhanced dark matter annihilation from light dark-sector mediators that could be kinetically mixed with elecroweak gauge bosons (see, e.g., [378–380]).

<sup>&</sup>lt;sup>3</sup>All the while, they continue to place strong constraints on particle parameters and open the window on solar neutrino searches (e.g.,[374, 375]).

Several authors pointed out that this could lead to enhanced elastic dark matter selfinteractions as well [381–383], leading to significant theory work to characterize the cross section as a function of velocity [384, 385], and many cosmic numerical simulation studies for signatures of this kind of self-interaction on a wide variety of scales [170, 172, 214, 386–388].

All the while, new annihilation searches in gamma rays and direct detection searches on Earth constrained the coupling of these "hidden sector" models to the Standard Model [389, 390], and new searches for the "dark matter photon" in these models commenced at a variety of colliders [391–393].

To this day, simulators and observers are working to sharpen predictions and tests for Yukawa coupling of dark matter in the smallest halos to nearly horizon scales [172, 173, 175, 386, 388, 394–402]. More broadly, if dark matter exists in a rich hidden sector, its physics may be primarily accessible through cosmic probes if its interaction with the Standard Model is small. But, only when measurements of dark matter in the sky are coupled with terrestrial experiments can we fully characterize dark matter's particle properties.

For most applications (perhaps most notably for neutrinos and dark matter), there is a strong foundation of interdisciplinary work among observational cosmology and laboratory experiments, united by theory, to reveal new physics. We expect this interaction among fields to be even more critical to suss new physics out of the next generation of cosmological and laboratory data sets.

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