Computational Resources for Lattice QCD: FY25 – 29

Robert Edwards[1,*], Thomas Blum[2,†], Norman Christ[3], Carleton DeTar[4], William Detmold[5], Anna Hasenfratz[6], Andreas Kronfeld[7], Swagato Mukherjee[8], Kostas Orginos[9], Peter Petreczky[8], and Phiala Shanahan[5]

[1] *Theory Center, Thomas Jefferson National Accelerator Facility, Newport News, Virginia 23606*
[2] *Department of Physics, University of Connecticut, Storrs, CT 06269*
[3] *Department of Physics, Columbia University, New York, New York 10027*
[4] *Department of Physics and Astronomy, University of Utah, Salt Lake City, Utah 84112*
[5] *Center for Theoretical Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139*
[6] *Department of Physics, University of Colorado, Boulder, Colorado 80309*
[7] *Theoretical Physics Department, Fermi National Accelerator Laboratory, Batavia, Illinois 60510*
[8] *Physics Department, Brookhaven National Laboratory, Upton, New York 11973*
[9] *Department of Physics, College of William and Mary, Williamsburg, Virginia 23187*

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∗ Spokesperson, USQCD, `edwards@jlab.org`
† Deputy spokesperson, USQCD, `thomas.blum@uconn.edu`

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1 Introduction

This document outlines the scientific rationale for the Lattice Quantum Chromodynamics (LQCD) Computing Initiatives from fiscal year 2025 to 2029. Its goal is to obtain funding for computational resources at Brookhaven National Laboratory (BNL), Fermi National Accelerator Laboratory (Fermilab), and Thomas Jefferson National Accelerator Facility (JLab) for conducting numerical simulations of lattice gauge theories, with a focus on lattice QCD. This initiative builds on the success of the original LQCD Infrastructure Project (FY2005–FY2009) and its three subsequent extensions (LQCD-ext I: FY2010–FY2014, LQCD-ext II: FY2015–FY2019, LQCD-ext III: FY2020–FY2024), as well as the Nuclear and Particle Physics Lattice Computing Initiative (NPPLCI, FY2018–FY2024).

Quantum Chromodynamics (QCD) plays a crucial role in the missions of two divisions within the Department of Energy's Office of Science: the Office of High Energy Physics (HEP) and the Office of Nuclear Physics (NP). For NP, the significance of long-distance QCD interactions is evident in the study of hadrons, nuclei, extreme states of matter, and symmetry violations. In HEP, the phenomenon of color confinement ensures that strongly interacting particles are detected as hadrons, and often used in experiments as beams or targets. Consequently, a wide range of data – from fundamental QCD parameters to specific hadronic matrix elements – is essential for interpreting HEP experiments, necessitating a deep understanding of QCD at nonperturbative scales. Numerical lattice gauge theory stands as the sole comprehensive, quantitative method for investigating nonperturbative QCD from first principles.

The synergy of leadership-class computing facilities and USQCD cluster hardware, combined with shared SciDAC and Exascale Computing Project software, has transformed lattice QCD into a highly precise tool. During the LQCD-ext II and LQCD-ext III phase, these clusters served as platforms for developing calculations crucial for predicting the muon's anomalous magnetic moment according to the Standard Model. These efforts have since secured substantial resources from leadership-class computing. USQCD clusters have also been instrumental in advancing calculations of nucleon matrix elements, addressing new challenges such as nucleon form factors (vital for neutrino experiments), parton distribution functions (PDFs, crucial for Large Hadron Collider experiments), and the nucleon's strangeness content (relevant for direct dark matter detection and muon-to-electron conversion). Additionally, USQCD has dedicated a portion of its resources to exploring strongly-coupled lattice gauge theories beyond QCD, which hold potential for applications in theories beyond the Standard Model, including composite dark matter, composite scalar bosons akin to the Higgs, and supersymmetric lattice gauge theories.

It is important to recognize that many lattice-QCD calculations are pertinent to both the HEP and NP missions of the DOE. For example, the momentum-fraction dependence of PDFs, an expanding area of lattice-QCD research, is vital for calculating proton-proton collision cross-sections at the LHC from a HEP perspective and fosters important discussions between lattice QCD and phenomenology from an NP standpoint. This dialogue supports the case for a future Electron-Ion collider. Similarly, certain nucleon form factors measurable in electron-proton experiments, such as those conducted at JLab, can be compared with lattice QCD predictions. Additional nucleon form factors are necessary for analyzing neutrino-oscillation experiments, with lattice-QCD calculations providing valuable input for experimental analyses.

