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## Lattice QCD and Particle Physics

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## EXECUTIVE SUMMARY

Lattice field theory provides a mathematically rigorous definition of quantum field theory, including gauge theories. The rigor provides a platform for computation of strongly-coupled gauge theories, not only quantum chromodynamics (QCD) at long-distances but also strongly-coupled sectors that might lie beyond the Standard Model (BSM) of particle physics. Indeed, the interpretation of many experiments in particle physics, nuclear physics, and astrophysics relies, often crucially, on results from lattice QCD or BSM.

In quark-flavor physics, lattice QCD is essential for grounding theoretical predictions. Together with experimental measurements, lattice QCD is used to determine many of the fundamental parameters of the Standard Model's flavor sector: five out of six quark masses and the three mixing angles and  $CP$ -violating phase of the Cabibbo-Kobayashi-Maskawa (CKM) matrix. Further Standard-Model predictions requiring lattice QCD are for processes that could reveal signatures of new physics. This area of lattice QCD has become a precision science, as has the determination of the strong coupling,  $\alpha_s$ , which is key in many areas, for example for understanding Higgs-boson decay to gluons.

Lattice-QCD calculations of the hadronic contributions to the anomalous magnetic moment of the muon are another area for which precision is both mandatory and achievable. While these contributions can be estimated via a combination of certain measurements and general theoretical concepts, a direct *ab initio* calculation from QCD is desirable to confirm robustly the tantalizingly large discrepancy between experiment and the Standard Model.

Other indirect searches for new physics are complementary to quark-flavor physics and the muon anomalous magnetic moment. Lattice QCD is an essential tool for understanding newly discovered hadrons with quark content different from the usual baryons and mesons. Lattice-QCD calculations are needed to interpret bounds on electric dipole moments, proton decay, neutron-antineutron oscillations, neutrinoless double-beta decay, and charged-lepton flavor violation. These topics all entail matrix elements of the nucleon, usually in concert with nuclear many-body theory.

The theory of the neutrino-nucleus cross section also requires these two ingredients. To first approximation, neutrino-nucleus scattering consists of a neutrino-nucleon interaction followed by propagation of the struck nucleon, and any produced hadrons, in a nuclear medium. Having results with full error budgets for nucleon-level quantities will solidify theoretical treatments of this complicated process. Any improvement in nuclear modeling will pay dividends in extending the power of neutrino-oscillation experiments. Lattice QCD can also be used to provide information needed in nuclear many-body theory, via calculations of multihadron interactions.

The LHC experiments (among many others) rely on parton distribution functions for cross sections, both within and beyond the Standard Model. This is an area of rapid development, with precise lattice-QCD calculations foreseeable in the coming decade. Lattice BSM is used to understand the spectrum of composite Higgs models and other strongly-coupled theories that motivate LHC searches. Composite models are also a popular explanation for dark matter, requiring spectroscopy from lattice gauge theory. Lattice QCD is needed to understand the properties of the axion, a field introduced to explain the absence of observed strong  $CP$  violation, and a dark matter candidate in its own right. Lattice field theory is also increasingly pertinent to theoretical physics in general, for example in strongly-coupled supersymmetric theories and in conformal field theories studied in several fields.

This contribution to Snowmass is drawn from seven whitepapers prepared by the USQCD Collaboration in 2019 [1–7], with numerous updates as appropriate.

## I. INTRODUCTION

This contribution to the U.S. Community Study on the Future of Particle Physics (aka “Snowmass”) outlines the physics program of the USQCD Collaboration, as it pertains to particle physics. The USQCD Collaboration<sup>1</sup> is a federation of scientific collaborations and individuals engaged in computational research on lattice gauge theory and other lattice field theories, principally quantum chromodynamics (QCD). It is a steward of infrastructure—both hardware and software—for lattice-QCD calculations. In 2019, USQCD published seven whitepapers to build the case for funding mid-sized computing facilities. They spell out a comprehensive program for the coming 5–10 years in particle and nuclear physics [1–6] and a perspective on computing [7]. Most of the material in this document is drawn from those works, with updates to the references and, in cases where developments have been rapid, exposition and perspective.

The role of QCD in particle physics is easy to summarize: QCD is everywhere. The LHC collides beams of protons; the SuperKEKB and BEPC II  $e^+e^-$  colliders are designed to produce flavored hadrons; neutrino-oscillation experiments and searches for dark matter or charged-lepton-flavor violation use nuclear targets; collider experiments keep discovering new (and often weird) hadrons. Even purely leptonic experiments, if they are sensitive enough, probe virtual hadrons—the anomalous magnetic moment of the muon,  $g - 2$ , is the foremost example. To interpret these experiments, it is necessary to have some level of control over hadrons and nuclei. In some cases sub-percent total uncertainty is required and, as discussed below in several sections, increasingly feasible.

The techniques of numerical lattice gauge theory are not limited to QCD. Models beyond the Standard Model (BSM) of particle physics often include confining gauge theories. For example, dark matter could consist of hadron-like bound states. The Higgs boson could well be composite, although if so, the dynamics will have to differ from QCD; in particular, it seems necessary that the gauge coupling runs more slowly. Various aspects of composite dark matter and composite Higgs are well suited to numerical lattice gauge theory. A simple and general example is to examine a viable model to see whether the transition from high temperatures to low generates gravitational waves. Another question is whether a confining gauge theory could yield a light scalar with properties of the Standard-Model Higgs boson, with the rest of its spectrum (just) out of reach of the LHC.

Stemming from its focus on QCD, the lattice community’s relevance spans funding agencies’ programs in particle physics and in nuclear physics. In the United States, this means the DOE Office of High Energy Physics (HEP) and Office of Nuclear Physics (NP), as well as the NSF Division of Physics programs in Elementary Particle Physics (EPP) and in Nuclear Physics. In addition to DOE and NSF funding for researchers, the DOE supports infrastructure for numerical lattice gauge theory. DOE HEP and NP support medium-scale computer clusters at Brookhaven National Laboratory, Fermi National Accelerator Laboratory, and Thomas Jefferson National Accelerator Facility. These computer clusters support large, albeit not the largest, lattice-QCD and -BSM projects. USQCD’s allocation process has an excellent record of supporting innovative projects that might not sway a multidisciplinary allocation committee. (Early work on muon  $g - 2$  started this way.) USQCD also uses its stewardship of these clusters to foster the careers of junior researchers in lattice gauge theory. (Several by-now mid-career scientists established their reputations this way.) The largest-scale lattice-QCD calculations run on the leadership-class supercomputers available

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<sup>1</sup> More on USQCD can be found in Appendix A.

at several NSF and DOE facilities. The high precision demanded by the Muon  $g - 2$  Experiment and several quark-flavor experiments is not possible without computing campaigns spanning the clusters and the leadership-class facilities.

Computational science cannot prosper without code and algorithm development. The DOE Office of Advanced Scientific Computing Research (ASCR) supports development of QCD software and algorithms for the next-generation supercomputers coming on line this year via the Exascale Computing Project (ECP). These machines—Frontier at Oak Ridge National Laboratory and Aurora at Argonne National Laboratory—are designed to be capable of  $10^{18}$  double-precision floating-point operations per second, or 1 exaflop/s, which is comparable to the human brain [8]. (ECP also supports application development in accelerator science, computational cosmology, and many other subjects [9].) ASCR and the other DOE offices together fund programs in Scientific Discovery through Advanced Computing (SciDAC): for lattice gauge theory, these are collaborations between ASCR and HEP as well as ASCR and NP. SciDAC grants support research into algorithms for lattice gauge theory, in collaboration with applied mathematicians.

At the community level, lattice-gauge-theory research plays important roles in (at least) three units of the American Physical Society (APS): the Division of Particles and Fields (DPF), the Division of Nuclear Physics (DNP), and the Topical Group on Hadronic Physics (GHP). Lattice methodology has an even broader influence. For example, the hybrid Monte Carlo (HMC) algorithm [10] invented for full QCD with dynamical quarks is widely used<sup>2</sup> in Bayesian inference [11], cosmological signal processing [12], and condensed-matter physics [13].

Given this breadth of interests, it is impossible to cover everything. We limit the material in this contribution to the intersection of the Snowmass topical groups and the physics program of the 2019 USQCD whitepapers [1–6]. Many contributions to Snowmass cover these topics and are cited in the main text. Interesting topics not covered here include the following. A large part of the USQCD physics program supports nuclear physics; a similar document emphasizing nuclear physics will be prepared for the next long-range plan of the Nuclear Science Advisory Committee (NSAC). Several USQCD members engaged in the ECP discuss lattice simulations in a Snowmass contribution to the Computing Frontier [14], building on Ref. [7], so that material is not repeated here. The fast-moving topics of machine learning, quantum information science, and quantum computing—discussed briefly in Ref. [7]—are not yet central to USQCD collaboration activities. Several USQCD members have, however, co-authored contributions to Snowmass on these topics [15–19].

This contribution is organized as follows. Section II covers the Rare and Precision Frontier. It discusses how USQCD plans to continue to sharpen the search for new physics in the quark-flavor sector, to complete calculations of the hadronic contributions to muon  $g - 2$  with the required precision on the timescale of Fermilab E989, and some aspects of a program of precision nucleon matrix elements with comprehensive error budgets (i.e., electric dipole moments, proton decay,  $n - \bar{n}$  oscillations, and nucleon matrix elements involved in muon-to-electron conversion). Following Snowmass organization, hadron spectroscopy is also in Sec. II. Section III covers the Neutrino Physics Frontier, including the theory of neutrinos. Here again nucleon matrix elements appear, but now they must be folded into nuclear many-body theory [20, 21] and event generators [21, 22]. Sections IV and V cover the Energy Frontier and Cosmic Frontier, respectively. In addition further nucleon matrix elements, these frontiers also profit from the exploration of gauge theories other than QCD.

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<sup>2</sup> In other fields, HMC is often thought to stand for Hamiltonian Monte Carlo.



Again following Snowmass organization, hot, dense QCD appears in Sec. IV. Section VI is short, covering topics at the Theory Frontier with a less obvious connection to the HEP experimental program. Appendices give some background on the USQCD Collaboration, describe the landscape for computing (in the U.S.), and list contributions to Snowmass mentioning lattice QCD.

## II. RARE AND PRECISION FRONTIER

The rare and precision frontier covers a broad range of experiments and correspondingly broad range of lattice-QCD calculations. The U.S. lattice community has been influential in this area [1, 3, 5]. Among the topics covered in this frontier, hadronic spectroscopy and decay and mixing properties of  $B$ ,  $D$ , and  $K$  mesons are especially well developed. Recent years have witnessed rapid development in computing the hadronic contributions to the anomalous magnetic moment of the muon, namely the amplitude for hadronic vacuum polarization and for hadronic light-by-light scattering. Calculations of nucleon properties related to rare processes should be mentioned [1, 5]. As a rule [23, 24], nucleon correlation functions are noisier than their meson counterparts, so the results are less precise. Precision is less of an issue, though, because the corresponding experiments are still at the stage of setting limits. Some examples are matrix elements for nucleon electric dipole moments, proton-decay form factors, and the first calculation of operators that induce neutron-antineutron oscillations.

### A. Weak decays of quarks

Quark-flavor physics is, perhaps, the area of particle physics in which lattice QCD has had its greatest impact [3]. In many cases, the way QCD enters the Standard-Model expression for a measurable rate is very simple. Schematically,

$$d\Gamma = \left( \frac{\text{CKM}}{\text{factor}} \right) \left( \frac{\text{kinematic}}{\text{factor}} \right) \left( \frac{\text{QCD}}{\text{factor}} \right) + \left[ \frac{\text{BSM}}{\text{term}} \right]. \quad (2.1)$$

If the BSM term can be assumed to be small, as in processes that proceed at the tree level of the electroweak interactions, the combination of measurements and (lattice) QCD calculations can be used to determine the Cabibbo-Kobayashi-Maskawa (CKM) matrix. Correspondingly, if the CKM matrix is known and the Standard-Model contribution is suppressed, the same approach can be used to put constraints on physics beyond the Standard Model. Indeed, in many cases a single matrix element, or set of related matrix elements, is needed to interpret a single measurement. For example, in leptonic decays of charged mesons the QCD factor is parametrized by a single number, known as the decay constant, and the decay vertex entails a single CKM matrix element.

An important by-product of these studies are determinations of the quark masses, which are relevant to Higgs-boson decay. They are discussed in Sec. IV A together with the strong coupling  $\alpha_s$ , which is relevant to Higgs-boson production and decay. Of course, as the fundamental parameters of QCD,  $\alpha_s$  and the quark masses are important in many areas, not least the quark-flavor physics discussed in this section.



### 1. Weak decays of $b$ and $c$ quarks

For many years, lattice QCD has been a vital contributor to  $B$  and  $D$  physics [3]. Here the experiments aim to (over)determine the CKM quark-mixing matrix and search for new sources of  $CP$  violation (which are needed to explain the observed baryon asymmetry of the universe) by measuring  $B$ - and  $D$ -meson decay rates,  $CP$  asymmetries, and mixing frequencies of neutral mesons. Amplitudes of leptonic and semileptonic decays and neutral-meson mixing have been a major focus throughout the past 20 years, and many are now at or approaching a watershed of sub-percent uncertainties. In particular, the leptonic decay constants of  $B$  and  $D$  mesons (including those with strangeness) have now reached sub-percent precision [25], which is beyond the needs of the flavor factories BES III, Belle II, and LHCb for the foreseeable future.

