Computational Resources for Lattice QCD: 2019–2024

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I. INTRODUCTION

This document provides the scientific justification for Field Work Proposal (FWP) FNAL 20-24, the purpose of which is to secure funding for access to institutional clusters at Brookhaven National Laboratory (BNL) and Fermi National Accelerator Laboratory (Fermilab), to be deployed towards numerical simulations of lattice gauge theories, especially lattice QCD. FWP FNAL 20-24 follows the successful LQCD Infrastructure Project (LQCD, FY2005–FY2009) and its two extensions, abbreviated below as LQCD-ext (FY2010–FY2014) and LQCD-ext II (FY2015–FY2019). For lack of a better name, the research program described here is referred to as LQCD-ext III, which is envisioned to cover federal fiscal years FY2020–FY2024.

QCD is pervasive throughout the missions of two parts of the United States Department of Energy's Office of Science (DOE SC): the Office of High Energy Physics (HEP, to which FWP FNAL 20-24 is addressed) and the Office of Nuclear Physics (NP). For NP's mission of hadrons, nuclei, matter in extreme conditions, and violations of fundamental symmetries, the role of long-distance QCD is clear. In the case of HEP, color confinement implies that the detected strongly-interacting particles are always hadrons; further, many experiments use hadrons as a beam or a target. Therefore, many quantities—from the fundamental parameters of QCD to specific hadronic matrix elements—are needed to interpret HEP experiments. In particular, it is necessary to understand QCD at long distances, where the dynamics are nonperturbative. The only general, quantitative tool to study nonperturbative QCD from first principles is numerical lattice gauge theory.

The combination of access to leadership-class computers and USQCD cluster hardware, sharing the common SciDAC software, has allowed U.S.-based researchers to turn lattice QCD into a precision tool. As discussed further below, several quantities of direct relevance to quark-flavor physics and to Higgs physics now have total uncertainties below 1%. During LQCD-ext II, the clusters were the testbed for developing calculations needed for the Standard-Model prediction of the muon's anomalous magnetic moment. These calculations now secure significant leadership-class resources. USQCD clusters have also fostered the development of calculations of nucleon matrix elements, which present new challenges. Some examples are nucleon form factors (crucial for neutrino experiments), parton distribution functions (PDFs, which are key to experiments at the Large Hadron Collider (LHC)), and the strangeness content of the nucleon (pertinent to direct dark-matter detection and muon-to-electron conversion). At the same time, USQCD has used a relatively small fraction of its resources for studying strongly-coupled lattice gauge theories other than QCD. These theories are fascinating in their own right and may find application beyond the Standard Model. Some examples are models of composite dark matter, models containing composite scalar bosons with Higgs-like properties, and supersymmetric lattice gauge theories.

One should bear in mind that many lattice-QCD calculations are important to both DOE Offices. Consider, for example, calculations of the momentum-fraction dependence of PDFs, which are a growing part of lattice-QCD research. From a HEP perspective, PDFs are needed to compute cross sections of *pp* collisions for the LHC; from an NP perspective, the dialog about PDFs between lattice QCD and phenomenology constitutes an important part of the case for a future electron-ion collider. Similarly, some nucleon form factors can be measured in electron-proton experiments—for example, at the Thomas Jefferson National Accelerator Facility (JLab)—and compared with lattice QCD. Additional nucleon form factors are needed for neutrino-oscillation experiments, and lattice-QCD calculations of them can be used as inputs to the experimental analysis.

The rest of this proposal is organized as follows. Section II explains how the USQCD collaboration manages funding from various parts of DOE SC. Section III reviews the key high-energy physics accomplishments made possible by the most recent Project, LQCD-ext II. This discussion sets the stage for the scientific objectives and milestones of LQCD-ext III, which are set out in Sec. IV. Finally, in Sec. V, we summarize the most important aspects of the proposed management of LQCD-ext III. An Appendix provides some information on the USQCD collaboration. Much of the material on achievements and plans is drawn from a series of whitepapers that the USQCD Collaboration posted in April 2019 [1–7].

II. LATTICE-QCD LANDSCAPE

Before discussing scientific accomplishments and plans, it is 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, the earlier projects LQCD, LQCD-ext, and LQCD-ext II were funded jointly by HEP and NP. In January 2019, the funding model at HEP changed from dedicated clusters to institutional clusters (for the distinction, see below), leading to a split of the HEP- and NP-funded efforts. The HEP-funded part retained the LQCD-ext II name and project structure and focused on BNL and Fermilab, while NP began a new research initiative, the Nuclear and Particle Physics Lattice-QCD Computing Initiative (NPPLC), to continue installing dedicated clusters at JLab.

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. In addition to the cluster projects, the major source of lattice-QCD computing comes from the leadership-computing facilities: the Argonne Leadership Class Facility (ALCF), the Oak Ridge Leadership Class Facility (OLCF), the National Energy Research Scientific Computing Center (NERSC), and supercomputers funded and operated by the U.S. National Science Foundation (NSF). A group functioning outside of the USQCD umbrella has access to supercomputers at Lawrence Livermore National Laboratory.

Much, but not all, of these computing resources are coordinated by the USQCD Collaboration [8], which is a federation of many, smaller scientific collaborations. USQCD started when the DOE (HEP, NP, and SciDAC[1]) encouraged several senior lattice-QCD researchers to form a committee to explore ways to collaborate on software and to coordinate computing resources. This committee evolved into the USQCD Executive Committee, which now leads a collaboration of approximately 150 U.S.-based scientists. Resources on the LQCD–LQCD-ext II projects were allocated by USQCD, and now LQCD-ext II and NPPLC have both asked USQCD to allocate their clusters as a unified computing facility.[2] We propose to continue this arrangement for LQCD-ext III.

USQCD also coordinates proposals to the DOE's INCITE program for large grants of time on leadership-class computers at ALCF and OLCF. It does not coordinate proposals to the ALCC program (which also allocates the ALCF and OLCF machines) or proposals to

[1] "SciDAC" stands for the DOE SC Office for Scientific Discovery through Advanced Computing.

[2] This setup is not new: as part of the American Recovery and Reinvestment Act of 2009, NP secured funding for a significant build-out of the JLab clusters in a separate project referred to as LQCD ARRA.

the supercomputers at NERSC or at NSF centers. The constituent scientific collaborations apply, often successfully, to these programs. While USQCD's main scientific goals evolve slowly (at the pace of corresponding opportunities in experimental physics), details are influenced by these external factors. For example, some members might not participate in a given year's annual USQCD Call for Proposals, if their work has received sufficient resources from ALCC, NERSC, NSF, or via overseas collaborators.

The USQCD Collaboration has organized and led community software development, funded through a series of grants from SciDAC and, more recently, through the Exascale Computing Project (ECP). The SciDAC software stack enables optimized codes to run on a variety of hardware: CPUs and GPUs, clusters built from commodity hardware and more specialized supercomputers at national computing centers. The lattice-QCD ECP focuses on the exascale computers scheduled to come on line over the next few years at ALCF, NERSC, and OLCF. The exascale computers will deploy several different compute architectures. Thanks to ECP, USQCD will have software to enable incorporation of the most cost-effective architectures into LQCD-ext III.