Uncovering the internal structure of nucleons and nuclei is one of the primary objectives of the DOE NP mission. Lattice QCD calculations have expanded to include generalized parton distributions and other descriptions of their constituent quark and gluons, providing a more comprehensive picture of the internal structure of nucleons and nuclei including the decomposition of their spin and internal binding forces. In close coordination with NP and HEP phenomenologists, these calculations are guiding the experimental programs at JLab 12GeV and the Electron-Ion Collider (EIC). Hadron and nuclear spectroscopy is critical to understanding the masses and excitations of hadrons and nuclei as well as to learning about hadronic and nuclear interactions. These calculations are relevant to the experimental programs at JLab, the EIC, the Facility for Rare Isotope Beams (FRIB), as well as to nuclear astrophysics. Exotic and heavy-quark spectroscopy that lattice calculations provide is also a key area of investigation at LHCb, Belle-II and other HEP facilities. Lattice calculations have provided a solid theoretical foundation for the RHIC Beam Energy Scan program as well as at the LHC.

The remainder of this proposal is structured as follows: Section 2 provides an overview of how the USQCD collaboration manages DOE SC funding. Section 3 reviews the key significant achievements in high-energy and nuclear physics enabled by the most recent projects (LQCD-ext III and NPPLCI), and the scientific goals and milestones for the proposed LQCD Computing Initiatives. This includes discussions in Section 4 on the relevance of the project to HEP and NP priorities, in Section 5 the computational needs for the planned LQCD facilities at BNL, FNAL, and JLab, and in Section 7 a summary of the proposed management strategy for these initiatives. An appendix offers insights into the USQCD collaboration. Much of the material draws extensively from whitepapers presented during the Snowmass and Nuclear Science Advisory Committee (NSAC) planning processes [396, 397].

2 Lattice-QCD Landscape

To effectively discuss the progress and future directions in lattice gauge theory research within the United States, it is beneficial to first review the current state of the field. The study of the long-range aspects of Quantum Chromodynamics (QCD) is vital for the scientific goals of both HEP and NP, which is why funding for researchers and computational resources is sourced from both divisions. Historically, projects such as LQCD and its extensions were jointly financed by HEP and NP. However, in January 2019, the HEP funding approach shifted from dedicated clusters to institutional clusters, resulting in a division of efforts funded by HEP and NP. The HEP-funded initiatives continued under the name LQCD-ext II, focusing on Brookhaven National Laboratory (BNL) and Fermilab, while NP initiated a new project, the Nuclear and Particle Physics Lattice QCD Computing Initiative (NPPLC), to maintain dedicated clusters at Jefferson Lab (JLab).

In May 2023, a combined review of the LQCD-ext III and NPPLC initiatives took place. One of the outcomes was the decision that the HEP initiative could also invest in dedicated clusters, with an open bidding process currently in use for procurement at BNL under LQCD-ext III. Another result was the agreement that the HEP and NP LQCD initiatives would jointly seek renewal for the fiscal years 2025 to 2029, with a business plan for each DOE office – HEP and NP – and a joint scientific proposal.

The computing clusters at BNL, Fermilab, and JLab are significant sources of computational power for lattice gauge theory in the U.S. Additional computing time is available at some university facilities, though it represents a smaller portion of the total resources. Beyond these clusters, major computational support for lattice QCD comes from leadership computing facilities such as the Argonne Leadership Class Facility (ALCF), the Oak Ridge Leadership Class Facility (OLCF), the National Energy Research Scientific Computing Center (NERSC), and supercomputers funded by the U.S. National Science Foundation (NSF).

The USQCD Collaboration, which is a collective of numerous smaller scientific collaborations, coordinates much of these resources. It originated when the DOE encouraged leading lattice QCD researchers to form a committee to explore collaborative opportunities in software development and computing resource coordination. This committee evolved into the USQCD Executive Committee, which now oversees a collaboration of around 150 scientists based in the U.S. The allocation of resources for the LQCD-I through LQCD-ext II projects was managed by USQCD, and currently, the Scientific Program Committee for USQCD allocates resources for the LQCD-ext III and NPPLC initiatives. The proposed initiative aims to continue this coordinated approach.