Semileptonic decays are experimentally more accessible than leptonic decays, for which the rates are suppressed by the square of the lepton mass. Combined with lattice QCD, experimental measurements of exclusive semileptonic decays yield the most precise determinations of most of the elements of the CKM matrix:  $|V_{us}|$  from  $K \rightarrow \pi \ell \nu$  [26–29],  $|V_{cd}|$  from  $D \rightarrow \pi \ell \nu$  and  $D_s \rightarrow K \ell \nu$  [30, 31],  $|V_{cs}|$  from  $D \rightarrow K \ell \nu$  [31, 32],  $|V_{ub}|$  from  $B \rightarrow \pi \ell \nu$  [33–36] and  $B_s \rightarrow K \ell \nu$  [33, 37–39], and  $|V_{cb}|$  from  $B_{(s)} \rightarrow D_{(s)}^{(*)} \ell \nu$  [38, 40–45]. In all cases, not only is the normalization of the corresponding form factors computed, but also the shape, namely the dependence on the lepton-pair invariant mass  $q^2$ . A sample joint fit to the lattice-QCD and experimental shapes is shown in Fig. 1 (left) [44], with a floating normalization that yields  $|V_{cb}|$ . Further information on  $|V_{ub}|/|V_{cb}|$  comes from the ratio of  $b$ -flavored baryon decay distributions using form factors from lattice QCD [46]. The precision of calculations of semileptonic  $D$ - and  $B$ -meson form factors is expected to reach the percent level over the coming few years.

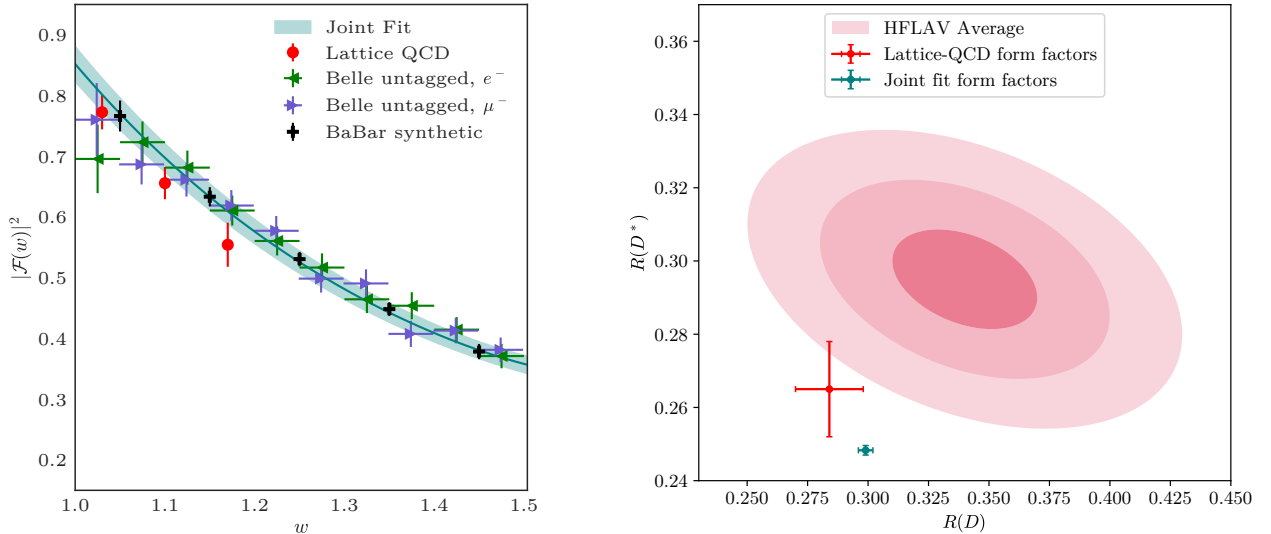


FIG. 1. Semileptonic decays  $B \rightarrow D^* \ell \nu$  [44]. Left: A joint fit to experimental and lattice data, which determines the CKM element  $|V_{cb}|$ . The variable  $w$  is related to the momentum transfer,  $q$ , by  $q^2 = M_B^2 + M_{D^*}^2 - 2wM_B M_{D^*}$ . Right:  $R(D^*)$  vs.  $R(D)$ . An average of experimental measurements (red ellipses) is compared with the Standard-Model prediction either using shape information only from lattice QCD (red point with error bars) or using the combined fit of the shape from the  $|V_{cb}|$  determination (green point). The discrepancy is several  $\sigma$ .

Recent measurements of semileptonic decays, in both charged-current and flavor-changing-neutral-current (FCNC) processes, have shown an abundance of deviations from the Standard Model [47, 48]. In lattice QCD, the corresponding calculations [49–52] are an offshoot of those just discussed for CKM determinations. A sample result relying on lattice QCD is the  $q^2$  distribution for the FCNC decay  $B \rightarrow K\mu^+\mu^-$  [50], where  $q$  is the four-momentum of the  $\mu^+\mu^-$  pair. The experimental results from BaBar, Belle, CDF, and LHCb lie  $1.8\sigma$  ( $2.2\sigma$ ) below the prediction, for  $q^2$  below the  $J/\psi$  (above the  $\psi(2S)$ ) resonance. Note that the uncertainty from the form factors dominates the error in the prediction. Beyond the differential rate of  $B \rightarrow K\mu^+\mu^-$ , other tensions in  $b \rightarrow s$  transitions have been observed. The differential rate and angular distributions of  $B \rightarrow K^*\mu^+\mu^-$  and  $B_s \rightarrow \phi\mu^+\mu^-$  [52, 53], and ratios of the branching fractions of  $K^{(*)}\mu^+\mu^-$  relative to the  $K^{(*)}e^+e^-$  final state all are in poor agreement with the Standard Model [54–56]. In addition, many measurements of the rate for the rare leptonic decay  $B_s \rightarrow \mu^+\mu^-$  (i.e.,  $b\bar{s}$  annihilation) have been in tension with the Standard Model [25, 57, 58], although a recent one is not [59]. The baryon decay  $\Lambda_b \rightarrow \Lambda\mu^+\mu^-$  has also been studied using lattice QCD [60–64].

The  $K^*$  decays to  $K\pi$ , so the rigorous calculation of the amplitude for  $B \rightarrow K^*$  is very challenging. An analysis with the appropriate finite-volume<sup>3</sup> formalism [65] is underway [66], as is an analysis of  $B \rightarrow \rho(\pi\pi)$ . These results will inform future computing projects, but the difficulty is such that the rates obtained from the lattice-QCD form factors will be less precise than the measured rates for several years.

Neutral-meson mixing, which entails the oscillation from particle  $P$  to its antiparticle  $\bar{P}$  and back, is also an FCNC. The frequency,  $\Delta M_P$ , is measured from the time dependence of decays, and, as is often the case with frequencies, the measurements are very precise. Thus, the precision of lattice-QCD calculations of these quantities have lagged experiment. In the laboratory, this phenomenon has been observed for all stable neutral-meson systems:  $K^0$ - $\bar{K}^0$ ,  $D^0$ - $\bar{D}^0$ ,  $B^0$ - $\bar{B}^0$  and  $B_s$ - $\bar{B}_s$ . The most accurate theoretical results are for the  $B$  systems, because these mixing processes are dominated by short-distance virtual particles, leading to local four-quark operators. The past few years witnessed significant improvement of all five operators that could mediate  $B_{(s)}$ - $\bar{B}_{(s)}$  mixing in the Standard Model and any extension thereof [67, 68]. The two most precise calculations of the  $B_{(s)}$ - $\bar{B}_{(s)}$  mixing matrix elements are in imperfect agreement [67, 68]. For this reason, and because the precision lags experiment, further work on the  $B_{(s)}$  systems,  $\Delta M_B$  and  $\Delta M_{B_s}$ , is planned. For remarks on the long-distance contributions that are crucial to  $K^0$ - $\bar{K}^0$  and  $D^0$ - $\bar{D}^0$  mixing, see Sec. II A 2.

The measured ratios  $R(D^{(*)}) = \text{BR}(B \rightarrow D^{(*)}\tau\nu)/\text{BR}(B \rightarrow D^{(*)}\ell\nu)$  of charged-current processes also disagree with the Standard Model, by approximately  $3\sigma$  combined [69]. The Standard-Model prediction of these ratios requires the form factors over the full kinematically allowed range. Results are available for  $R(D)$  [41, 42] and, since 2021, for  $R(D^*)$  [44]. The status after the first full lattice-QCD calculation of  $R(D^*)$  [44] is shown in Fig. 1 (right). Lattice-QCD results and measurements are also available for the similar ratios  $R(J/\psi)$  [70, 71] and  $R(\Lambda_c)$  [46, 72]. Lattice-QCD results for all ratios are of sufficient precision to meet the demands of LHCb and Belle II for the next several years. Even so, their precision will improve, because the relevant form factors are needed to determine the CKM element  $|V_{cb}|$ .

The most persistent puzzles in  $B$  physics are the discrepancies in the values  $|V_{cb}|$  and  $|V_{ub}|$  determined via exclusive vs. inclusive semileptonic decays [73]. The theory input for exclusive decays consists of the form factors mentioned above, while the theory input for inclusive decays employs the operator-product expansion and heavy-quark expansion, which require

<sup>3</sup> See Sec. II E for more information on using finite-volume effects to understand hadronic resonances.

coefficients calculated in perturbation theory<sup>4</sup> with operator matrix elements obtained from kinematic distributions. Lattice QCD can be used to compute (a few of) the matrix elements [74–77]. More recently, interesting ideas have been put forward to compute quantities related to the spectral function, such that a weighted integral yields the inclusive rate [78–83]. One of these new methods [81] has recently been implemented in a full lattice-QCD study [84].

The possible hints of new physics in several measurements of  $B$  decays lends renewed urgency to quark-flavor physics. On the experimental side, both LHCb and Belle II will be making more precise measurements during the coming five years, as will CMS and ATLAS. The  $B$  program is complemented by the charm program at these experiments and BES III. Better precision on the fundamental parameters of the Standard Model is essential to establishing any new-physics effect in the processes mentioned above. For quark masses, current precision [77, 85–87] suffices for the time being, although further confirmation is, of course, desirable. The magnitudes of the CKM matrix can be determined from leptonic (e.g.,  $B \rightarrow \tau\nu$ ) and charged-current semileptonic decays. For leptonic decays, precision again suffices for the time being, although confirmation is, of course, desirable. New calculations of the form factors for  $B \rightarrow \pi\ell\nu$  and  $B \rightarrow D^{(*)}\ell\nu$  are needed to match the precision of Belle II for  $|V_{ub}|$  and  $|V_{cb}|$ , respectively. Work is underway using the same general strategy that made the leptonic decays constants so precise; this work will automatically include semileptonic  $D$  decays [88]. In addition, there is ongoing effort to support future measurements of  $b$ -baryon decays.

Further discussion of these and other issues related to  $b$ - and  $c$ -quark physics can be found in contributions to Snowmass; see Ref. [89] for lattice QCD, Refs. [47, 90, 91] for phenomenology, and Refs. [92–94] for experiment summaries, and Refs. [95, 96] for new analysis tools.

## 2. Weak decays of strange and light quarks

In addition to the short-distance processes analogous to those that dominate  $B_{(s)}\text{--}\bar{B}_{(s)}$  mixing,  $K^0\text{--}\bar{K}^0$  ( $D^0\text{--}\bar{D}^0$ ) oscillations are also mediated by processes [97, 98] with two  $\Delta S = 1$  ( $\Delta C = 1$ ) transitions separated by long, hadronic distances, such as  $K^0 \rightarrow \pi\pi \rightarrow \bar{K}^0$  ( $D^0 \rightarrow \pi K \rightarrow \bar{D}^0$ ). These long-distance effects are a challenge. Lattice-QCD must employ a finite volume (because any computer’s memory is finite), and the two-particle intermediate state is very sensitive to finite-volume effects. This sensitivity is, however, well understood mathematically for elastic processes such as  $K \rightarrow \pi\pi$  [99]. First calculations of the long-distance contribution to  $\Delta M_K$  have been carried out [100, 101], although again the precision achieved so far lags that of experiment. These calculations are part of a broader campaign to study the  $K \rightarrow \pi\pi$  reaction. In 2015, the first lattice-QCD calculation with a complete error budget of the quantity  $\text{Re}(\epsilon'/\epsilon)$ , which quantifies direct  $CP$  violation, appeared [102]. Further work [103] led to a result  $\text{Re}(\epsilon'/\epsilon) = 21.7(8.4) \times 10^{-4}$  [104] in agreement with  $\text{Re}(\epsilon'/\epsilon) = 16.6(2.3) \times 10^{-4}$  from the 2002 measurements of the KTeV [105] and NA48 [106] experiments (at Fermilab and CERN, respectively).