It is useful to spell out the difference between the "institutional clusters" being operated at BNL and Fermilab and the "dedicated clusters" of NPPLC and the earlier LQCD projects. A dedicated cluster is procured and operated directly with an infrastructure project's funding. An institutional cluster is procured and operated by the host laboratory, and a research program purchases annually a certain number of node-years. In the first case, all decisions are contained within the project, whereas in the second, the research program negotiates with the host laboratories to optimize computational effectiveness. In practice, the institutional clusters have been designed and procured with USQCD/LQCD-ext II input. The advantage of an institutional cluster is that BNL and Fermilab have several communities requiring high-performance computing (HPC), leading to economies of scale when running a single facility. In addition, the more experienced users of HPC (e.g., the lattice community) can share know-how with those learning to use HPC on an institutional cluster before moving to the leadership-class facilities.

It is important to appreciate that leadership-class computers and the clusters proposed here 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 $(6\ \mathrm{fm})^3$, 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.

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 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.

III. SCIENTIFIC ACCOMPLISHMENTS OF LQCD-ext II

To set the stage for the work proposed below, let us review some of the accomplishments of the most recent five-year project. These, in turn, rest on the foundation from earlier LQCD projects. Taken as a whole, the series of LQCD projects can be seen as a research facility that allowed the U.S. lattice-gauge-theory community to develop lattice QCD into a precision science, while fostering innovation and the exploration in new ideas. To show the connection to the Particle Physics Project Prioritization Panel (P5) plan for high-energy physics [9], we organize the section around the five science drivers spelled out in the P5 report: use the Higgs boson as a new tool for discovery (Sec. III A); pursue the physics associated with neutrino mass (Sec. III B); identify the new physics of dark matter (Sec. III C); understand cosmic acceleration, namely dark energy and inflation (Sec. III D); explore the unknown: new particles, interactions, and physical principles (Sec. III E). Finally, Sec. III F briefly describes highlights from the nuclear-physics side of the LQCD-ext II and NPPLC program.

A. The Higgs boson as a new tool for discovery

The 2012 discovery of the Higgs-like resonance at 126 GeV by the ATLAS [10] and CMS [11] experiments at the Large Hadron Collider (LHC) provided a watershed insight into the origin of electroweak symmetry breaking. Three sets of recent lattice-QCD results help turn experimental studies of this particle into a tool for discovery. First are analyses that determine from hadronic properties the strong coupling α_s [12, 13][3] and the quark masses [12–17], particularly those of charm and bottom. In both cases, several methods yield consistent results, with uncertainties below the percent level. Figure 1 shows comparisons of recent lattice-QCD results for the charm- and bottom-quark masses, compiled by the Flavor Lattice Averaging Group [18]. As one looks forward to future e^+e^- colliders at energies needed for Higgs production [19], some refinement in the precision of α_s is warranted, but the present level of precision in the quark masses sufficient.[4] These quantities are needed to confront measurements of Higgs-boson branching ratios with Standard-Model predictions. 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 [16].

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 [20–22]. One component of the recent USQCD program is the study of 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 [23–26]. This behavior is completely different from QCD, where the scalar (the $f_0(500)$, often called the σ) is a massive, broad resonance, while the pseudoscalars (the

[3] In this section, the lattice-QCD results we cite are those enabled by LQCD-ext II.

[4] Confirming determinations of quark masses with domain-wall or clover-Wilson quarks are still worthwhile.

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.

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). Following a new suggestion of Ji [27], a new class of nucleon matrix elements have attracted a lot of attention theoretically [28–34] and, especially from members of USQCD, numerically [35–38]. (More references can be found in recent reviews [39–41].) While these matrix elements do not yield the PDFs directly, the two quantities are related by a matching calculation that, after suitable renormalization of the lattice matrix elements, can be obtained in continuum perturbative QCD. This research direction is still exploratory but poised for more ambitious calculations in the future.

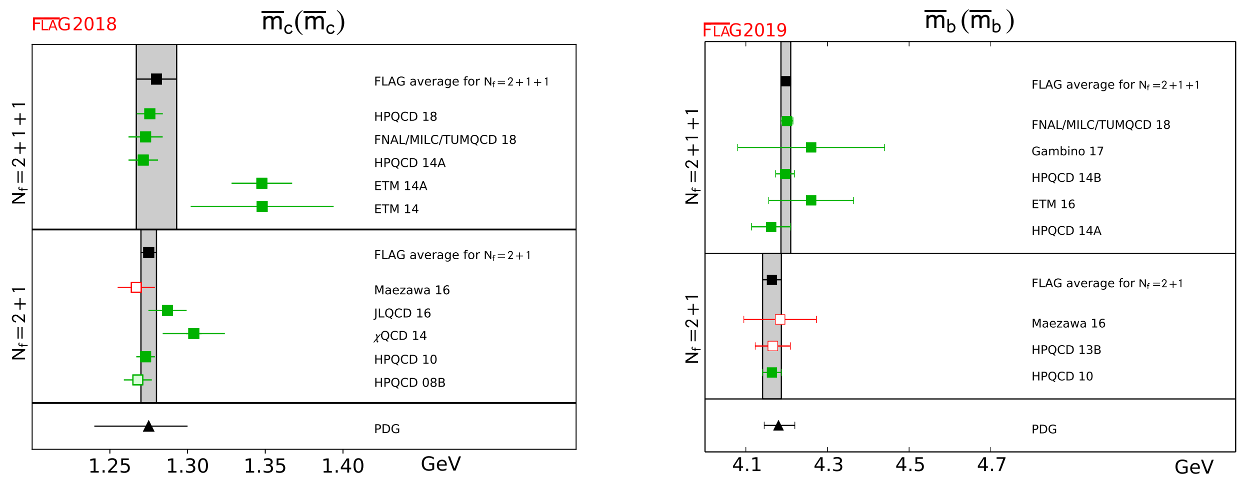

FIG. 1. Comparisons of charm (left) and bottom (right) quark masses, from Ref. [18]. Green symbols are included in the averages (gray bands); red symbols fall short of certain criteria and are omitted. Entries labeled "HPQCD" [14, 17], "FNAL/MILC/TUMQCD" [16], "χQCD" [15], and "Maezawa" [12] have used LQCD-ext II resources. Reference [13] appeared after the deadline for FLAG 2019.

B. Physics associated with neutrino mass

The physics associated with neutrino mass 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. The neutrino energy cannot be measured directly, and it is difficult or impossible to reconstruct the neutrino energy without a model of the nuclear physics of the neutrino-nucleus interaction [42, 43], because the energy of the struck nucleus also is not measured. Scattering amplitudes at the *nucleon* level are necessary ingredients to these models [3], whose uncertainties are extremely difficult to estimate [44, 45].

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 (with both high-energy and nuclear leanings) have studied this form factor's normalization and shape [46–52]. While the precision achieved so far is considerably less than for meson form factors, discussed below, the combination of increased computer power and the increased interest (stemming from the neutrino experiments) will lead to rapid progress. As illustrated in Fig. 2, lattice-QCD calculations [52] of the isovector electric, $G_E(Q^2)$, and axial, $F_A(Q^2)$, form factors are close to controlling all sources of systematic uncertainty.

Two additional CP-violating phases can arise if neutrinos are Majorana particles. The Majorana nature can be explored via the neutrinoless double-beta ($0\nu\beta\beta$) decay of certain nuclei. Relating the observations (limits or, eventually, discovery) to the Standard Model with Majorana neutrinos again requires nucleonic matrix elements as ingredients to nuclear many-body theory. Work on these challenging matrix elements began over the past few years in simulations with unphysically massive pions [53, 54]. The push to more realistic calculations is expected to take at least five more years [4].