The USQCD Collaboration has been at the forefront of community software development, supported by grants from SciDAC, and recently, the Exascale Computing Project (ECP), which concluded in December 2023. The SciDAC software stack is designed to run optimized codes on various hardware platforms, including CPUs and GPUs, commodity hardware clusters, and specialized supercomputers at national centers. The lattice QCD ECP project focused on exascale computers such as the operational Frontier at OLCF, the upcoming Aurora at ALCF, and future facilities at NERSC. The exascale computers feature diverse computing architectures, and thanks to the ECP, USQCD has developed software to integrate the most cost-effective architectures into the LQCD Computing Initiatives. Currently, there are two SciDAC-5 projects – ASCR & NP and ASCR & HEP – that are developing a new generation of algorithms for Exascale systems and beyond, tackling the challenges of lattice QCD calculations as they increase the fidelity of their calculations.

USQCD members can leverage this considerable software infrastructure development into competitive allocation requests on the leadership computing facilities at ALCF, NERSC, OLCF and NSF centers. USQCD computing facilities are guided by the success of these group projects, and inform future directions for both hardware acquisitions, as well as the science programs for USQCD.

Leadership class computers and the clusters discussed here serve complementary functions. Leadership class computers are designed for high capability, suitable for the largest lattices or for mature problems with highly automated workflows. On the other hand, high-capacity computing is essential for the calculation and statistical analysis of hadron correlation functions, which are foundational for the extraction of amplitudes and estimating systematic uncertainties. This requires close interaction between researchers and computers, with a need for quick turnaround. The moderate capability of USQCD clusters makes them ideal for the analysis phase of a long scientific workflow, and for developing new computing strategies and conducting numerous simulations on small to medium-sized lattices, which would be impractical on leadership class machines. The flexibility of the queues on both dedicated and institutional clusters supports innovation and can be easily adjusted in unexpected situations. The LQCD projects also provide significant computing resources for outstanding proposals from junior researchers, who might not yet have the standing to compete for access to DOE or NSF leadership class facilities.

USQCD members have been at the forefront of algorithmic and architectural development, including the construction of dedicated computing hardware platforms, and collaboration with industry in the design of state of the art systems optimized for lattice field theory calculations. Members are actively involved in new projects involving industry partners centered on applying techniques for Machine Learning. And while years away from production level calculations, members of the USQCD community are leading national efforts in the development and potential application of quantum computing systems for computations relevant to HEP and NP.

3 Scientific Accomplishments of LQCD-ext III and NPPLCI and Plans

This section reviews key scientific achievements in HEP and NP enabled by the most recent initiatives (LQCD-ext III and NPPLCI), and the scientific goals and milestones for the proposed LQCD Computing Initiatives.