In addition to  $\Delta M_K$  and  $\text{Re}(\epsilon'/\epsilon)$ , a few calculations in kaon physics are needed to get the most out of some older experiments. Even better precision than that now available (sub-percent [26–29]) for the form factor in  $K \rightarrow \pi\ell\nu$  is needed to resolve a possible  $5\sigma$

<sup>4</sup> Lattice QCD for  $\alpha_s$  is discussed Sec. IV A.

tension in first row of the CKM matrix.<sup>5</sup> Such improvement requires a complete treatment of electromagnetism and isospin breaking via  $m_d \neq m_u$ . This advance will require new ensembles of gauge-field configurations, which are already planned for muon  $g - 2$ . Now that the ingredients of a full calculation of  $\text{Re}(\epsilon'/\epsilon)$  are understood, it is time to aim for the precision of KTeV and NA48 [105, 106]. Last, CERN experiment NA62 is underway to improve BNL E949’s measurement of the branching ratio of  $K^+ \rightarrow \pi^+ \nu \bar{\nu}$ . With the recent improvement in the charm-quark mass and expected improvements in the CKM matrix, the leading theoretical uncertainty in the Standard-Model prediction is a long-distance effect of charmed intermediate states [110]. Technology similar to that used for  $\Delta M_K$  will be used to attain a first-principles result to replace phenomenological estimates currently in use. For further discussion of these and other issues related to kaon physics, see the Snowmass contributions on lattice QCD [111], phenomenology [112, 113], and experiment [114].

Lattice-QCD calculations of properties of isoscalar mesons, such as  $\eta$  and  $\eta'$  are more difficult, because the conversion of  $q\bar{q}$  into gluons and back again is computationally more challenging, making results less precise. Basic properties, such as the masses and mixing angle have been studied [115–119]. The prospect of the REDTOP experiment [120] makes further pertinent calculations compelling.

## B. Fundamental physics in small experiments

Among the many “small” experiments exploring fundamental physics, two kinds benefit from high-quality lattice-QCD calculations: measurements of the (anomalous) magnetic moment of the muon [3] and searches for permanent electric dipole moments in the neutron, proton, and (in principle) other hadrons [5].

### 1. Muon magnetic moment ( $g - 2$ )

In the Standard Model or any extension of it, the muon anomalous magnetic moment, denoted  $g - 2$  or  $a_\mu = (g - 2)/2$ , is a sum of quantum fluctuations from photons, hadrons, the top quark,  $W$  and  $Z$  bosons, the Higgs boson, and any as-yet undetected particles that couple to the muon or any of the other Standard-Model particles. Except for the hadronic contributions, perturbation theory can be used to obtain sufficient precision to match the experiments’ needs. Thus, the hadronic contributions dominate the error budget. The two most important hadronic contributions to  $g - 2$  are the leading-order HVP and the much smaller hadronic light-by-light (HLbL; again, leading order). To obtain these contributions, the hadron current-current correlation function (for HVP) or the four-current scattering amplitude (for HLbL) are convolved with kernels derived in perturbative QED [121, 122]. Further hadronic contributions are the next-to-leading order (NLO) HVP and HLbL, which use the same QCD calculations but higher-order QED kernels.

As recently as 2015, precise calculations of the HVP were beginning, and work on HLbL scattering was in an exploratory phase. Both began to receive increasingly large computing allocations as the Fermilab experiment was being built. By now, HVP is a fully mature subject. Recent results for the HVP from lattice QCD come from many collaborations in the U.S., Europe, and Japan [123–143].

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<sup>5</sup>  $5\sigma$  is attained when using a new result for a certain radiative correction in nucleon  $\beta$  decay [107–109].

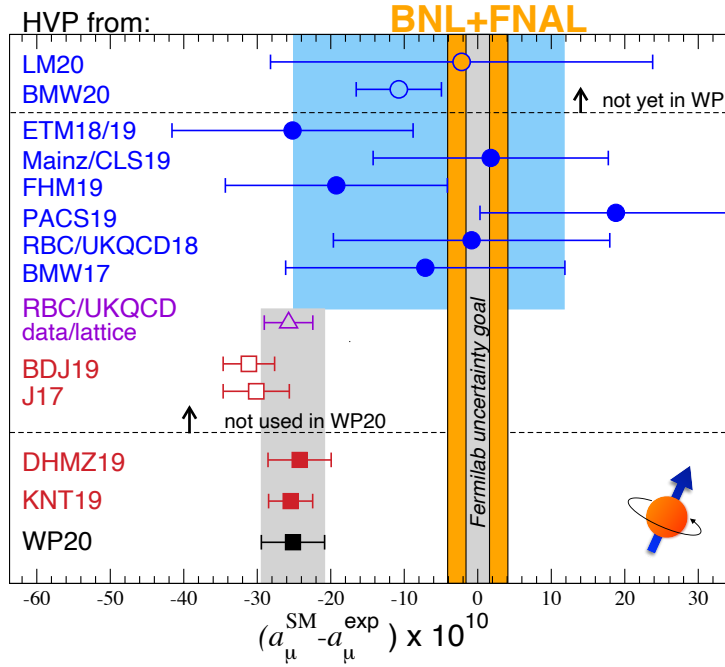


FIG. 2. Comparison of  $a_\mu = (g-2)/2$  calculations of the full HVP with experiment. To obtain  $a_\mu^{\text{SM}}$  the other Standard-Model contributions as given in Ref. [148] are added to the calculation of the HVP. Averages for dispersion-theory (gray band, lower left) and lattice-QCD (blue band) results are based on the filled symbols; results shown with unfilled symbols are omitted for various reasons. The orange band shows the average of the BNL and Fermilab experiments, with the narrow gray band the target uncertainty of Fermilab E989. From Ref. [149].

Since the publication of the 2019 USQCD whitepaper [3] on quark- and lepton-flavor physics, the landscape of the  $g-2$  has developed dramatically. The Fermilab experiment reported a new result with 0.46 ppm precision [144, 145], in agreement with an earlier BNL result measured to 0.54 ppm [146]. In support, the Muon  $g-2$  Theory Initiative [147] produced consensus values for the hadronic contributions [148], with an update contributed to Snowmass [149]. A comparison plot [149] of the combination of the BNL and Fermilab experiments,  $a_\mu^{\text{exp}}$ , with the consensus Standard-Model prediction,  $a_\mu^{\text{SM}}$ , is reproduced in Fig. 2. Figure 2 also shows individual theoretical predictions that use data for  $e^+e^- \rightarrow$  hadrons and dispersion theory to determine the HVP [150, 151], which lead to the consensus value. The average of the experiments [144–146] and Standard-Model consensus disagree by  $4.2\sigma$ . This discrepancy is not new, and explanations of it with new physics constitute an enormous literature; see, for example, Ref. [152] and references therein.

Meanwhile, the Budapest-Marseille-Wuppertal (BMW) collaboration [140] has published the first lattice-QCD result for the HVP with a total error comparable to the latest data-driven results [150, 151]. Using the BMW result for the HVP (labeled “BMW20” in Fig. 2) would relieve the disagreement with experiment. Even so, it would not be the end of the drama, because the HVP with a different QED weight enters the running of  $\alpha_{\text{QED}}$  up to the  $Z$  pole [153, 154]. Most of the lattice groups cited above are aiming at precision targets [149] of 0.5% for the leading-order HVP (thus surpassing the precision of the BMW calculation [140]) and 1% for the NLO and NNLO HVP. Assuming consistency, the NLO calculations could be averaged, bringing the overall uncertainty down to the level of the Fermilab experiment.



Even with exascale computing resources, it will be extremely difficult to attain a single such precise calculation for the leading-order HVP ( $a_\mu^{\text{HVP, LO}}$  in Table I). In particular, effects of isospin breaking are needed, requiring additional ensemble generation with  $m_u \neq m_d$ . Electromagnetism in finite-volume systems is also a challenge. It is crucial to have independent efforts with enough differences in analysis to ameliorate correlations in the systematic errors. These calculations will receive rigorous scrutiny from the Muon  $g - 2$  Theory Initiative. Once the uncertainties are comparable to the dispersive method, they will be folded into the consensus. The higher-order HVP,  $a_\mu^{\text{HVP, NLO}}$ , requires the same QCD calculation [129], so the same lattice-QCD work will hit the 10% target for this contribution too.

As a four-point function, the HLbL contribution,  $a_\mu^{\text{HLbL}}$ , is more computationally demanding (for comparable precision). It is smaller, however, so the precision target is less demanding, again 10%. In the past, the HLbL contribution was suspected as the origin of the discrepancy between the BNL measurement and contemporary Standard-Model predictions, in large part because there was no rigorous way to determine it. The community relied on values bracketing model-based calculations [155–158], without having a firm grasp on the uncertainties or even the robustness of those estimates. These suspicions can now be dismissed, thanks to advances in lattice QCD and a relatively recent data-driven dispersive method [159]. Building on the earlier development of viable techniques [160–164], RBC/UKQCD [165] and Mainz [166, 167] and both have published results with  $\sim 20\%$  uncertainty, comparable to the data-driven dispersive method [149, 159]. While still short of the ultimate goal, the consistency of these results makes it implausible that the HLbL contribution can be large enough to explain the discrepancy between the consensus Standard-Model value and the experiments. Now that the lattice-QCD methods are mature, it is expected that with exascale resources the uncertainty in HLbL can be reduced further, again matching the needs of the final Fermilab result.

It is impossible to predict how HVP, HLbL, and the experiments will land as the work continues to unfold. As already mentioned,  $a_\mu^{\text{HLbL}}$  is too small to affect the outcome. If one assumes the new data from the Fermilab experiment agree with Refs. [144–146] and reduce the uncertainty as planned, and *further* assumes that lattice-QCD confirms the dispersive results for HVP, then a very significant discrepancy would arise. Less exciting scenarios are also possible, for example if other lattice-QCD groups confirm BMW’s result for the HVP. That would imply some sort of misunderstanding of  $e^+e^- \rightarrow \text{hadrons}$ , which would have repercussions elsewhere [153].

## 2. Electric dipole moments

Permanent EDMs of elementary particles, nucleons, atoms and molecules in the ground state, if observed, are signals of  $CP$  violation. CKM-induced contributions are orders of magnitude tinier than experimental sensitivity [168]. In the Standard Model, EDMs could stem from a  $CP$ -violating gluonic operator in the QCD Lagrangian, commonly known as strong- $CP$  violation. Limits on the neutron EDM lead to the strong- $CP$  problem, one of the outstanding puzzles associated with the Standard Model [169]. Briefly, the current bound on the neutron EDM implies  $\theta_{\text{QCD}} - \arg \det Y \lesssim 10^{-10}$ , where  $\theta_{\text{QCD}}$  is the coefficient of the strong- $CP$  term, and  $Y$  is the Yukawa coupling matrix between the Higgs and quark fields. The cancellation is baffling. A statistically significant calculation of the required nucleon matrix element directly from (lattice) QCD is not yet available; see Ref. [170] for discussion and Ref. [171] for a review. These matrix elements are challenging, because of the need to

sample fully the topological sectors of QCD [172].

A popular explanation<sup>6</sup> for the smallness of strong- $CP$  violation is the axion [169], a field that couples to the strong- $CP$  term in a way that dynamically cancels  $\theta_{\text{QCD}} - \arg \det Y$ . Then a nonzero EDM would be a signal of new physics. The axion is of further interest as a dark matter candidate; lattice-QCD input on its viability is discussed in Sec. VB.

Several new experiments aimed at the neutron EDM are planned [176, 177] and an experiment aimed at the proton EDM is being developed [178–180]. In addition to the strong- $CP$  term, several higher-dimension operators induced by physics at energies at or beyond the electroweak scale can generate EDMs; for more information, see the recent reviews [171, 176] or a contribution to Snowmass [177]. Lattice-QCD calculations of nucleon matrix elements of the Standard-Model operator and BSM operators have been carried out or are underway [170, 172, 181–187]. Of these, the nucleon EDM induced by the quark EDM operator is a technically straightforward calculation, and results with  $\lesssim 5\%$  uncertainty have been obtained [188–190]. The calculations of the matrix elements of other leading BSM operators can be challenging because of the low statistical signal and issues of renormalization [191–194]. Progress has, however, been steady and over the next five years, estimates with around 20% uncertainty are expected for many EDM matrix elements.

### C. Baryon- and lepton-number violating processes

On their own, baryon number,  $B$ , and lepton number,  $L$ , are accidental symmetries of the Standard Model. The Standard Model does allow for changes in  $B - L$  via instantons or sphalerons, which are both suppressed at temperatures below the electroweak phase transition. Many extensions of the Standard Model break  $B$  and  $L$  while preserving  $B - L$ : an observation of baryon-number violation via proton decay or neutron-antineutron oscillations would lend support to these ideas. Extensions of the Standard Model that accommodate nonzero neutrino masses sometimes introduce Majorana fermions (for example, right-handed neutrinos), leading to  $\Delta L = 2$  neutrinoless double- $\beta$  decay ( $0\nu\beta\beta$ ) of nuclei. As hadronic and nuclear transitions, proton decay,  $n-\bar{n}$  oscillations, and  $0\nu\beta\beta$  require a solid understanding of the strong interactions in order to make Standard-Model predictions.

The large-scale neutrino detectors, DUNE [195] and HyperK [196], will set new limits on proton decay and  $n-\bar{n}$  oscillation processes [197]. Dedicated  $n-\bar{n}$  experiments are also being developed [198] including a proposed experiment at the European Spallation Source [199]. The  $n-\bar{n}$  transition rates probed by these experiments can be directly connected to constraints on BSM theories using lattice-QCD calculations of the corresponding nucleon matrix elements. The extraction of BSM theory constraints from experimental searches for nuclear instability at DUNE and HyperK will require a combination of lattice-QCD calculations of nucleon-level processes with nuclear effective theories [200, 201] and event generators describing experimental signatures of these processes in nuclei [202, 203] that are under active development. Lattice-QCD calculations of proton-decay matrix elements have been carried out for several proton decay modes [204–208], accurately enough for current limits. During the coming decade, it will be feasible to improve them to the 10-percent level. For  $n-\bar{n}$  oscillations, the matrix elements turn out to be 5–10 times larger in lattice-QCD calculation [209–211] than had previously been estimated using the MIT bag model and, thus, extend the reach of current and future experiments. A second round of calculations is

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<sup>6</sup> The solution of the strong- $CP$  problem with  $m_u = 0$  is ruled out [77, 173–175].



needed to obtain a fuller understanding of the systematic uncertainties, but the 10-percent level again seems feasible.