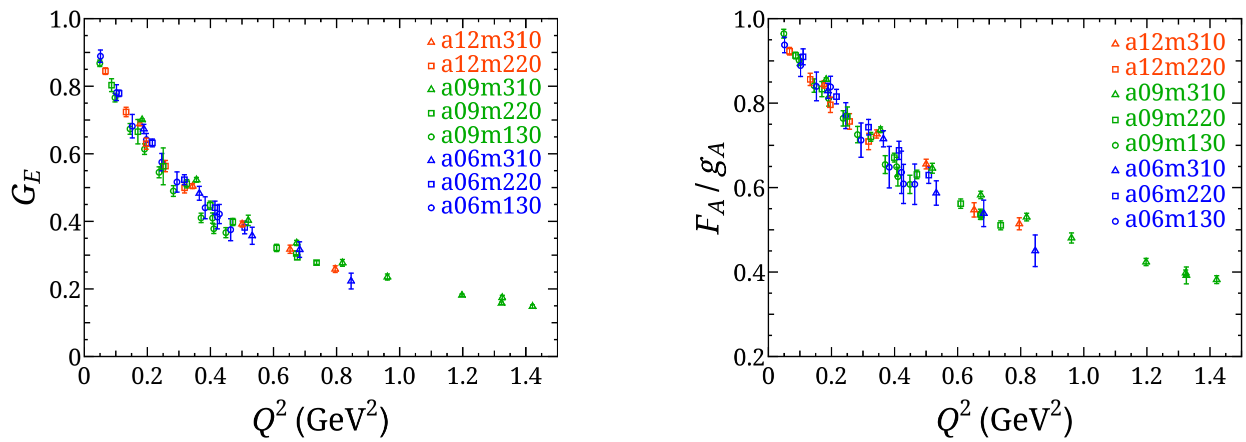

FIG. 2. Electric (left) and isovector axial (right) form factors of the nucleon vs squared momentum transfer $Q^2 = -q^2$. Plots from Ref. [3] based on data from USQCD members PNDME [52].

C. New physics of dark matter

The interplay between lattice-QCD calculations of nucleon properties and nuclear many-body theory, introduced above for neutrinos, arises in many places. 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. On the other hand, the interaction may be flavor singlet, so in addition to the "connected" diagrams needed for isovector (i.e., charged current) processes, a class of computationally challenging "disconnected" diagrams are also needed.[5]

For spin-independent dark-matter detection, the most important nucleonic quantities are $\sigma_{\pi N} = \frac{1}{2}(m_u + m_d)\langle N|(\bar{u}u + \bar{d}d)|N\rangle$, the strangeness content $\sigma_s = m_s\langle N|\bar{s}s|N\rangle$, and the ratio

[5] The terminology "(dis)connected" refers to quark lines—in lattice-QCD simulations the gluon field is treated nonperturbatively. In a disconnected diagram, the vertex of the dark-matter mediator with the struck quark appears not on a valence quark but on a sea quark. These diagrams entail the propagation of a quark from anywhere in spacetime to everywhere and back again. To be computationally feasible, noisy sources are needed; in the end these diagrams are still more demanding than valence propagators and introduce more noise.

$\langle N|(\bar{u}u-\bar{d}d)|N\rangle/\langle N|(\bar{u}u+\bar{d}d)|N\rangle$. Before lattice-QCD calculations became available [55–58], 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 clearly are needed. Note that the same matrix elements are needed to set bounds (or interpret a signal) in muon-to-electron conversion near a nucleus [59], a topic more closely related to the science driver covered in Sec. III E. In addition to the spin-independent matrix elements shown in Fig. 3, spin-dependent matrix elements are also relevant [60] and computable with lattice QCD. First attempts to address nuclear effects on both spin-independent and spin-dependent operators are underway [61].

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. [62].

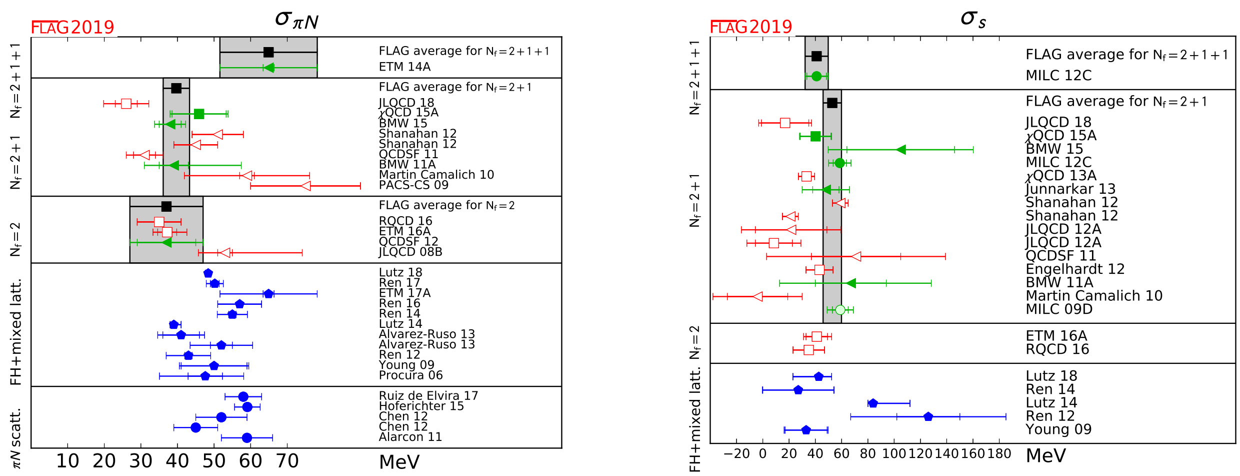

FIG. 3. Comparisons of the "nucleon sigma term" $\sigma_{\pi N}$ (left) and the strangeness content of the nucleon σ_s (right), from Ref. [18]. Green symbols are included in the averages (gray bands); red symbols fall short of certain criteria and are omitted. Entries labeled "χQCD" [58], "Junnarkar" [57], "MILC" [56] (green), and "Engelhardt" [55] (red) used USQCD resources. Blue pentagons denote analyses of several data sets, usually including USQCD data. NB: the $N_f = 2$ results omit the strange sea and are, thus, not recommended for phenomenology.

D. Understand 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 just mentioned, 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) 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 [1], leveraging the extensive experience with QCD [6]. 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 [63].

E. Explore the unknown: New particles, interactions, and physical principles

This science driver is both P5's broadest and the one benefiting most from lattice QCD. U.S. researchers working under the USQCD/LQCD framework have been especially influential in this area [2]. In many cases, a single matrix element, or set of related matrix elements, is needed to interpret a single measurement. In those cases, the role of lattice QCD is especially easy to quantify. Two examples have been given under the Higgs science driver in Sec. III A: the strong coupling α_s, which is obtained from simple observables such as quarkonium correlators and small Wilson loops, and quark masses, which are tuned to reproduce measured meson masses and then renormalized to the customary $\overline{\text{MS}}$ scheme.

QCD correlation functions are needed to compute the hadronic contributions to the anomalous magnetic moment of the muon, which is one of the most precise tests of the Standard Model and places constraints on many extensions of the Standard Model [64]. To obtain these contributions, the hadronic vacuum polarization (HVP) and the much smaller hadronic light-by-light (HLbL) four-point scattering amplitude are convolved with kernels derived in perturbative QED [65, 66]. At the outset of LQCD-ext II, precise calculations of HVP were beginning and work on HLbL was in an exploratory phase. Both began to receive increasingly large allocations on USQCD resources and have also been successful in, for example, the ALCC program. By now, HVP is a mature subject. Figure 4 shows a compilation of results obtaining the HVP from lattice QCD [67–69], from a dispersion relation involving the ratio $R(s) = \sigma(e^+e^- \to \text{hadrons}, s)/\sigma(e^+e^- \to \mu^+\mu^-, s)$ [71–73], and from a combination of the two. These results are compared to the result from the the Standard Model, assuming no new physics and the Glasgow consensus for HLbL [70]. One sees a discrepancy between experiment and the Standard Model (based on $R(s)$) around 3σ. The experiments underway at Fermilab (E989) and planned at J-PARC (E34) aim to improve

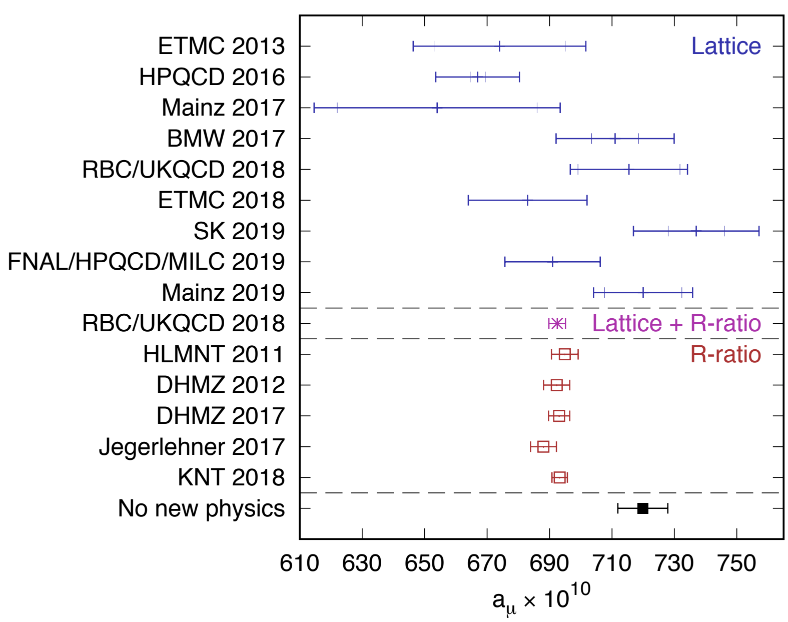

FIG. 4. Comparison of calculations of the full HVP from Ref. [2]. Results labeled "HPQCD" [67], "RBC/UKQCD" [68], and "FNAL/HPQCD/MILC" [69] used USQCD resources. The value with "no new physics" assumes the value for HLbL from the Glasgow consensus [70].

on the current 0.54 ppm measurement at BNL [74] by a factor of four (to 0.14 ppm). Prospects for reducing the uncertainty in lattice QCD hinge mostly on increased computing power although, as discussed in Sec. IV, it remains challenging.

In contrast, lattice-QCD calculations of HLbL may well profit from new ideas. These are needed, because the "Glasgow consensus" employed, for example, in Fig. 4 brackets a set of representative model estimates [70]. Five years ago, the proposal for LQCD-ext II could not guarantee a calculation meeting the needs of the new experiments. The situation changed thanks to a new approach developed during LQCD-ext II [75]. A first result for the value of HLbL from this method [76] suggests that the estimate in Ref. [70] is not so inaccurate that the discrepancy with the Standard Model will go away. Moreover, a lattice-QCD calculation of HLbL delivering the needed precision is now a viable milestone [77].

For many years, lattice QCD has been a vital contributor to quark flavor physics [2]. Here the experiments aim to (over)determine the Cabibbo-Kobayashi-Maskawa (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-, D-, and K-meson decay rates, CP asymmetries, and mixing frequencies of neutral mesons. Amplitudes of leptonic and semileptonic decay decays and neutral-meson mixing have been a major focus throughout every LQCD project and many are now at a watershed, due primarily to USQCD. In particular, the leptonic decay constants of B and D mesons (including those with strangeness) have now reached sub-percent precision [78], 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, because the latter rates are suppressed by the square of the lepton mass. Combined with lattice QCD, they offer the most precise determinations of most of the elements of the CKM matrix: $|V_{us}|$ from $K \to \pi\ell\nu$ [79, 80], $|V_{cd}|$ from $D \to \pi\ell\nu$ [81, 82], $|V_{cs}|$ from $D \to K\ell\nu$ [82, 83], $|V_{ub}|$ from $B \to \pi\ell\nu$ [84, 85], and $|V_{cb}|$ from $B \to D^{(*)}\ell\nu$ [86–89]. In some cases, only the normalization of the corresponding form factors is computed, but for $B \to \pi\ell\nu$ [84, 85] and $B \to D\ell\nu$ [87, 88] the shape, namely the dependence on the lepton-pair invariant mass q^2, is available too; for $B \to D^*\ell\nu$, the shape will be published soon [90]. A sample joint fit to the lattice-QCD and experimental shapes is shown in Fig. 5 (left) [85], with a floating normalization that yields $|V_{ub}|$. Further information on $|V_{ub}|/|V_{cb}|$ comes from the ratio of b-flavored baryon decay distributions using form factors from lattice QCD [91].

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. In lattice QCD, such calculations [92–94] are an offshoot of those just discussed for CKM determination. A sample result relying on lattice QCD is shown in Fig. 5 (right) [93], namely the q^2 distribution for the FCNC decay $B \to K\mu^+\mu^-$, where q is the four-momentum of the $\mu^+\mu^-$ pair. The experimental results from BaBar, Belle, CDF, and LHCb lie 1.8σ (2.2σ) below the prediction, for q^2 below the J/ψ (above the $\psi(2S)$) resonance. Note that the uncertainty from the form factors dominates the error in the prediction.

Neutral-meson mixing entails the oscillation frequency, ΔM_P from particle P to antiparticle $\bar{P}$, and, as is often the case with frequencies, the measurements are very precise. 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 processes are dominated by short-distance virtual particles, leading to local four-quark operators. In contrast to the semileptonic decays discussed above, the precision of lattice-QCD calculations of these quantities have lagged experiment. During LQCD-ext II, USQCD fostered significant improvement of all five operators that could mediate $B_{(s)}$-$\bar{B}_{(s)}$ mixing in the Standard Model and any extension thereof [95]. Similarly to the FCNC decays, the Standard-Model prediction for ΔM_{B^0} (ΔM_{B_s}) is 1.8σ (1.1σ) larger than the corresponding measurements.

In addition to the same kind of short-distance processes, K^0-$\bar{K}^0$ and D^0-$\bar{D}^0$ oscillations are also mediated by long-distance processes [96], such as $K^0 \to \pi\pi \to \bar{K}^0$ or $D^0 \to \pi K \to \bar{D}^0$. Lattice-QCD must employ a finite volume (the 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 $K \to \pi\pi$ [97]. First calculations of the long-distance contribution to ΔM_K were made possible by LQCD-ext II although again the precision achieved so far again lags that of experiment [98]. These calculations are part of a broader campaign to study the $K \to \pi\pi$ reaction. For example, during LQCD-ext II, the first lattice-QCD calculation with a complete error budget of the quantity $\mathrm{Re}(\epsilon'/\epsilon)$, which quantifies direct CP violation, appeared [99]. Although the errors are still large, the result is in tension with the 2002 measurements of the KTeV [100] and NA48 [101] experiments (at Fermilab and CERN, respectively).

Finally, several calculations of nucleon properties should be mentioned. As a rule [102, 103], nucleon correlation functions are noisier than the 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 (nonzero EDMs violate CP) [104–107], proton-decay form factors [108], and the first calculation of operators that could induce neutron-antineutron ($n\bar{n}$) oscillations [109, 110]. The $n\bar{n}$ matrix elements turn out to be 5–10 times larger than had previously been estimated using MIT bag model results and, thus, extend the reach of current and future experiments.