An observation of  $0\nu\beta\beta$  would demonstrate that neutrinos are Majorana fermions, unlike the charged leptons and quarks [212]. Nuclear effective field theory analysis has recently demonstrated that a short-distance  $nn \rightarrow pp$  interaction is required to consistently describe  $0\nu\beta\beta$  processes in nuclei [213]. The corresponding low-energy constant has been estimated [214] and shown to lead to  $\sim 30\%$  or larger modifications of experimentally relevant nuclear matrix elements [215–217]. Lattice QCD calculations of the  $nn \rightarrow ppe^-e^-$  process can be used to accurately determine this low-energy constant and reduce associated uncertainties in  $0\nu\beta\beta$  nuclear matrix element predictions. This undertaking will be challenging. Techniques similar to those developed for  $K^+ \rightarrow \pi^+\nu\bar{\nu}$  and  $a_\mu^{\text{HLbL}}$  are expected to be helpful. First results are becoming available for “warm-up” lattice-QCD calculations: the Standard Model  $2\nu\beta\beta$  process  $nn \rightarrow ppe^-e^-\bar{\nu}_e\bar{\nu}_e$  [218, 219], as well as  $\pi^- \rightarrow \pi^+e^-e^-$  and related mesonic processes involving light Majorana neutrino exchange [220–222]. Lattice-QCD calculations have also been performed for four-quark operator matrix elements needed to predict  $0\nu\beta\beta$  rates from other BSM scenarios involving TeV-scale  $B-L$  violation instead of long-distance Majorana neutrino propagation [223]. The push toward realistic calculations of the  $nn \rightarrow ppe^-e^-$  process is expected to take at least five more years [5, 224].

#### D. Charged lepton flavor violation

With nonzero neutrino masses and mixing, the Standard Model allows charged-lepton flavor violation (CLFV), similarly to FCNCs in the quark sector, but the rate is too small to observe, because the neutrino mass differences are so small. An example is a muon converting to an electron, either through electromagnetic decay (i.e.,  $\mu \rightarrow e\gamma$ ) or in the field of a nucleus ( $\mu A \rightarrow eA$ , often referred to as  $\mu 2e$ ). Other possibilities include meson decays, for example  $B^+ \rightarrow K^+\mu^-e^+$  or  $B_s^0 \rightarrow \tau^\pm\mu^\mp$ . The latter require the lattice-QCD calculations discussed in Sec. II A, while  $\mu 2e$  requires isoscalar nucleon properties, as the (BSM) mediator interacts with quarks inside a nucleon inside the nucleus. Many experiments searching for charged-lepton flavor violation are running or are on the horizon, for example the Mu2e Experiment at Fermilab, which aims to reduce the sensitivity to  $\mu A \rightarrow eA$  by four orders of magnitude. Mediators with similar couplings to quarks are posited to couple to dark matter (DM), so the same nucleon matrix elements are needed for limits on direct DM detection.

In the lepton conversion or DM scattering off nuclei, the energy transfers are low enough so that only  $q^2 = 0$  nucleon matrix elements are needed. The interaction may be flavor singlet, in which case the current can couple to a sea quark, instead of just a valence quark as in isovector (i.e., charged current) processes. The sea quark can propagate from anywhere in spacetime to anywhere else and back again, and such sea-quark propagators are simply more computationally challenging than valence-quark propagators.

To interpret Mu2e, lattice-QCD calculations of the light- and strange-quark contents of the nucleon are needed [225, 226]. These are the matrix elements known as the “sigma term”,  $\sigma_{\pi N} = \frac{1}{2}(m_u + m_d)\langle N|(\bar{u}u + \bar{d}d)|N\rangle$  and the strangeness content  $\sigma_s = m_s\langle N|\bar{s}s|N\rangle$ , as well as the ratio  $\langle N|(\bar{u}u - \bar{d}d)|N\rangle/\langle N|(\bar{u}u + \bar{d}d)|N\rangle$ . Before lattice-QCD calculations became available [227–233], estimates of these quantities from hadronic physics were very uncertain. The situation, as shown in Fig. 3 is much better now, thanks to lattice QCD, but further improvements are clearly needed. The heavy-quark content, defined in analogy with  $\sigma_s$  (for charm, bottom, and top), can be related to the trace anomaly [234]. Because charm

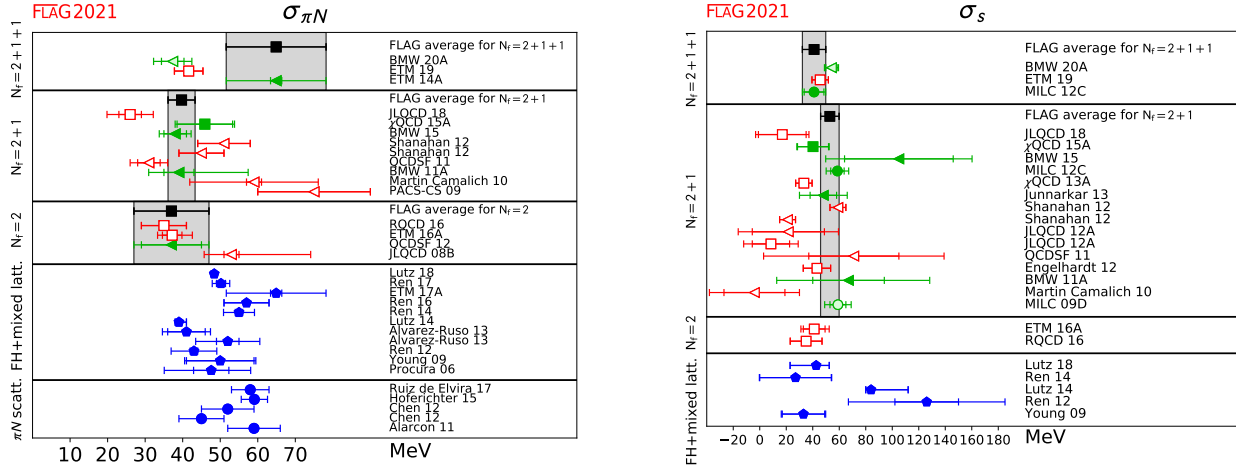


FIG. 3. Comparisons of the “nucleon sigma term”  $\sigma_{\pi N}$  (left) and the strangeness content of the nucleon  $\sigma_s$  (right), from Ref. [190]. Green symbols [228–233] are included in the averages (gray bands); red symbols fall short of certain criteria and are omitted. Blue pentagons denote analyses of several data sets, often including lattice-QCD results. NB: the  $N_f = 2$  results omit the strange sea and are, thus, not recommended for phenomenology.

might not be heavy enough, lattice-QCD calculations of the charm content have been carried out [235, 236]. In addition to the spin-independent matrix elements shown in Fig. 3, spin-dependent matrix elements are also relevant [237] and computable with lattice QCD. First attempts to address nuclear effects on both spin-independent and spin-dependent operators are underway [238].

The isovector versions of these matrix elements, or *charges*  $g_A^{u-d}$ ,  $g_S^{u-d}$ ,  $g_T^{u-d}$ , are important for ultraprecise neutron decay experiments. It is highly unlikely that lattice QCD will reach the uncertainty of the experimental average,  $g_A^{u-d} = 1.2754(13)$  [239] during the coming decade, but 1% calculations should be possible and could shed light on the disagreement among neutron-lifetime measurements [240].<sup>7</sup> The tensor and scalar charges at similar precision also will be possible [244–246]. Calculations of these charges at the 10% level, when combined with  $\beta$ -decay measurements, complement the LHC search for new quark interactions, probing effective scales of new physics close to 10 TeV [243, 247, 248].

## E. Hadron spectroscopy

The prospect of *ab initio* calculations of the hadron spectrum was one of the original attractions of numerical lattice QCD. For the most common mesons and baryons, this task was in a sense completed about a decade ago; see Fig. 2 of Ref. [249]. In more recent years, common hadron masses are studied carefully for technical purposes such as tuning the quark masses and converting from lattice to physical units.

At the same time, the community has moved on to more challenging and interesting questions [1, 250–252], such as determining resonance widths and the masses of more exotic

<sup>7</sup> In fact, 1% precision is claimed already [241, 242], although the tension of this result with that of Ref. [243] (computed on the same ensembles) leads FLAG [190] to quote an “average” with 2.2% error. See Sec. III for more details on  $g_A^{u-d}$

hadrons, such as those discovered at BaBar, Belle, CDF, D0, and LHCb—the “XYZ” states—tetraquarks, pentaquarks, and dibaryons [253–265]. Determining the structure of these states is a compelling and still unanswered question.

Also falling within the rubric of spectroscopy is the calculation of decay widths and scattering amplitudes, because they can be determined from finite-volume energy levels via various universal formulas [266–276]; for a review, see Ref. [277]. Thus, the resonance properties of the  $\rho$  and  $K^*$  mesons are now well studied. Future applications will include electromagnetic transitions such as  $N\gamma \rightarrow \Delta \rightarrow N\pi$  or similarly with a weak current. See Refs. [278, 279] for studies of the similar process  $\pi\gamma \rightarrow \rho \rightarrow \pi\pi$ . As mentioned in Sec. II A, weak decays to vector mesons, such as  $B \rightarrow K^*l\nu$  or  $B \rightarrow D^*l\nu$  play important roles in the “flavor anomalies”, and a completely rigorous treatment requires these finite-volume spectroscopic techniques.<sup>8</sup> Coupled-channel scattering in  $D\pi$ - $D\eta$ - $D_s\bar{K}$  has been used to gain a QCD-based understanding of the excited  $D$ -meson spectrum and its puzzling features [280–282].

Given the importance of heavy-quark physics in particle physics (cf., Sec. II A), it is worth noting that computations of the quarkonium [283–286] and heavy-light meson spectrum were important milestones in establishing lattice QCD for heavy quarks [287]. Indeed, the aim of lattice  $B$  physics played a role in the invention of nonrelativistic QCD (NRQCD) [288–291] and the leading terms of the heavy-quark effective theory [292–294]. NRQCD also played an important role in the predictions of the masses of the  $B_c$  [295, 296] (confirmed [297]),  $B_c^*$  [298] (not yet seen), and  $B_c(2S)$  [299] (confirmed [300]) mesons.

### III. NEUTRINO PHYSICS FRONTIER

The physics associated with neutrino mass and mixing is addressed principally through neutrino oscillation experiments, such as Daya Bay, NOvA, T2K, DUNE, and HyperK, which compare the neutrino energy spectra in detectors at short and long baselines. Deformations in the neutrino-energy spectrum yield the oscillation parameters of the Pontecorvo-Maki-Nakagawa-Sakata (PMNS) mixing matrix [301–303]. The incoming neutrino energy cannot be measured directly, and it is difficult or impossible to reconstruct it without a model of the nuclear physics of the struck nucleus [21, 304, 305], because the final-state energy of the nuclear remnant(s) is at best measured poorly. Scattering amplitudes at the *nucleon* level are necessary ingredients to these models [4]. The uncertainties are extremely difficult to estimate because they have so many moving parts [306, 307]: lattice QCD can provide a firm anchor at the nucleon level.

At low energies, the key signal process for neutrino-nucleus scattering is quasielastic scattering off a nucleon bound in the nucleus. Here, the main missing ingredient is the isovector axial form factor. In the past few years, several groups have studied this form factor’s  $Q^2$  dependence [308–319]. While the precision achieved so far is considerably less than for meson form factors, discussed in Sec. II A, the combination of increased computer power and the increased interest (stemming from the neutrino experiments) has led to rapid progress.

Calculations of the vector form factors, which can be measured in  $eN$  scattering [320], can provide validation. Charge conservation makes the normalization automatic, but the

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<sup>8</sup> In the case of the  $D^*$ , chiral perturbation theory is used to control and estimate uncertainties in  $D^* \leftrightarrow D\pi$ .

radii defined by ( $i$  labels form factors  $G$ )

$$r_i^2 \equiv \frac{6}{G_i(0)} \left. \frac{dG_i}{dq^2} \right|_{q^2=0}, \quad (3.1)$$

are of interest. As illustrated in Fig. 4, lattice-QCD calculations [319] of the isovector electric,  $G_E(Q^2)$ , and magnetic,  $G_M(Q^2)$ , form factors agree well with (a parametrization of) experimental measurements [321], overall and in particular for the radii: the Kelly parameterization gives  $r_E = 0.926(4)$  and  $r_M = 0.872(7)$  [321] while lattice QCD gives  $r_E = 0.92(12)$  and  $r_M = 0.84(18)$  fm [319]. Moreover, the shape agreement—as seen in Fig. 4—extends well beyond  $Q^2 = 0$ . The validation of lattice QCD in this case is very encouraging.

The status of the axial form factor is less settled. The normalization  $F_A(0) = g_A = 1.2754(13)$  [239] is known from neutron beta decay. FLAG [190] quotes averages that are consistent but much less precise:  $g_A = 1.246(28)$   $\{g_A = 1.248(23)\}$  for  $2+1+1$   $\{2+1\}$  flavors, based on Refs. [241–243]  $\{\text{Refs. [322, 323]}\}$ . The  $Q^2$  dependence is shown in Fig. 5, both from work with all sources of uncertainty under control [319] and from a compendium [324]. Several lessons can be taken from these plots and details inferred from them. The most striking is how the lattice data—for individual ensembles at nonzero lattice spacing and unphysical light-quark mass, but also for continuum–physical-mass extrapolations—lie systematically above inferences from experiment. That said, the *slopes* agree at  $Q^2 = 0$ . Two mature works obtain axial radii  $r_A = 0.654(47)$  fm [319] and  $r_A = 0.670(31)$  fm [317] in the continuum limit. These values are based on a model-independent parametrization of the shape founded on analyticity and unitarity, known as the  $z$  expansion. Turning to phenomenology, the same approach to the form-factor shape and minimal assumptions on modeling the deuteron has been used [325] finding  $r_A = 0.68(16)$  fm. Similar results with further assumptions obtain similar values with 3% quoted uncertainty [328, 329]. The agreement is (now) quite good. Note that these radii correspond closely to the black dashed line with axial “mass”  $M_A = 1.026$  GeV in the left panel of Fig. 5, which fails at larger values of  $Q^2$ .

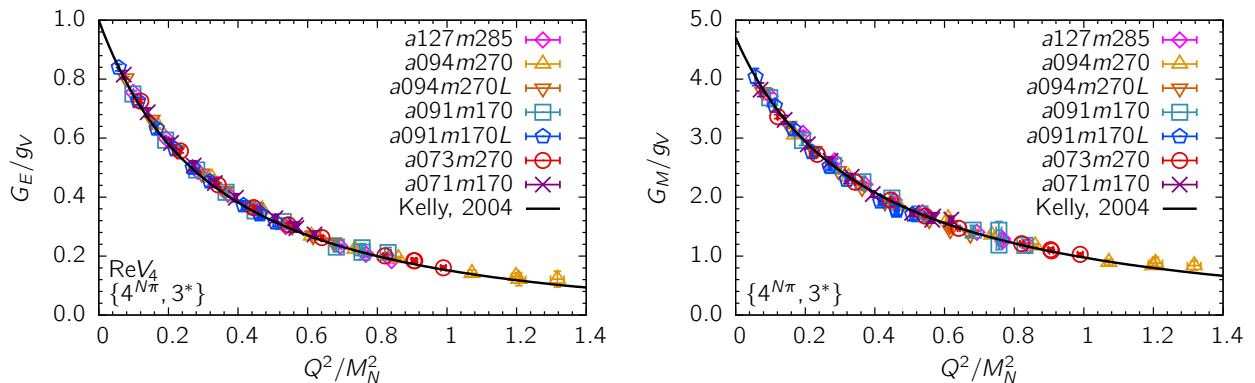


FIG. 4. Electric (left) and magnetic (right) form factors of the nucleon vs. squared momentum transfer  $Q^2 = -q^2$  in nucleon-mass units. The colored symbols denote explicit calculations at various lattice spacing ( $a \approx 0.13, 0.09$ , and  $0.07$  fm), pion mass ( $M_\pi \approx 285, 270$ , or  $170$  MeV), volumes (“large” or “larger  $L$ ”). The Padé parametrization of Kelly [321] of experimental measurement is shown for comparison (black curve). From Ref. [319].

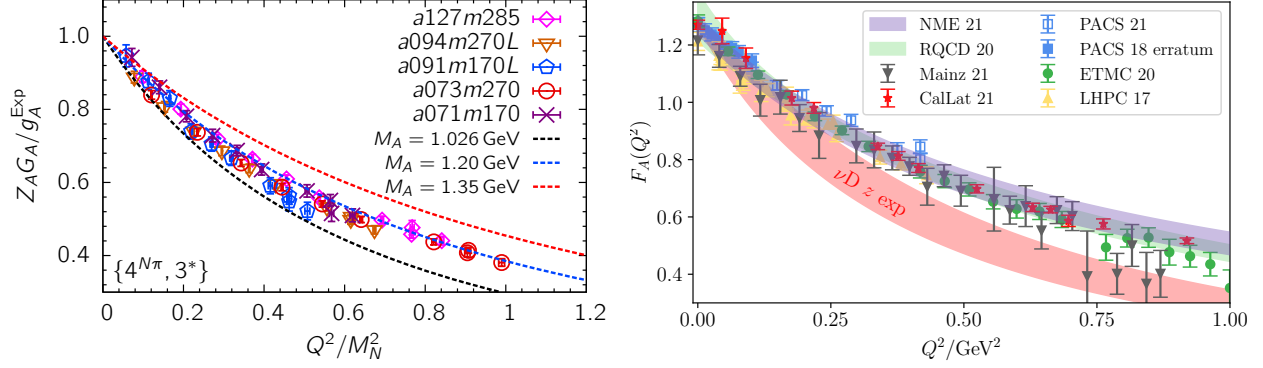


FIG. 5. Isovector axial form factors of the nucleon vs. squared momentum transfer  $Q^2 = -q^2$ . Left: results as in Fig. 4 compared with dipole parametrization for three choices of the axial “mass”  $M_A$ ; from Ref. [319]. Right: compendium of results [324] compared with the  $z$  expansion from  $\nu D$  scattering [325]; shown here are continuum limit fits from RQCD [317] and NME [319], and single-ensemble data points from LHPC [310, 311], PACS [314–316], ETMC [318], CalLat [326] and Mainz [327]; from Ref. [324].

Earlier lattice-QCD calculations reported smaller values of the axial radius. Such values can be extracted via the unphysical but traditional dipole form [317], but with higher statistics the dipole leads to fits of poorer quality [317, 319]. A smaller radius would increase the  $\nu A$  quasielastic cross section [330] with obvious implications for neutrino experiments. Even with agreement for the radius, i.e., the slope, the departure of the lattice-QCD results from phenomenology for  $Q^2 \gtrsim 0.3 \text{ GeV}^2$  influences the quasielastic cross section [324]. An important goal, which should be achievable during the next few years, is a continuum-limit, physical-pion-mass parametrization of the axial form factor up to, say,  $Q^2 = 1.3 \text{ GeV}^2$ .

At DUNE neutrino energies, it is also necessary to understand processes in which additional pions are produced, eventually reaching deep inelastic scattering (DIS). In the resonance region, lattice QCD can provide transition form factors, e.g.,  $N \rightarrow \Delta$ . In principle, the nonzero width can be treated rigorously using the techniques described in Sec. II A for  $B$  decays to vector mesons. For the shallow inelastic region, which has too many pions to identify hadronic resonances but too low energy for the operator-product expansion to hold as in DIS, there is very little information. In this region, one can use lattice QCD to compute the hadron tensor of the nucleon [4], which, as with the nucleon form factors, is used in nuclear many-body theory. Work in this direction has started recently [331]. It is difficult to forecast an uncertainty at this stage—the 20% listed in Table I is meant to suggest that a calculation with a full error budget may be feasible on this time scale. In the DIS region, calculations of nucleon parton distribution functions (PDFs), discussed in Sec. IV B, will play a role.

Beyond single-baryon matrix elements lie calculations of multi-nucleon systems. For practical reasons, these will be limited to a few nucleons, and often unphysically heavy pions, for at least a decade. These calculations will be relevant because they can be used to constrain low-energy constants of the chiral effective theory used to build up a systematic, theoretically based model of the nucleus. The most prominent example is the calculation of nuclear two-body currents: in QCD language, these are matrix elements of the form  $\langle NN | J | NN \rangle$ , where the  $NN$  states can be bound (the deuteron) or unbound. Exploratory calculations of axial-current matrix elements for  $A = 2$  and  $A = 3$  systems are underway [238,



[332, 333]. Calculations of moments of nuclear PDFs relevant to neutrino-nucleus scattering in the DIS region have also been performed, although only for unphysically large quark masses so far [334, 335]. See Ref. [336] for a recent review.

Also important for neutrino scattering is neutral-current elastic scattering. The technical issues run parallel to those for the charged current, except that the isoscalar current can interact with sea quarks, requiring propagators that are computationally much more demanding than those for valence quarks. As a consequence, the precision of neutral-current matrix elements will be lower than their connected counterparts.

The PMNS matrix contains two additional  $CP$ -violating phases if neutrinos are Majorana particles. This possibility can be explored via the neutrinoless double-beta ( $0\nu\beta\beta$ ) decay of certain nuclei, which is discussed in Sec. II C.

Further details can be found in a contribution to Snowmass on neutrino-nucleus scattering that contains perspectives from lattice QCD, nuclear many-body theory, experiment, and event generators [21]. Reference [320] examines the connection to electron-nucleus scattering, and Ref. [22] covers event generators throughout high-energy physics.

## IV. ENERGY FRONTIER

Most of the applications of computational lattice gauge theory to particle physics are QCD. At the energy frontier, lattice QCD is just as important as elsewhere, providing determinations of  $\alpha_s$  and the quark masses, as well as calculations of the parton distribution functions that inform both tests of QCD and searches for signals of new phenomena rising above the Standard-Model background. To a large extent, the searches are motivated by the desire to understand the origin of electroweak symmetry: is it the Standard-Model Higgs sector or something else? Some ideas for “something else” take inspiration from QCD and posit a confining gauge theory that (to be compatible with LHC measurements) is well-described by the Standard Model at sub-TeV energies. Lattice QCD for the energy frontier is discussed in Secs. IV A, IV B, and IV C; lattice BSM in Sec. IV D with related topics in Sec. V.

### A. Precision QCD and Higgs boson properties

The 2012 discovery of the Higgs-like resonance at 126 GeV by the ATLAS [337] and CMS [338] experiments at the Large Hadron Collider (LHC) provided a watershed insight into the origin of electroweak symmetry breaking. Lattice-QCD results help turn experimental studies of this particle into a tool for further discovery, starting with the fundamental couplings of QCD. Of particular importance are analyses that determine from hadronic properties the strong coupling  $\alpha_s$  and the quark masses, particularly those of charm and bottom. These quantities are needed to confront measurements of Higgs-boson branching ratios with Standard-Model predictions.

In both cases, several methods yield consistent results, with uncertainties below the percent level. Figure 6 shows comparisons of recent lattice-QCD results for  $\alpha_s(m_Z)$  (left) [85, 339–348] and for the bottom-quark mass (right) [76, 77, 85–87, 341, 342, 344, 349–351], compiled by the Flavor Lattice Averaging Group (FLAG) [190]. It is worth noting that lattice QCD is the only way to determine the light-quark masses,  $m_s$ ,  $m_d$ , and  $m_u$  with any meaningful precision. Here, too, the results have become impressively precise [77].

Although LHC measurements of Higgs coupling exceed expectations, the current precision of the quark masses, and probably also  $\alpha_s$ , suffices for the coming decade. For experiments at future  $e^+e^-$  or  $\mu^+\mu^-$  Higgs factories, some refinement in the precision of  $\alpha_s$  is warranted, while the present level of precision in the quark masses suffices [352]. That said, many of the most precise results for  $\alpha_s$  and quark masses stem from the same set of ensembles of gauge-field configurations [25, 353, 354], with staggered sea quarks. Confirming determinations of quark masses from sets of ensembles with domain-wall or improved-Wilson sea quarks are, thus, worthwhile; see, for example Ref. [355].

Bottom- and charm-quark masses and  $\alpha_s$  can also be extracted from high-energy decay and scattering processes, analyzed with perturbative QCD. A comprehensive survey of  $\alpha_s$  determinations can be found in a contribution to Snowmass [356].

## B. Parton distribution functions

At the LHC, the Higgs boson is produced in  $pp$  collisions. Therefore, like any process, the predictions of the production cross section depend on the parton distribution functions (PDFs). Indeed, given the crucial role the PDF description of structure functions in  $ep$  deep-inelastic scattering (DIS), it has been a long-standing goal of lattice QCD to compute them. This is a challenging problem, not least because the PDFs are functions of a kinematic variable, namely Bjorken  $x = -q^2/2p \cdot q$ , where  $p$  is the target 4-momentum and  $q$  the momentum transfer.