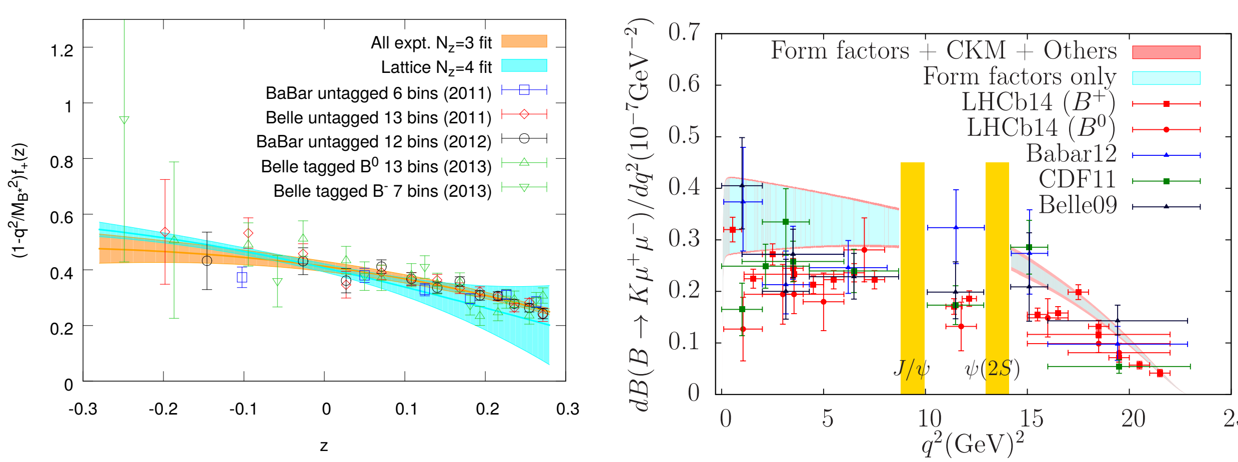

FIG. 5. Semileptonic decays $B \to \pi\ell\nu$ [85] (left) and $B \to K\ell^+\ell^-$ (right) [92, 93]. A joint fit to experimental and lattice data yields the CKM element $|V_{ub}|$ (left); the measured rate for $B \to K\mu^+\mu^-$ falls short of the Standard-Model prediction (right), an example of the anomalies seen in several semileptonic B decays. The variable z in the left panel is related to q^2 by a conformal mapping; see, for example, Ref. [85].

F. Nuclear physics

The nuclear-physics efforts in LQCD-ext II produced many interesting results, without which a discussion of USQCD accomplishments would not be complete. Full details are covered in USQCD's whitepapers "Hadrons and nuclei" [5], "Hot, dense QCD" [6], and "The role of lattice QCD in searches for violations of fundamental symmetries and signals for new physics" [4]. Here a small subset of this program is highlighted.

One of the focuses of the JLab experimental program is spectroscopy [111, 112], which has inspired wide ranging lattice-QCD studies of hadron spectroscopy. The HEP experiments Belle, BaBar, CDF, D0, and LHCb, have also made remarkable discoveries of new hadrons, for example the XYZ states in the charmonium region and the recently observed pentaquark state. In the context of U.S.-based lattice QCD, it is NP-leaning colleagues whose broad spectroscopy program will eventually address these states.

As the universe cooled, it passed through a phase transition in which a liquid of quarks and gluons condensed into a gas of hadrons [113]. A textbook result from lattice QCD is that this transition is a smooth crossover, not a first-order transition as had been assumed on the basis of chiral symmetry. In fact, for massless up, down, and strange quarks, the transition *is* first order, but the quark masses (i.e., the quark-Higgs Yukawa couplings) are just large enough to soften the transition. A major focus of QCD thermodynamics now is to find out whether there is a critical point at nonzero baryon chemical potential, where the transition becomes first order. 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 USQCD [6].

IV. SCIENTIFIC OBJECTIVES OF LQCD-ext III

The objective of LQCD-ext III is to enable numerical studies of QCD and BSM theories of the breadth and precision needed to have an important impact on high-energy physics. The full range of possibilities for the coming 5–10 years have been spelled out in the USQCD Collaboration's whitepapers on the physics program [1–6] and computing landscape [7].

This section narrows the focus to five milestones:

- complete calculations of the HVP and HLbL contributions to muon $g - 2$ with the required precision on the timescale of Fermilab E989;
- continue to sharpen the search for new physics in the quark-flavor sector;
- develop a program of precision nucleon matrix elements with comprehensive error budgets;
- continue the exploration of gauge theories other than QCD;
- provide a platform for innovation on these and further relevant areas.

Specific calculations supporting these milestones are listed in Tables I and II, below.

A. Muon anomalous magnetic moment

Fermilab E989, the experiment underway at Fermilab, aims to reduce the experimental uncertainty on the muon's anomalous magnetic moment to 0.14 ppm. This suggests precision targets of 0.2%, 10%, and 10% for the leading-order HVP, higher-order HVP, and HLbL, respectively. Even with exascale resources, it will be extremely difficult to attain a single such precise calculation for the leading-order HVP, $a_\mu^{\text{HVP, LO}}$. In particular, effects of isospin breaking are needed, requiring additional ensemble generation (cf. Table II). Within USQCD, however, there are two independent efforts on different ensembles and enough differences in analysis to minimize correlations in the systematic errors. In addition, several similarly promising and separate efforts are underway in Europe [114–116] and Japan [117]. These calculations will receive rigorous scrutiny from the Muon $g-2$ Theory Initiative [118] and from FLAG. These groups will produce averages of these results that may hit the target. The higher-order HVP, $a_\mu^{\text{HVP, HO}}$, comes from the same QCD calculation albeit folded with a higher-order QED kernel [69], so the same lattice-QCD work will hit this target too.

As a four-point function, the HLbL contribution is more difficult to compute. It is smaller, however, so the precision target is less demanding. We expect that the new techniques discussed above, combined with new developments from clusters and exascale computing will reach the target in a single calculation. If a second calculation emerges from the USQCD user community, it will be encouraged.

B. Quark flavor physics

The tension observed for several measurements of B decays lends new 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.

Several of the anomalies are in flavor-changing neutral currents (FCNCs). Let us start with $b \to s$ transitions. The differential rate of $B \to K\mu^+\mu^-$, the differential rate and angular distributions of $B \to K^*\mu^+\mu^-$, and ratios of the branching fractions of these two processes relative to the $K^{(*)}e^+e^-$ final state all are in poor agreement with the Standard Model. The pseudoscalar case $B \to K\ell\ell$ is part of a suite of calculations including charged-current processes $B_s \to K\ell\nu$ and $B \to \pi\ell\nu$, discussed below. The K^* decays to $K\pi$, so the amplitude for this process is very challenging. An analysis with the appropriate rigorous finite-volume formalism [119] is underway using LQCD-ext II resources [120], as is an analysis of $B \to \rho(\pi\pi)$. 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.

The measured ratios $R(D^{(*)}) = \text{BR}(B \to D^{(*)}\tau\nu)/\text{BR}(B \to D^{(*)}\ell\nu)$ of charged-current processes also disagree with the Standard Model, by 3σ combined [121]. The Standard-Model prediction of these ratios requires the form factors over the full kinematically allowed range. Results of sufficient precision for the next several years have been published for $R(D)$ [87, 88] and are soon to appear for $R(D^*)$ [90]. Even so, these results will improve, because the relevant form factors are needed to determine the CKM element $|V_{cb}|$.