PDFs (and the related distribution amplitudes of high-energy exclusive scattering processes) are defined via operators entailing a light-like separation, which is clearly inaccessible in the Euclidean framework of numerical lattice QCD. One way to circumvent these problems is to focus on moments of  $x^n$ , which the operator-product expansion (OPE) expresses as matrix elements of local operators, reducing the problem to that of the form factors and charges discussed in Secs. II A and III. Unfortunately, higher moments are related to high-dimension operators, which mix (with a lattice as the ultraviolet regulator) under renor-

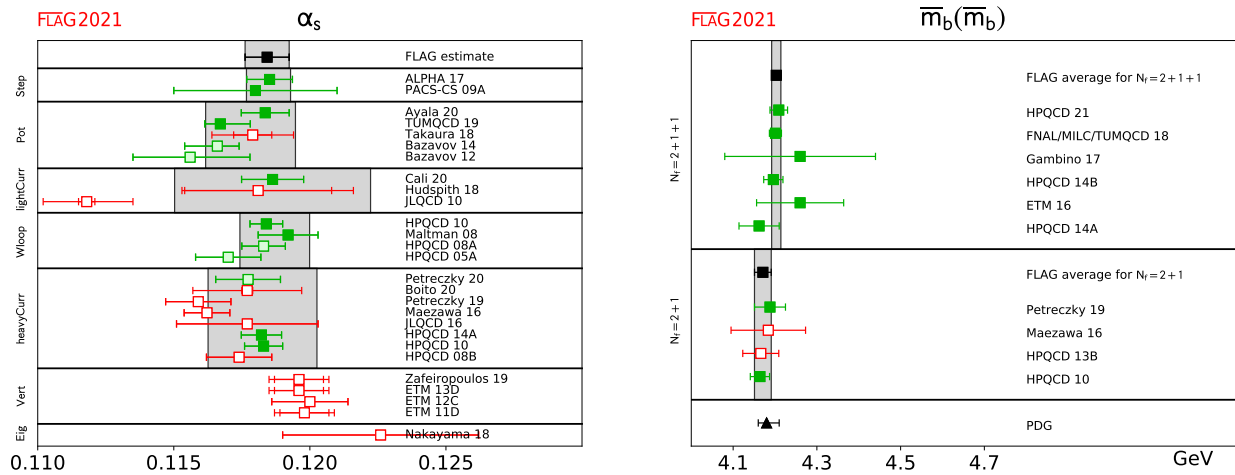


FIG. 6. Comparisons of  $\alpha_s(m_Z)$  [85, 339–341, 343, 345–347] (left) and bottom quark mass [76, 77, 87, 341, 349, 351] (right). From FLAG 2021 [190]. Green symbols are included in the averages (gray bands); red symbols fall short of certain criteria and are omitted from the average.



malization with lower-dimension operators. Thus, lattice QCD has been used to compute only the first few moments of several PDFs; for recent work on nucleon-PDF moments, see Ref. [357, 358]. Higher moments are accessible by introducing an intermediate “smearing” scale [359, 360], taking the continuum limit, and matching back to standard continuum renormalization schemes.

The moments can also be obtained by taking a step back to consider matrix elements of the form  $\langle N(p) | J(z) J'(0) | N(p) \rangle$ , where  $J^{(\prime)}$  are currents of some sort,  $p$  is the momentum of the hadron (e.g., the nucleon  $N$ ), and  $z$  is a (short) distance. For lattice QCD, these matrix elements are four-point functions depending on the Lorentz invariants  $z^2$  and  $\nu = z \cdot p$ . In the original DIS problem, the currents are electromagnetic, but here they can have different quantum numbers and even different quark content [361–363]. The continuum limit of these objects can then be analyzed with the OPE to obtain expressions with the same operator matrix elements as in DIS but different Wilson coefficients. Such factorizable current-current matrix elements can also be used to obtain the Bjorken- $x$  dependence, either via the hadron tensor [331, 364] of the matrix element of two electromagnetic currents or a more general class known as “good lattice cross sections” [365, 366].

Another way to compute the Bjorken- $x$  dependence of the PDFs directly is via the matrix element  $\langle N(p) | \bar{q}(z) W(z, 0) q(0) | N(p) \rangle$ , where now  $q$  ( $\bar{q}$ ) is an (anti)quark field. (For the gluon PDF, replace the quark fields with gluon field-strength tensors.) This idea was invigorated when Ji [367] introduced the large-momentum effective field theory to show how to relate a distribution—known as the quasi-PDF—with spacelike (i.e., Euclidean)  $z^2$  to the usual Minkowski PDF [368–370]. Early calculations of the quasi-PDF [371, 372] stimulated a lot of theoretical attention [373–390]. One of these developments is a distribution known as the pseudo-PDF, which can again be related via perturbative matching to the Minkowski PDF [376]. Starting from the position space matrix element, the quasi-PDF is defined as a Fourier transform in  $z$ , while the pseudo-PDF is a Fourier transform in  $\nu$  [391]. Recovering the PDF requires taking  $p_z \gg \Lambda_{\text{QCD}}$  at fixed  $x$  for the quasi-PDF or  $z^2 \rightarrow 0$  at fixed  $\nu$  for the pseudo-PDF. Both quasi-PDFs [392–399], and pseudo-PDFs [400–407] are areas of active study.

These calculations are very challenging, so many studies are carried out for the simplest hadron, namely the pion. In addition to obstacles facing all calculations, some of these methods require renormalization, and certain approaches require some sort of inverse transform—such as the inverse Laplace transform. On finite data sets, this problem is numerically ill-posed, so active dialog and research will be needed to attack or circumvent it.

For more information on lattice-QCD calculations of PDFs, see Ref. [408]. The interplay of traditional approaches to PDFs with lattice QCD is explored in a 2017 community whitepaper [409] and two contributions to Snowmass [410, 411]. Reference [409] argues that a calculation of the isovector proton PDF at the 12% level for  $x \in [0.7, 0.9]$  will improve our knowledge of the PDF at  $x \sim 1$  by more than 20%. This region is relevant for DUNE and for high-mass, new-physics searches at the LHC experiments ATLAS and CMS. Given recent progress, such precision may be possible during the coming decade. More difficult, but also under active research, are extensions of the collinear PDFs discussed here: generalized parton distributions and transverse momentum distributions describe short-distance hadron structure in greater detail [408], and their study with lattice QCD has synergy with the electron-ion collider [412].

### C. Hot, dense QCD

As the universe cooled, it passed through a phase transition in which a liquid of quarks and gluons condensed into a gas of hadrons [413]. The high-energy phase, which essentially follows from asymptotic freedom, is known as the quark-gluon plasma (QGP). Two landmark results from lattice QCD are that the transition (at zero baryon density) is a smooth crossover [414, 415] at a temperature around  $T_c \approx 155$  MeV [416–420]. In a world with massless light quarks, the transition would be second order, based on chiral symmetry. Before definitive lattice-QCD studies were available, a first-order transition was often assumed, which would mean that bubbles of hadronic matter would emerge from the QGP as the universe expands. The up, down, and strange masses (i.e., the corresponding quark-Higgs Yukawa couplings) are large enough to soften the transition: no bubbles. The crossover temperature can be directly tested from the freeze-out of particle production in heavy-ion collisions [421]. It is fair to say these results from lattice QCD and experiment have changed our conception of the universe.

At zero temperature, the equation of state has been further elucidated [422–424]. The phase transition might become first order at nonzero baryon density,  $\mu$ , with a line in the  $\mu$ - $T$  plane ending in a critical point. A major focus of QCD thermodynamics now is to find this critical point. The tools of this investigation are lattice QCD and the beam-energy scan of the Relativistic Heavy-Ion Collider at BNL. A coordinated investigation of the phase transition in this region has been devised by experimentalists and theorists, including several members of the U.S. lattice-QCD community [2]. The key challenge for Euclidean gauge theory is that nonzero  $\mu$  implies a quark determinant that is not positive definite and, hence, a sign problem for the Monte Carlo method. The phase diagram must therefore be explored at imaginary  $\mu$  (for which the sign problem goes away) or via Taylor expansions of thermodynamic observables around  $\mu = 0$ , variants of multiparameter reweighting, the density of state method, or a complex Langevin approach.

The study of hot, dense QCD is an enormous subject, and future plans will be spelled out in a future long-range plan for nuclear science, rather than at Snowmass. Some topics of ongoing and near-term interest include the phases and properties of baryon-rich QCD, microscopy of the QGP using heavy-quark probes, the nature of QCD phase transitions, electromagnetic probes of QGP, and jet-energy loss in and viscosities of the QGP [2].

### D. Higgs boson as a portal to new physics

If the measured Higgs-boson branching ratios deviate from the predictions of the Standard Model, speculation will ensue about the true nature of the observed state. One possibility is that it is a composite of more fundamental building blocks that interact via a new strong force [425–428]. The possible composite nature of the observed Higgs boson can be studied in lattice gauge theories with fermion content that slows the running of the gauge coupling, so that it is nearly conformal over several decades of energy scale. Computations of the spectrum of such theories have repeatedly found a light scalar boson, a scalar almost as low in mass as the pseudoscalars [429–437]. This behavior is completely different from QCD, where the scalar (the  $f_0(500)$ , often called the  $\sigma$ ) is a massive, broad resonance, while the pseudoscalars (the pions) are the lightest particles, owing to the Nambu-Goldstone mechanism. For this reason, near-conformal gauge theories are interesting in their own right, as well as being a part of particle-physics phenomenology beyond the Standard Model.

The light scalar boson in these scenarios is often called the “Higgs impostor” because (in part, by design, to comport with LHC measurements) its properties are close to the Standard-Model Higgs boson. To distinguish the composite scenario from the Standard Model, it is interesting to explore the rest of the spectrum. In analogy with QCD and chiral perturbation theory, these results can be mapped to an effective field theory framework to make contact with phenomenology [438–440]. Because it is unlikely that any of the simulated models are realized in nature, it is important to uncover general features [6]. If the additional states (beyond the Higgs) are seen at the LHC, the first step in identifying where to start dedicated studies is by matching these general features. More challenging is a study of the anomalous dimension of four-fermion operators, which are necessary to understand whether the composite scalar boson generates mass for quarks and leptons [426].

If the Higgs boson is the quantum of a fundamental field, as in the Standard Model, it could couple to non-Standard-Model fields. To the extent that such interactions are detected by the Higgs boson’s effect on nucleons, the sigma terms discussed in Sec. IID are relevant; for other hadrons analogous matrix elements are also straightforward to compute. These kinds of QCD matrix elements remain relevant in impostor scenarios too.

## V. COSMIC FRONTIER

Similarly to Higgs physics, lattice gauge theory can play a role in astrophysics and cosmology either through non-QCD confining gauge theories in a dark sector or through QCD itself to determine interaction strengths with Standard-Model matter. Below we mention a few points of contact of lattice calculations that play a supporting role at the cosmic frontier.

In the direct detection of dark matter, the energy transfers are expected to be low enough so that only  $q^2 = 0$  nucleon matrix elements are needed. As discussed in Sec. IID, these are the same matrix elements needed for CLFV. Calculations of the needed quantities, such as  $\sigma_{\pi N}$  and  $\sigma_q$  ( $q \in \{s, c, b, t\}$ ), at the few-percent level are expected to be possible over the next few years, which will solidify limits set on dark matter. As noted in Sec. IID, some choices made in the DM literature for  $\sigma_{\pi N}$  and  $\sigma_s$  suggested bounds that were more aggressive than what the latest results (cf., Fig. 3) support.

Below, three BSM points of interest are discussed: dark hadrons as dark-matter candidates (Sec. VA), the QCD axion (Sec. VB), and the possibility of the dark-hadron thermodynamics having a first-order phase transition (Sec. VC).

### A. Particle-like dark matter

Recently, models of the dark sector with QCD-like confining forces have been examined for their phenomenological viability. To make headway, lattice-gauge-theory calculations of the spectrum of the proposed confining theories have been undertaken. This topic is also noteworthy because it led to collaborations between dark-matter model builders and lattice experts, particularly in the U.S. This body of work is reviewed in Ref. [441].

The underlying strong coupling in a potential composite dark sector precludes the use of perturbation theory for calculating quantities of interest, so that lattice gauge theory is necessary to fully understand the physics of such models. As in QCD, one is interested in the thermodynamics of the dark sector, the spectrum of dark hadrons, and their form factors. The identity of the lightest dark hadron is also an open question: it could be a baryon (a

boson for an even number of dark colors), a meson, or a glueball. Definitive results for dark glueballs probably lie beyond the next few years, but otherwise, exciting developments can be expected in the near term.

## B. Wave-like dark matter

In QCD, the axion is a new field that couples to the strong  $CP$ -violating term in the Lagrangian, in such a way that it can dynamically remove the dependence on  $\theta_{\text{QCD}}$  and  $\arg \det Y$  (cf., Sec. II B 2). With nonzero up-quark mass a firm result from lattice QCD [77, 173–175], the motivation for the QCD axion is strong. In recent years, there have been several works using lattice gauge theory to study axion phenomenology, with some emphasis on cosmology. The axion mass (and decay constant  $f_a$ ) is related to the topological susceptibility  $\chi_t = \int d^4x \langle q(x)q(0) \rangle$  ( $q$  is the topological charge density) by  $m_a^2 f_a^2 = \chi_t$ . The task is then to compute  $\chi_t$  to temperatures well above the QCD phase transition, which has been done for pure-gauge theory [442, 443] and for QCD [444–446]. (See also Ref. [447] for further considerations.) From the (steep,  $\chi_t \sim T^{-8}$ ) fall-off, the axion relic density can be computed and a mass inferred from assuming all dark matter consists of axions [169, 448].

## C. Dark energy and cosmic acceleration

As the universe evolved from the Big Bang, the phase transitions of particle physics influenced the expansion and cooling. If a confining dark sector exists, as in the models mentioned in Sec. V A, then it is important to understand whether the confining transition is a smooth crossover (as it is for QCD with physical up-, down-, and strange-quark masses; cf. Sec. IV C) or a first-order transition (as it would be in QCD with smaller quark masses). Thus, in addition to studying the spectrum of confined dark hadrons, it is useful to study the thermodynamics of these models as well [6], leveraging the extensive experience with QCD [2]. An especially intriguing idea is that the violent behavior accompanying a first-order phase transition of the dark sector would leave an imprint on gravitational waves [449].

# VI. THEORY FRONTIER

This section provides short summaries on topics not covered in detail elsewhere: the connection of lattice supersymmetry to holography, the AdS/CFT correspondence, and string theory (TF01 in Sec. VI A); a short survey on the application of effective field theories in numerical lattice QCD (TF02 in Sec. VI B); and computational work on conformal field theories (TF03 in Sec. VI C).

Material for most of the other topical groups in the Theory Frontier can be found in other sections. In applications to weak decays and the vacuum polarization for the muon  $g - 2$ , lattice QCD is now a precision technique (TF06 in Secs. II A and II B 1). Collider phenomenology is at the Energy and Rare & Precision Frontiers (TF07 in Secs. II and IV). Lattice gauge theories beyond the Standard Model provide information on composite Higgs bosons and composite dark matter (TF08 in Secs. IV D and V A). Section V contains further information related to astroparticle physics and cosmology (TF09): axion properties (Sec. V B) and composite dark sector implications for gravitational waves (Sec. V C). Lat-

tice QCD influences the theory of neutrino physics via inputs to neutrino cross sections (TF11/NF08 in Sec. III).

### A. Supersymmetry and gravity

Because supersymmetry is a spacetime symmetry, it is not straightforward to formulate a lattice field theory with exact supercharges. Recent developments with orbifolding and with topological field theory have, however, made the construction of (some) supersymmetric lattice gauge theories possible [450]. It is now possible to address several nonperturbative questions in supersymmetric field theories.

One set of questions has to do with holography and the gauge/gravity duality, which is often used to relate a strongly coupled (supersymmetric) gauge theory to a weakly coupled and, thus, tractable gravity problem. Lattice supersymmetric Yang-Mills (SYM) simulations start by checking reliable analytic results and then proceed to weaker coupling to learn about strongly coupled gravity. For example, simulations of SYM quantum mechanics agree well with predictions for Dirichlet-0 branes [451]. Similarly,  $2d$  lattice SYM with maximal supersymmetry confirms results of the black-hole–black-string phase transition [452, 453].

The 2019 USQCD whitepaper proposes a few lines of investigation [6]. One avenue of exploration is to test  $S$  duality—the relationship in  $\mathcal{N} = 4$  SYM between  $g^2/4\pi$  and  $4\pi/g^2$ —with numerical simulations. In the Coulomb phase of a model with spontaneous symmetry breaking, the vector boson mass is (as usual) proportional to  $g^2$ , while a monopole in the model has a mass proportional to  $1/g^2$ . Charged particles (electric or magnetic) can be accommodated on a torus with charge-conjugate-periodic boundary conditions [454–456], so commonplace lattice gauge theory calculations yield the masses. Another possibility is to monitor the free energy as a function of  $g^2N$  in large- $N$ ,  $\mathcal{N} = 4$  SYM at nonzero temperature, to test whether the known weak- and strong-coupling limits are connected by a continuous or discontinuous function of  $g^2N$ . A longer-term goal is to study supersymmetric QCD in four dimensions; work in two dimensions [457, 458] may provide a starting point, particularly the Sugino construction [459–461].

Further ideas can be found in Snowmass contributions on lattice  $\mathcal{N} = 4$  SYM [462] and on generalized symmetries in quantum field theory [463]. Researchers who would like to work on numerical lattice supersymmetry can consider a publicly available software package [464] to get started.

### B. Effective field theory techniques

Numerical simulations generate data, which then must be combined to yield a result in the continuum limit and, in the case of QCD, physical quark masses. In principle, the data all have nonzero lattice spacing and (slightly) mistuned quark masses; in practice, some data sets have quark masses that are considerably different from their physical values. A framework is needed to combine the data into final results: that framework is effective field theory [465].

The guide to the continuum limit is the Symanzik effective field theory [466–468], which grew out of Symanzik’s work on renormalization (i.e., the Callan-Symanzik equation) [469]. It posits a renormalized continuum field theory with a local Lagrangian, which is simply the target theory plus higher-dimension operators multiplied by the power of the lat-



tice spacing needed to get back to dimension 4. Symanzik described the formalism for scalar field theories [466–468], while others extended the idea to gauge theories [470–473] and fermions [474, 475]. The Symanzik formalism provides a framework for suppressing discretization effects order-by-order in perturbation theory (known as Symanzik improvement) [476–478] or even by additional powers of the lattice spacing (nonperturbative improvement) [479].

A large fraction of lattice-QCD data is generated with up and down quarks whose mass is larger than physical. The tool for combining data over a range of light-quark masses is chiral perturbation theory ( $\chi$ PT) [480, 481], which incorporates constraints from QCD’s chiral symmetries in the massless limit. Although the original arguments for the chiral effective Lagrangian were generality, the cluster property of correlation functions, analyticity, and unitarity, in lattice QCD unitarity is sometimes broken by choosing different sea and valence quark masses or even different sea and valence discretizations. The jargon for such simulations is “partially quenched” and “mixed action” with corresponding versions of  $\chi$ PT [482–485]. It has been argued that a bounded transfer matrix can substitute for unitarity [486] as a foundational element [481] of  $\chi$ PT. Numerous one-loop calculations have been worked out to support numerical computations; in the most precise cases, two-loop calculations are necessary and available [487].

Finite-volume effects for multihadron states [266, 267] are discussed in Sec. II E in connection with scattering and resonance properties. That work was based on a general massive quantum field theories, which Lüscher had used earlier to demonstrate that the finite-volume effects on single-particle properties are exponentially suppressed [488]. Because physical pions are so light, finite-volume effects in  $\chi$ PT are also considered [489], as well as syntheses of  $\chi$ PT and Lüscher’s approach [490]. Power-law finite-size effects can arise if the system samples topological charge incompletely, another circumstance that can be handled with  $\chi$ PT [491–494]. With some lattice-QCD calculations reaching a precision such that QED effects are relevant, it is also necessary to deal with massless photons in a box; see Refs. [495–497] and a review [498] for more information.

As mentioned in Sec. II E, lattice QCD was part of the motivation for the heavy-quark effective field theories nonrelativistic QCD (NRQCD) [289–291] and heavy-quark effective theory) [292–294]. Discretized versions of NRQCD [289–291] and HQET [499, 500] are used in heavy-quark phenomenology. Effective field theories of heavy quarks are also used to understand and control cutoff effects of the standard fermion formulations [501–506].

Effective field theories can extend the impact of lattice-QCD results in the single-, two-, and few-nucleon sectors to nuclear many-body systems in a systematic manner. For example, nuclear effective field theories organize the two- and few-nucleon interactions and currents at low energies within a given power-counting scheme, assigning them given low-energy coefficients that encode the knowledge of short-distance dynamics that are being integrated out; see Ref. [507] for a recent review. These coefficients, in the absence of experimental data, need to be constrained by direct QCD calculations using lattice QCD. Furthermore, direct matching of lattice QCD to infinite volume can be bypassed by matching finite-volume effective-field-theory calculations directly to lattice-QCD results in the same volume, with the same boundary conditions. Such interplay between lattice QCD and effective field theories, combined with nuclear many-body calculations, is important for many topics discussed in this document: electric dipole moments (Sec. II B 2), charged-lepton-number violation (Sec. II D), neutrino physics (Sec. III), and direct dark-matter detection (Sec. V A).

### C. Conformal field theory

Conformal symmetry plays an important role in the composite Higgs models discussed in Sec. IV D, at least as a limiting behavior. The methods of numerical lattice field theory are widely applied to conformal systems as theoretically interesting quantum field theories, perhaps with real applications in condensed-matter or statistical physics. A famous example is the computation of the critical exponents of the three-dimension  $O(2)$  model [508, 509], one of which disagreed with a comparably precise experiment (on the space shuttle) [510], only to be confirmed by the numerical conformal bootstrap [511].

Of course, both the lattice and the finite spacetime volume break conformal invariance explicitly. Universality (in the sense of critical phenomena) can wash out the discretization (as in real crystals at second-order phase transitions), and well-established relations from finite-size scaling are used to treat the finite box size; see, for example, Ref. [512]. The lattice community is developing new general purpose tools for studying conformal field theories numerically, for example the gradient-flow renormalization group [513–517] and radial quantization [518–521].

Further details can be found in the USQCD whitepaper [6] and (for the complementary numerical conformal bootstrap) in a Snowmass contribution [522].

## VII. SUMMARY & OUTLOOK

The preceding sections outline a program of lattice-QCD and -BSM calculations designed to make an impact on the experimental program in high-energy physics. To summarize many of the calculations needed, Table I lists several specific quantities (grouped into rough categories) together with forecasted precision targets over the coming decade. As “forecasts”, they are contingent on many uncontrollable factors, especially funding for research and allocations of computer time. Historically, the least accurate USQCD forecasts have been for multiyear calculations abandoned by junior researchers taking jobs outside the field.

The first column of Table I lists categories, with links to the sections in which they are discussed, and the second column lists quantities of interest. Here,  $a_\mu = (g - 2)_\mu/2$  is the anomalous magnetic moment of the muon,  $f(q^2)$  denotes form factors for the process in the superscript,  $\Delta M$  the mass difference of a neutral-meson system, and  $\epsilon^{(\prime)}$  is well-established notation for kaon  $CP$  violation. The nucleon matrix elements are isovector axial, tensor, and scalar charges; the “sigma” terms (defined in Sec. II D); radii of nucleon form factors and axial form factor  $F_A(q^2)$  itself. The third column of Table I provides these forecasts, and the fourth column the corresponding experiments.

In many cases, the feasible precision matches that of the relevant experimental measurements. In some cases (marked with an asterisk), the corresponding experiments require better precision than that possible in the near term. These are simply more challenging computationally, and they represent a minimal set of topics in lattice gauge theory that will remain relevant to particle physics beyond the coming decade. In further cases (labeled “NA”), precision is not the right metric; instead some aspect of the dynamics of gauge theories must be understood via a synthesis of complementary experimental, theoretical, and numerical information. For example, in QCD spectroscopy the structure (e.g., tetraquark vs. molecule) of exotic hadrons is more interesting than absolute precision in the mass; in BSM spectroscopy, the main issues are the separation of a light scalar (the Higgs imposter) from the rest of the spectrum and the imposter’s couplings to Standard-Model particles.



TABLE I. Lattice-QCD calculations supporting the U.S. and worldwide program in particle physics, with target precision over the coming few years. An asterisk \* indicates that the target precision *falls short* of the experimental uncertainty.

Category	Milestone	Target precision	Experiment(s)
$a_\mu = (g_\mu - 2)/2$ (Sec. II B 1)	$a_\mu^{\text{HVP, LO}}$	0.5%	Muon $g - 2$ (E989)
	$a_\mu^{\text{HVP, NLO+NNLO}}$	1%	Muon $g - 2$ (E989)
	$a_\mu^{\text{HLbL}}$	10%	Muon $g - 2$ (E989)
CKM $B$ & $D$ physics (Sec. II A 1)	$f^{D \rightarrow \pi, K}(q^2)$	1%	Belle II, BES III
	$f^{B \rightarrow D^{(*)}}(q^2)$	1%	Belle II
	$f^{B \rightarrow \pi}(q^2)$	2%	Belle II
	$f^{\Lambda_b \rightarrow p/\Lambda_c}(q^2)$	2%	LHCb
FCNC $B$ physics (Sec. II A 1)	$f^{B \rightarrow K}(q^2)$	2%	Belle II, LHCb, ATLAS, CMS
	$f^{B \rightarrow K^*}(q^2)$	10%*	Belle II, LHCb, ATLAS, CMS
	$f^{\Lambda_b \rightarrow \Lambda}(q^2)$	2%	LHCb
	$\Delta M_{B(s)}$	5%*	Belle II, LHCb, BaBar
$K$ physics (Sec. II A 2)	$f^{K \rightarrow \pi}(0)$	0.1%	First-row CKM unitarity
	$\Delta M_K$	20%*	KTeV, NA48
	$\epsilon'/\epsilon$	15%	KTeV, NA48
	$K \rightarrow \pi \nu \bar{\nu}$	3%	NA62, K0T0
Nucleon matrix elements (Secs. II D and V) (Sec. III) (Secs. III and IV B) (Sec. II C) (Sec. II B 2)	Nucleon $g_A^{u-d}$	1%*	Neutron lifetime puzzle
	Nucleon $g_T^{u-d}$	1%	UCNB, Nab
	Nucleon $g_S^{u-d}$	3%	UCNB, Nab
	$\sigma_{\pi N}, \sigma_s$	5%	Mu2e, LZ, CDMS
	Nucleon $r_E, r_M, r_A$	5%	DUNE, MicroBooNE, NOvA, T2K
	Nucleon $F_A(q^2)$	8%	DUNE, MicroBooNE, NOvA, T2K
	Nucleon tensor	20%	DUNE, MicroBooNE, NOvA, T2K
	Nucleon PDFs	12%*	ATLAS, CMS, DUNE, EIC expts
	Proton decay	10%	DUNE, HyperK
	$nn \rightarrow pp$	50%*	EXO, other $0\nu\beta\beta$ experiments
Higgs + BSM (Sec. IV D) (Sec. V A) (Sec. IV A) (Sec. VI A)	Nucleon EDM	10%*	Neutron, proton EDM experiments
	$g_{A,T,S}, 1 < A \leq 4$	20%*	All neutrino, DM, EDM, ...
	Light BSM spectrum	NA	ATLAS, CMS
	Anomalous dimension	NA	ATLAS, CMS
	Composite DM	NA	LZ, CDMS
Spectroscopy (Sec. II E)	$\alpha_s(m_Z)$	0.3%	ATLAS, CMS, FCC, ILC
	Susy	NA	ATLAS, CMS
	$XYZ$	NA	Belle (II), LHCb, BaBar, CDF, D0
Heavy ions (Sec. IV C)	pentaquarks	NA	LHCb
	exotic light hadrons	NA	BES III, CLAS, COMPASS, GlueX
	QCD phase transition	NA	(s)PHENIX, ALICE, ATLAS, CMS

Some quantities (e.g., quark masses and decay constants of pseudoscalar mesons) are not listed in Table I because current precision suffices for the time being.