Neutral-meson mixing is also an FCNC. As discussed above, the associated measurements are of frequencies and are very precise. Further work on the $B_{(s)}$ systems, ΔM_B and ΔM_{B_s}, will resume during LQCD-ext III, and work on the long-distance part of ΔM_K is underway. The long-distance contributions D^0-$\bar{D}^0$ entail multiparticle intermediate states, making this topic an exploratory one that would benefit from theoretical and computational innovations.

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, no new work is required during LQCD-ext III.[4] Some improvement to α_s is desirable and new calculations are underway. The magnitudes of the CKM matrix can be determined from leptonic (e.g., $B \to \tau\nu$) and charged-current semileptonic decays. For leptonic decays, again no new work is required during LQCD-ext III.[4] New calculations of the form factors for $B \to \pi\ell\nu$ and $B \to D^{(*)}\ell\nu$ are needed to match the precision of Belle II for $|V_{ub}|$ and $|V_{cb}|$, respectively. Work is underway using both cluster and INCITE resources for the former, using the same general strategy that made the leptonic decays constants so precise; this work will automatically include semileptonic D decays. Analysis of $B \to D^{(*)}\ell\nu$ will start when the analysis of an older dataset is finished. In addition, there is ongoing effort to support future measurements of b-baryon decays.

In addition to ΔM_K, a few results in kaon physics are needed to get the most out of some older experiments. Even better precision than that now available for the form factor in $K \to \pi\ell\nu$ is needed to resolve a possible 5σ tension in first row of the CKM matrix.[6] Such improvement requires a complete treatment of electromagnetism and isospin breaking via $m_d \neq m_u$, thus requiring the same new ensembles as needed for muon $g-2$. Now that the ingredients of a full calculation of $\mathrm{Re}(\epsilon'/\epsilon)$ are understood, we plan in LQCD-ext III to reach the precision of KTeV and NA48 [100, 101]: $10^4\,\mathrm{Re}(\epsilon'/\epsilon) = 16.6 \pm 2.3$. Last, experiment NA62 is underway to improve BNL E949's measurement of the branching ratio of $K^+ \to \pi^+\nu\bar{\nu}$. 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 [123]. Technology similar to that used for ΔM_K will be used to attain a first-principles result to replace phenomenological estimates currently in use.

C. Nucleon matrix elements

Nucleon matrix elements are the most prominent area in which, from the HEP perspective, conversation and collaboration among nuclear physicists and particle physicists are necessary. Starting with the quenched approximation[7] decades ago, nuclear physicists have carried out calculations of nucleon structure. Meanwhile, particle physicists were developing quark-flavor physics—with mesons—into a precision science with full error budgets. Thus, nuclear physicists' efforts discussed in this section are served by the nuclear-physics side of USQCD's INCITE proposals. Some particle physicists have begun complementary calculations, using the USQCD clusters for computation. To employ these matrix elements to interpret HEP experiments, everyone's expertise will be needed.

This subsection covers many topics—neutrino physics, PDFs, dark-matter detection, fundamental symmetries, and small nuclei—which are labeled for ease of reference.

[6] 5σ is a attained when using a new result for a certain radiative correction in nucleon β decay [122].

[7] The "quenched approximation" omits sea quarks loops and absorbs the leading effect of this omission into the bare couplings.

TABLE I. Calculations supporting the principal milestones of the proposed research program. The meanings of the categories and milestones are explained in the text. The compute percentages reflect 2019 planning and will change in time in response to many external factors. "LCF" refers to the high-energy-physics part of USQCD's resources on the leadership-class computers at ALCF and OLCF. "NP" means that these topics are covered by the nuclear-physics part of USQCD's leadership-class resource. An asterisk * indicates that the target precision *falls short* of the experimental uncertainty.

Category	Milestone	Target precision	Compute %-age LCF	Compute %-age cluster	Experiment(s)
$a_\mu = (g_\mu - 2)/2$	$a_\mu^{\text{HVP, LO}}$	0.5%	10%	4%	Muon $g-2$ (E989)
	$a_\mu^{\text{HVP, HO}}$	10%	with $a_\mu^{\text{HVP, LO}}$		Muon $g-2$ (E989)
	a_μ^{HLbL}	10%	–	2.5%	Muon $g-2$ (E989)
CKM B physics	$f^{B\to D^{(*)}}(q^2)$	1%	10%	2%	Belle II
	$f^{B\to\pi}(q^2)$	2%	10%	5%	Belle II
	$f^{\Lambda_b\to p/\Lambda_c}(q^2)$	2%	–	–	LHCb
FCNC B physics	$f^{B\to K}(q^2)$	2%	with $f^{B\to\pi}(q^2)$		Belle II, LHCb
	$f^{B\to K^*}(q^2)$	10%*	–	–	Belle II, LHCb
	$f^{\Lambda_b\to\Lambda}(q^2)$	2%	–	–	LHCb
	$\Delta M_{B_{(s)}}$	5%*	8%	–	Belle II, LHCb, BaBar, CDF, D0
D physics	$f^{D\to\pi,K}(q^2)$	1%	with $f^{B\to\pi}(q^2)$		Belle II, BES III
K physics	$f^{K\to\pi}(0)$	0.1%	5%	–	First-row CKM unitarity
	ΔM_K	20%*	12%	2.5%	KTeV, NA48
	ϵ'/ϵ	15%	–	2.5%	KTeV, NA48
	$K\to\pi\nu\bar{\nu}$	3%	5%	1%	NA62, K0T0
Nucleon matrix elements	Nucleon g_A^{u-d}	1%*	with $F_A(q^2)$		Neutron lifetime puzzle
	Nucleon g_T^{u-d}	1%	NP	1.5%	UCNB, Nab
	Nucleon g_S^{u-d}	3%	NP	1.5%	UCNB, Nab
	$\sigma_{\pi N}$, σ_s	5%	NP	2%	Mu2e, LZ, CDMS
	Nucleon r_E, r_A	5%	with $F_A(q^2)$		DUNE, MicroBooNE, NOvA, T2K
	Nucleon $F_A(q^2)$	8%	NP	15%	DUNE, MicroBooNE, NOvA, T2K
	Nucleon tensor	20%	NP	3%	DUNE, MicroBooNE, NOvA, T2K
	Nucleon PDFs	12%*	NP	15%	ATLAS, CMS, DUNE
	Proton decay	10%	NP	–	DUNE, HyperK
	$nn\to pp$	50%*	NP	4%	EXO, other $0\nu\beta\beta$ experiments
	Nucleon EDM	10%*	NP	3.5%	Neutron, proton EDM experiments
	$g_{A,T,S}$, $A\le 4$	20%*	NP	3%	All neutrino, DM, EDM, ...

TABLE II. Additional calculations supporting the milestones of the proposed research program. "NA" means that precision is not a useful metric. Other notation is the same as in Table I.

Category	Milestone	Target precision	Compute %-age LCF	cluster	Experiment(s)
Ensemble generation	DWF	–	13%	–	
	HISQ	–	7%	–	
Higgs[a] + BSM	$\alpha_s(m_Z)$	0.3%	with quark flavor		ATLAS, CMS, FCC, ILC
	Light spectrum	NA	10%	2%	ATLAS, CMS
	Anom. dim.	NA	5%	1.5%	ATLAS, CMS
	Composite DM	NA	3%	–	LZ, CDMS
	Susy	NA	2%	1%	ATLAS, CMS
Spectroscopy	XYZ	NA	NP	–	Belle (II), LHCb, BaBar, CDF, D0
	P_c	NA	NP	–	LHCb

[a] Note also the PDFs under "Nucleon matrix elements" in Table I.