Almost everything will rely on the mid-scale computers at BNL, Fermilab, and JLab that USQCD administers. Many of them also require leadership-class facilities. The underlying reason is simple: lattice gauge theory calculations proceed through a sequence of lattices with finer and finer spacings and, hence, larger and larger lattices. The smaller, coarser lattices are the first steps, both in developing innovative ideas and in beginning an “industrial-strength” campaign of aimed at a specific result. Only exploratory work (i.e., new topics not in Table I) can be completed in a few months to a year. To make an impact on experiment require multiyear campaigns spread over many computing facilities.

Common to all numerical lattice-gauge-theory analyses are ensembles of gauge-field configurations. Many such ensembles already exist with  $2 + 1 + 1$  flavors<sup>9</sup> of sea quark from the MIMD Lattice Computation (MILC) Collaboration [25, 353, 354] and the Extended Twisted Mass (ETM) Collaboration [523, 524], and with  $2 + 1$  flavors of sea quark from the RIKEN Brookhaven Columbia and United Kingdom QCD (RBC/UKQCD) Collaborations [525–527], the Coordinated Lattice Simulations (CLS) consortium [528, 529], and a similar effort in the U.S. [530]. These sets of ensembles will be the starting point for the physics calculations discussed throughout this contribution. For the most precise calculations, additional ensembles with  $1 + 1 + 1 + 1$  flavors and/or explicit photon fields will be generated.

Table I suffers from the serious shortcoming that it does not highlight exploration and innovation. Many lattice-QCD calculations are underway or in a stage of development that makes forecasts impossible. For example, transverse momentum distributions are similar to but more difficult than the collinear PDFs in the table. The transverse motion they describe may be relevant when the precision on the  $W$ -boson mass reaches that of the 2022 measurement from CDF [531]. PDFs are challenging enough: adding another layer of complexity is exciting to think through but postpones calculations of direct relevance to experiment. Calculations for the muon anomalous magnetic moment,  $a_\mu$ , are an example from recent history. As little as ten years ago, exploration had begun but it was not clear whether useful calculations could be carried out. Innovative methods were developed on mid-sized computer systems to bring us within reach of the precision needed by the current Fermilab and future JPARC experiments. It should also be noted that the enthusiasm for lattice expressed by the from  $g - 2$  experimental community inspired both new ideas and hard work.

## Appendix A: USQCD Collaboration

USQCD is a collaboration of almost all high-energy and nuclear physicists in the United States who are working on lattice gauge theory. Around 100 of USQCD’s 170 members are involved in numerical projects at any given time. The USQCD website [532] covers all aspects of the USQCD collaboration and includes the [charter](#), the [code of conduct](#), and the current [list of members](#).

Overall leadership of USQCD is vested in its Executive Committee (EC). This committee was established in 1999, with encouragement from the DOE, to organize the community,

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<sup>9</sup> The notation  $2 + 1$  means two equal-mass quarks, for up and down, with another tuned to the strange quark;  $2 + 1 + 1$  adds charm to the sea;  $1 + 1 + 1 + 1$  implies the different masses for up and down.

develop plans for the infrastructure, obtain funding to carry out these plans and oversee the implementation of them. There are nine standing members, who rotate at the rate of roughly one replacement per year. For example, in 2018 there were three changes, in 2017, 2019, and 2021 there were none, and in 2020 there was one. For the past six years, one member of USQCD has been an early-career scientist elected by the USQCD membership (apart from students). The current EC members are Robert Edwards (Chair, and USQCD Spokesperson), Thomas Blum (Deputy), Tanmoy Bhattacharya (*ex officio*), Norman Christ, Carleton DeTar, William Detmold, Anna Hasenfratz, Andreas Kronfeld, Huey-Wen Lin (elected), Swagato Mukherjee, and Kostas Orginos.

The principle role of the EC is to prepare proposals for mid-scale computing clusters to the DOE Offices of High Energy Physics (HEP) and Nuclear Physics (NP), followed by oversight of said systems. For many years, HEP and NP funded a single project that designed, procured, and operated dedicated clusters for the U.S. lattice-QCD community. NP continues with this model, deploying clusters at Jefferson Lab. HEP has moved to a different model, known as the institutional cluster, in which Fermilab and BNL design, procure, and operate the cluster, while the LQCD project purchases access to a certain number of nodes each year. With an institutional cluster, there are typically several communities purchasing access. In this way, nodes are only idle if all parts of a large, broad user base are in a lull.

The EC also coordinates proposals for software and algorithm development. For approximately 20 years, the main funding stream has been the Scientific Discovery through Advanced Computing (SciDAC) program, which is a partnership between the DOE Office for Advanced Scientific Computing Research (ASCR) and HEP and/or NP. Over the past several years, USQCD has also been part of the Exascale Computing Project (ECP). The software created under the SciDAC grants has greatly enhanced the effectiveness with which USQCD use the hardware resources, whether leadership-class or clusters. Software development continues under SciDAC 4 (NP only) and the ECP. All of the software developed under the SciDAC grants is publicly available, and can be found at <https://usqcd-software.github.io/>. At present, a NP-ASCR SciDAC 4 project is coming to a close, a proposal to the HEP-ASCR SciDAC 5 funding opportunity was recently awarded, and a proposal to the NP-ASCR SciDAC 5 funding opportunity has been submitted.

The EC appoints the Scientific Program Committee (SPC), which plays a major role in setting scientific priorities and allocating USQCD resources. Members serve terms of 3–4 years. The current members are Tanmoy Bhattacharya (Los Alamos, Chair), Alexei Bazavov (Michigan State), Martha Constantinou (Temple), George Fleming (Yale), Jack Laiho (Syracuse), Meifeng Lin (BNL), and Sergey Syritsyn (Stony Brook). The SPC Chair is an *ex officio* member of the EC. Annually, the SPC issues a call for proposals for computer time on the mid-scale computer clusters and long-term storage. As part of its deliberations, the SPC organizes the annual USQCD All Hands’ Meeting (AHM), to share its thinking and receive input from collaboration members. The AHM also provides structured dialog between the EC and collaboration members.

The EC and the SPC solicit advice from the Scientific Advisory Board (SAB) consisting of experimenters and phenomenologists in the various subfields of high energy and nuclear physics that depend on lattice-gauge-theory calculations. The current members of the SAB are Ayana Arce (Duke, ATLAS), Roy Briere (Carnegie Mellon, BES III, Belle II), Abhay Deshpande (Stony Brook, PHENIX, EIC), Lawrence Gibbons (Cornell, Muon  $g - 2$ , CMS), Kendall Mahn (Michigan State, T2K, DUNE), Krishna Rajagopal (MIT, theory), Matthew

Shepherd (Indiana, GlueX, BES III), and Jure Zupan (University of Cincinnati, theory).

In February 2020, USQCD founded a Committee on Diversity, Equity, and Inclusion (CDEI). The current members of the CDEI are Will Detmold (MIT, chair), Kimmy Cushman (Yale), Joel Giedt (RPI), Robert Edwards (*ex officio*, EC Chair), Aida El-Khadra (UIUC), and Huey-Wen Lin (MSU). The committee has conducted a survey on the climate in the USQCD collaboration and is currently analyzing the results. A similar survey was conducted in 2018 at the International Symposium on Lattice Field Theory, with results reported in the proceedings [533].

## Appendix B: Computing Landscape

To supplement remarks about computing in the rest of this document, it may be helpful to survey the landscape of lattice-gauge-theory research in the United States. As discussed above, understanding the long-distance properties of QCD is crucial to the scientific missions of both HEP and NP. Consequently, funding for scientists and computing comes from both Offices. Thus, both provide funding for mid-sized computing projects aimed at lattice QCD and other gauge theories. The HEP initiative, known as the Lattice QCD Infrastructure Research Program extension III (LQCD), allows USQCD to purchase resources from the institutional clusters at BNL and Fermilab. The NP initiative, known as the Nuclear and Particle Physics Lattice-QCD Computing Initiative (NPPLC), designs and builds dedicated clusters at JLab. The difference between “institutional” and “dedicated” has to do with the funding model, without impact on the science. All three sites operate, as a rule, mix of CPU and GPU clusters, and they support long-range storage of large, valuable files of broad community interest.

The BNL, Fermilab, and Jlab clusters are a major source of computing for lattice gauge theory in the U.S. Further computer time is available for lattice QCD on some university computing facilities, although the fraction of the total is modest. The largest source of lattice-QCD computing comes from the leadership-computing facilities (LCFs), funded by both the DOE and the NSF. The DOE facilities are the Argonne Leadership Class Facility (ALCF), the Oak Ridge Leadership Class Facility (OLCF), and the National Energy Research Scientific Computing Center (NERSC). Some of the recent, current, and future supercomputers that have had a big impact on lattice QCD are Mira, Theta, and Aurora (ALCF); Titan, Summit, and Frontier (OLCF); and Edison, Cori, and Perlmutter (NERSC). The supercomputers funded and operated by the NSF are located at many universities, for example the Texas Advanced Computing Center (TACC), which houses two computers well-suited for lattice QCD, Frontera and Stampede2.

Computing time at the LCFs is allocated via several calls for proposals. Most of the supercomputers at ALCF and OLCF is allocated annually via the Innovative & Novel Computational Impact on Theory & Experiment (INCITE) program, managed by ALCF and OLCF, aiming to maximize science. Most of the resources at NERSC are allocated annually via the Energy Research Computing Allocations Process (ERCAP) in support of the mission of the DOE Office of Science, with mid-year supplements. Most of the rest of the ALCF and OLCF resources, as well as a small part of NERSC computing, is allocated annually via the ASCR Leadership Computing Challenge (ALCC), in which the other program Offices in the DOE Office of Science (e.g., HEP and NP) have considerable influence. NSF supercomputers are mostly allocated through the Extreme Science and Engineering Discovery Environment (XSEDE) on a quarterly basis. Frontera, however, is allocated separately via

three programs, the largest of which is the annual Leadership Resource Allocation (LRAC) call for proposals. In all cases, the allocation review panels are multidisciplinary.

It is important to appreciate that leadership-class computers and the clusters fill complementary roles. The leadership-class computers are designed for high capability; they are suited for the largest lattices, namely those with the smallest lattice spacing at a large volume, say  $(6\text{ fm})^3$ , or a somewhat coarser lattice spacing with an even larger volume. They are also best suited for mature problems with a highly automated, industrialized workflow, because the queues on leadership-class computers are set up to accommodate such job streams. For lattice gauge theory, high-capability computing consists of Markov chains running as long as several years, involving the solution of many large linear systems of equations (scaling as lattice size  $\times$  lattice size) within every link of the chain. As complicated as this sounds, the atomic operation is three-by-three matrix multiplication (and similar operations), which is the kind of operation any computing device can carry out.

Lattice-QCD results also rely on high-capacity computing for the statistical analysis of millions of small to medium-sized files containing hadron correlation functions. These analyses are the foundation of estimates of systematic uncertainties, so they require close interaction between human researchers and the computer. In this mode, quick turnaround is essential. The USQCD clusters also are of moderate capability, which makes them ideal for developing new ideas into viable computing strategies, which can entail dozens of nontrivial simulations on small or medium-sized lattices. Such workflows would be all but impossible on leadership-class machines. On the other hand, in USQCD's experience the queues of both dedicated and institutional clusters are not only set up to offer the flexibility needed to foster such innovation but also can be refined with little bureaucratic effort in unforeseen circumstances. The LQCD and NPPLC projects have also provided significant computing for excellent proposals from junior researchers (postdocs and even advanced graduate students), who would not yet have the reputation to fare well in competition with senior scientists from all disciplines for access to DOE or NSF leadership-class facilities.

## Appendix C: List of Snowmass Whitepapers

For easy reference, we list here all contributions to the Snowmass Study that mention lattice QCD and/or lattice BSM.

- Properties of  $B$  and  $D$  mesons: lattice [89], phenomenology [47, 48, 90, 91], summaries of experiments [92–94]; new experimental tools [95, 96].
- Properties of kaons and hyperons [111–114].
- Properties of  $\eta^{(\prime)}$  mesons [120].
- Standard-Model prediction of muon  $g - 2$  [149].
- Electric dipole moments [169, 177, 180]
- Baryon-number violation: proton decay and  $n-\bar{n}$  oscillations [197].
- Neutrinoless double-beta decay ( $0\nu\beta\beta$ ) [224].
- Hadron spectroscopy [251, 252].

- Neutrino-nucleus scattering [21, 22, 320]
- Determination of the strong coupling  $\alpha_s$  [356]
- Parton distribution functions: lattice [408]; phenomenology and experiment [410, 411].
- The Electron Ion Collider (EIC) [412].
- Composite Higgs models [428]
- Axion dark matter [448] (connection to EDMs [169])
- Supersymmetric lattice gauge theories [462].
- Generalized symmetries [463].
- Conformal field theories [522].
- Machine learning in lattice field theory [15].
- Quantum information science and quantum computing, including quantum simulation of lattice field theories [16–19].
- Computing needs of numerical lattice gauge theory [14].

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