1. Neutrino physics

The increasingly central role of neutrino experiments in the U.S. onshore HEP program naturally raises the question of how lattice QCD can contribute [124]. To reiterate Sec. III B, many nucleon-level matrix elements are needed as ingredients to nuclear many-body theory, which in turn is employed to reconstruct the neutrino energy.

The first targets are the radii of the vector and axial form factors, defined by

$$r_i^2 \equiv \frac{6}{F_i(0)} \left. \frac{dF_i}{dq^2} \right|_{q^2=0}, \tag{4.1}$$

where the form factor F_i is either the electric form factor, $G_E(q^2)$, leading to r_E, or the axial form factor, $F_A(q^2)$, leading to r_A. By electric charge conservation, $G_E(0) = 1$, while $F_A(0) = g_A$, the (isovector) axial charge.

The value and justifiable uncertainty on r_A are controversial, with several values quoted in the literature [3]. With minimal assumptions on nuclear modeling and form-factor shape, Ref. [125] finds $r_A = 0.68(16)$. A lattice-QCD calculation [51] (a precursor of the results shown in Fig. 2) obtains $r_A = 0.46(06)$. These results both use a model-independent parametrization of the shape founded on analyticity and unitarity. With more assumptions on the shape of the form factor, uncertainties as small as 3% have been reported [126]. A definitive lattice-QCD calculation with a fully controlled 5% uncertainty will be achievable during LQCD-ext III, and would reduce the uncertainty in the νN quasielastic cross section below the level of other uncertainties [127] and also settle the controversy.

The calculations that yield the axial radius also yield the shape of $F_A(q^2)$ more generally. At larger momentum transfer, $Q^2 \approx 1$ GeV^2, we aim to achieve 8% uncertainty during LQCD-ext III. This uncertainty can be reduced in the future, if warranted.

At DUNE neutrino energies, it is also necessary to understand processes in which additional pions are produced, eventually reaching deep inelastic scattering (DIS). 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, which, as with the nucleon form factors, is used in nuclear many-body theory. Work in this direction has started recently [128]. 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 PDFs, discussed below, will also play a role.

Also important for neutrino scattering is neutral-current elastic scattering. The technical issues run parallel to those for the charged current, except that disconnected diagrams are needed for the isoscalar matrix element. As a consequence, the precision of neutral-current matrix elements will be lower than their connected counterparts.

2. Parton distribution functions

For many years, lattice QCD has been used to compute the first few moments of several PDFs; for reviews, see Ref. [39–41]. The development of the large-momentum effective theory [27] permits a connection between Euclidean lattice QCD and the desired Minkowski distributions. Suitable Fourier, Laplace, or Mellin transforms of kinematic variables yield the PDFs' dependence on the parton momentum fraction x [28–34]. Reference [39], an effort led by USQCD members, demonstrates 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 [35–38], such precision may be possible during LQCD-ext III.

3. Dark-matter detection, muon-to-electron conversion, precision neutron decay

In the Standard Model extended to incorporate neutrino masses and mixing in a minimal way, charged-lepton flavor violation is possible, but unobservably small. Thus, any observation of $\mu A \to eA$, where A is a nucleus, or the related process $\mu \to e\gamma$ would be an unambiguous sign of new physics. 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 $\mu A \to eA$ by four orders of magnitude.

To interpret Mu2e, lattice-QCD calculations of the light- and strange-quark contents of the nucleon are needed [59, 129]. As discussed in Sec. III, these are the same matrix elements needed for direct dark-matter detection. Calculations of the needed flavor-singlet quantities, such as $\sigma_{\pi N}$ and σ_s, at the few-percent level are expected to be possible even with disconnected diagrams.

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, $g_A^{u-d} = 1.2732(23)$ [130], but 1% calculations should be possible and could shed light on the disagreement among neutron-lifetime measurements [131].[8] The tensor and scalar charges at similar precision also will be possible. Calculations of these charges at the 10% level, when combined with β-decay

[8] In fact, 1% precision is claimed already [132], although the tension of this result with that of Ref. [51] (computed on the same ensembles) leads FLAG [18] to quote an "average" with 2.6% error.

measurements, complement the LHC search for new quark interactions, probing effective scales of new physics close to 10 TeV [51, 133, 134].

4. Fundamental symmetries

The large-scale neutrino detectors, DUNE [135] and HyperK [136], will set new limits on baryon-number violation via proton decay and neutron-antineutron oscillations. During LQCD-ext III, calculations of proton-decay matrix elements at the 10-percent level are feasible. A second calculation of n-$\bar{n}$ oscillations is needed to obtain a fuller understanding of the systematic uncertainties, but the 10-percent level again seems feasible.

Permanent EDMs, if observed, are signals of CP violation beyond the Standard Model (because CKM-induced contributions are tiny). Several new experiments aimed at the neutron EDM are planned and a possible experiment aimed at the proton EDM is under discussion [137]. Several matrix elements enter here, the usually neglected CP-violating θ term in QCD and several higher-dimension operators induced by physics at energies at and beyond the weak scale. The isovector quark-EDM-induced neutron and proton EDMs and their isoscalar counterparts are technically straightforward calculations, albeit requiring very high statistics. Many of these matrix elements are challenging, however, making them another exploratory area where innovation will be crucial.

For $0\nu\beta\beta$ decay, the most important near-term calculations are of the $nn \to pp$ process, because the chiral EFT framework [138] requires a low-energy constant that can be determined only via matching to (lattice) QCD. This undertaking will be challenging. Using techniques similar to those developed for $K^+ \to \pi^+\nu\bar{\nu}$ and a_μ^{HLbL}, progress on a "warm-up" calculation of $\pi^- \to \pi^+$ should be pursued first. First results over a range of (unphysical) quark masses will become available in the next 1–2 years.

5. Small nuclei

Beyond the single nucleon, Table I lists a set of matrix elements for small nuclei with atomic number $A \leq 4$. While not a component of this proposal per se, they represent many calculations of the properties of small nuclei that are being carried out by nuclear physicists in USQCD. Calculations of this type are needed to begin testing nuclear models important to many of the experiments discussed in this section. They will probably mature into calculations with full error budgets near the end of LQCD-ext III.

D. Strongly coupled gauge theories beyond the Standard Model

Now that light composite Higgs-like scalar bosons have been seen in the spectrum of several near-conformal gauge theories [23–26], 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 [139–141]. Because it is unlikely that any of the simulated models are realized in nature, it is more important to uncover general features. 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 [21].

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 LQCD-ext III, but otherwise, exciting results can be expected over the next several years.

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 [142]. It is now possible to address several nonperturbative questions in supersymmetric field theories, including the concept of holography encompassing gauge/gravity duality. A computationally straightforward example is to use thermodynamics to test conjectures about the content of a dual string theory, by simulating a supersymmetric pure gauge theory.

E. Innovative projects

By definition, it is impossible to say in advance where unexpected innovations will lie, but in USQCD's experience it is crucial to reserve some cluster computing for such projects. For an example of how USQCD cluster computing has fostered innovation, consider the new idea for the muon $g-2$ HLbL contribution [75], mentioned in Sec. III E. In fact, this idea came from a graduate student's extensive research involving dozens of nontrivial simulations. The underlying problem in earlier approaches was a poor signal-to-noise ratio. After gaining insight into the origin of the problem, various theoretical solutions had to be tested before finding a practical solution. More generally, many of the junior faculty and staff hires in lattice QCD have led USQCD projects, with the opportunity to expose their ideas boosting their careers.

This part of the research program is also where we will study the potential impact of machine learning. The main simulation algorithm of choice for the last thirty years, hybrid Monte Carlo [143],[9] has many internal parameters that affect the efficacy of the Markov chain without changing the physics. During LQCD-ext III, we expect studies exploring how machine learning can be used to tune these parameters. Another prospect is to improve (or replace) this algorithm [144–146]. Further ongoing work studies matrix traces (e.g., for disconnected diagrams) [147] and observables [148]. For more details on these topics and the full computing landscape of lattice QCD, see the USQCD whitepaper on computing [7].

The research program proposed here does not explicitly address quantum information science. Many members of the lattice community are engaged in this direction through other proposals. USQCD has appointed a subcommittee chaired by Martin Savage (University of Washington) to devise a strategy. That said, if USQCD members need small amounts of cluster time, such proposals will be considered seriously.

[9] Invented for lattice QCD, this algorithm is known as Hamiltonian Monte Carlo in other fields.

F. Setting priorities

The stewards of the research program outlined in this proposal are the Executive Committee (EC) and the Scientific Program Committee (SPC) of USQCD. (For current membership, see Appendix A.) As discussed above, many goals are mature enough to use the leadership-class facilities (LCFs). In those cases, the EC will (as in the past) submit proposals to the INCITE program designed to achieve these goals. At present, USQCD holds a collaboration-wide INCITE award on the ALCF machines Mira and Theta as well as two separate INCITE awards for quark- and lepton-flavor physics and for QCD thermodynamics on the OLCF machine Summit. For 2020, USQCD is submitting a unified proposal for all aspects of lattice gauge theory, aimed at Summit and Theta. As noted in the introduction, most of these projects also require cluster computing to turn the LCF outputs (namely, millions of files containing hadron correlation functions) into physics results. The SPC will (as in the past) allocate time on the clusters, both the institutional clusters supported via this proposal and the dedicated clusters at JLab, which are supported by NP's NPPLC initiative. In addition to supporting the INCITE-ready work, the SPC receives and supports dozens of proposals for research limited to small–to–medium-sized lattices that the clusters can capably process.

One should anticipate that new goals will arise during the coming five years, while some may decline in importance. For example, should two groups reach the target precision for $a_\mu^{\text{HVP, LO}}$, this calculation will no longer require such significant resources. If a major discovery is made—either a new particle or a 5σ flavor anomaly—new topics may bubble up or existing ones rise in importance. A new experiment requiring certain lattice-QCD calculations might be approved, again prompting a change in priorities. Finally, one or more of the medium-sized simulations mentioned above may mature into a central part of an INCITE proposal.

USQCD can respond to such changes in three ways. First, the annual discussion with the Scientific Advisory Board (SAB) provides a stimulus to anticipate new developments. For example, the SAB's advice helped guide the contents of the 2019 USQCD whitepapers [1–7]. Further, the DOE's annual review of the research program's technical milestones has always also addressed both the progress towards and the continued relevance of the scientific milestones. Third, the SPC allocation process, being proposal driven, responds to the lattice-QCD user community—each user's expertise is tapped to judge both the importance and feasibility of new calculations.

Finally, the review of this proposal will (as in the past) provide HEP the opportunity to guide USQCD's strategy. In LQCD-ext III and NPPLC, the guidance from HEP and NP has been to pursue the best possible program of lattice-QCD research without undue attention to the distinction between the two Offices' missions. For QCD, this approach makes sense, because so many calculations serve the needs of both Offices. Recall that nucleon form factors and PDFs, in particular, are relevant to HEP and NP: it is worth noting that the SPC's most allocation of cluster time for 2019–2020 is approximately 30:40:30 for HEP:both:NP.

V. MANAGEMENT

Although this document focuses on the science case for funding LQCD-ext III, the proposed research program cannot be completed without sound management. Full details concerning project management can be found in the Program Execution Plan accompanying FWP FNAL 20-24, and further details on USQCD can be found in Appendix A and the website [8], particularly the USQCD Charter.

William Boroski (Fermilab) will be the Program Manager, with overall responsibility for the effort. He will be responsible for negotiating Memoranda of Understanding with the participating laboratories for access to institutional clusters, deciding the optimal distribution of funds, and tracking the technical milestones in FWP FNAL 20-24. He is the key interface to the DOE for financial matters, reporting, and reviews. He will be assisted by the Associate Program Manager, Josephine Fazio (Fermilab). She will be responsible for maintaining documentation, tracking expenditures, and monitoring progress in achieving the FWP FNAL 20-24 milestones. Boroski and Fazio are carrying the same roles for LQCD-ext II; USQCD is very fortunate to be supported by such talented, experienced, and dedicated project managers.

In the institutional-cluster model, the host laboratories have several roles: designing, procuring, building, and operating the clusters. During the institutional-cluster phase of LQCD-ext II, the management team and USQCD have had a constructive relationship, for example participating in the design. Each participating laboratory has a Site Manager, currently Ken Schumacher and Amitoj Singh at Fermilab and Tony Wong at BNL. In addition to their part of the roles listed above, they are the key personnel for user support. At BNL, Robert Mawhinney (Columbia University) serves as a further liaison between the USQCD user community and the laboratory. BNL and Fermilab laboratory management are providing letters in support of this proposal, presenting their view of the interactions between their lab, the research program management, and USQCD.

The Chair of the USQCD Executive Committee, Andreas Kronfeld (Fermilab), serves as the scientific Spokesperson for the effort; Robert Edwards (JLab) serves as Deputy Chair and Deputy Spokesperson. They are the principal points of contact with the DOE on scientific matters. They are also the liaison between the Executive Committee and the research-program management team, relaying the Executive Committee's priorities to the Program Manager, and the Program Manager's progress reports to the Executive Committee. The Program Manager, Associate Program Manager, and Scientific and Deputy Spokespersons meet by conference call with each other and the LQCD-ext II and NPPLC Site Managers approximately every other week to discuss major issues. They report to HEP staff monthly and (with NPPLC personnel) to NP staff quarterly.

Appendix A: The 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 150 members are involved in numerical projects at any given time. The USQCD website [8] covers all aspects of the USQCD collaboration and includes the current list of members.

Overall leadership of USQCD is vested in its Executive Committee (EC), whose current members are the authors of this proposal. This committee was established in 1999, with encouragement from the DOE, to organize the community, develop plans for the infrastructure, obtain funding to carry out these plans and oversee the implementation of them. Membership currently rotates at the rate of roughly one replacement per year. For example, in 2018 there were three changes, but in 2017 and 2019 there were none. For the past four years, one member of USQCD has been an early-career scientist elected by the USQCD membership (apart from students).

The EC appoints the Scientific Program Committee (SPC), which plays a major role in setting scientific priorities and allocating USQCD resources, as described in Sec. IV F. Members serve terms of 3–4 years. The current members are Aida El-Khadra (UIUC, Chair), David Richards (JLab, deputy Chair), Alexei Bazavov (Michigan State), Jack Laiho (Syracuse), Meifeng Lin (BNL), Keh-Fei Liu (Kentucky), and Ethan Neil (Colorado).

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 University, ATLAS), Daniel Cebra (UC Davis, STAR), Lawrence Gibbons (Cornell University, Mu2e), Krishna Rajagopal (MIT, theory), Alan Schwartz (University of Cincinnati, Belle II), Matthew Shepherd (Indiana University, GlueX, BES III), and Jure Zupan (University of Cincinnati, theory).

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/`.

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