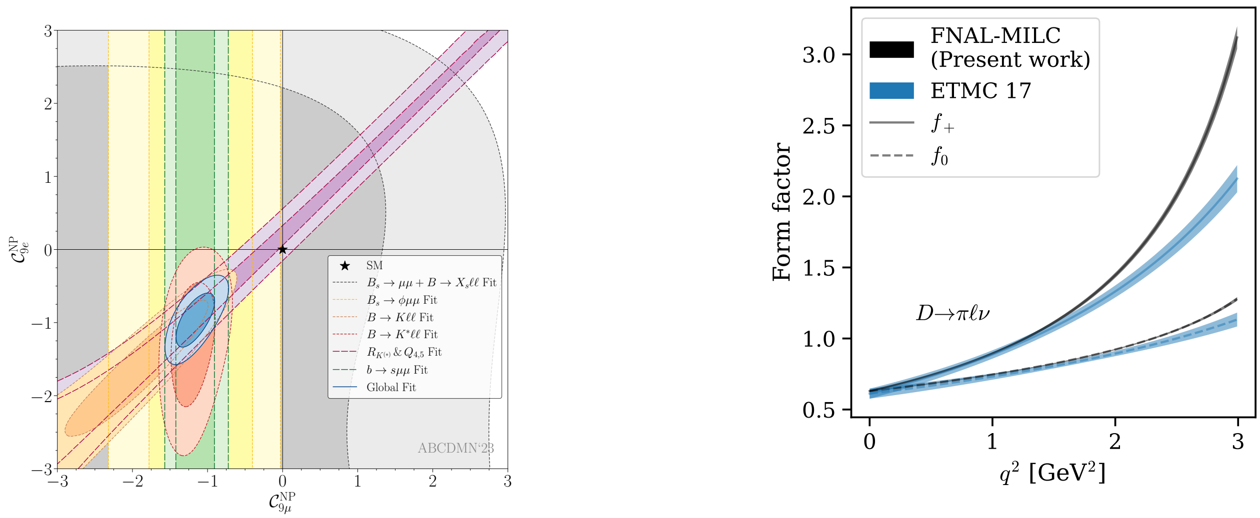


Figure 1: Left: Constraints on new-physics Wilson coefficients resulting from a combination of SM discrepancies in decays involving $b \to s\mu^+\mu^-$ and $b \to se^+e^-$ [401]. The global fit is inconsistent with the SM as indicated. Right: Form factors for $D \to \pi\ell\nu$ from the all-HISQ method [2] compared with the best previous result [402]. The width of the bands indicates the theoretical uncertainty. The improvement in uncertainty is striking. For the first time it matches the experimental uncertainty.

3.1 Quark flavor physics and SM parameters

For the past decade, lattice QCD flavor-physics calculations have made critical contributions to determinations of CKM matrix elements (fundamental parameters of the SM for transitions between quark flavors) and to searches for beyond-the-SM effects [1] [398–400]. Earlier results for the leptonic B, B_s, D, and D_s decay constants [356, 357] have sub-percent errors and provide a template for the more complicated semileptonic-decay processes. Semileptonic decays of these mesons, such as $B \to D^*\ell\nu$ and $B \to \pi\ell\nu$, permit a more precise determination of the CKM matrix elements than leptonic decays. The Belle II, BES III, and LHCb experiments are supplying much more accurate experimental measurements of these processes, which demands timely, commensurate SM precision improvements. For several quantities, differences at the 2σ level or greater between SM predictions and experimental measurement provide tantalizing hints of new physics. These quantities include the ongoing 3σ discrepancy in the determination of the CKM matrix element $|V_{cb}|$ between exclusive and inclusive semileptonic decays of the B meson, the combined 3.1σ discrepancy between measurements and SM predictions of $R(D)$ and $R(D^*)$ that test lepton flavor universality, and the theory/experiment discrepancy in several semileptonic flavor-changing neutral-current processes involving transitions from bottom to strange ($b \to s$) quarks that, when combined, approaches 5σ. For all of these, controlling the hadronic physics is crucial to establish the discrepancy, and lattice calculations will play an important role. Implications that might favor a weak effective theory of new physics are shown in Fig. 1.

The weak interactions of the light quarks (up, down and strange) are an important component of the P5 science driver: "Pursue Quantum Imprints of New Phenomena". Because of the structure of the standard model (for example, the need for three quark families for the violation of CP symmetry), the high precision of past and future experiments involving these light quark flavors and the ability to obtain subpercent *ab initio* results from lattice QCD, the electroweak properties of the light quarks are especially sensitive to the fleeting presence of virtual particles and interactions not yet seen in Nature. Increasingly accurate lattice QCD calculations of the standard model predictions for direct and indirect CP violation in kaon decay, the mass difference ΔM_K between the long- and short-lived K mesons, and the two- and three-particle semileptonic decays of the pion and kaon, among others, are placing limits on beyond-the-standard-model physics. Future work promises to make these constraints substantially tighter and possibly lead to discovery.

3.1.1 Accomplishments

High precision semileptonic D and B decays: The three most widely used lattice quark formulations for light quarks are "HISQ", "DWF" and "Wilson-Clover". Computations of semileptonic decays with the first two are underway, providing an opportunity for cross checks. A recent study of D and D_s meson decays with all HISQ quarks was completed and published [2]. A sample result is shown in Fig. 1 right. The improvement in precision over previous results is dramatic, and led to the most precise result to date for the CKM matrix element $|V_{cd}|$. A companion study of several B and B_s decays will be completed in the next two years. As with many USQCD projects, the procedures were developed and tested on LQCD resources with the coarsest lattice spacings before being moved to the LCFs for the finest spacings.

A parallel USQCD study of the decay $B_s \to K\ell\nu$ with light "DWF" fermions and a "relativistic" b quark, was also recently completed [403]. The resulting value of $|V_{ub}|$ is currently limited by experiment, but higher statistics experimental results are expected soon.

Semileptonic decays of heavy baryons: Members of USQCD have also been engaged in lattice calculations of semileptonic decays of baryons containing b or c quarks [358–360][3–5]. These calculations provide the SM predictions for several recent experimental measurements by LHCb [404, 405] and BESIII [406–408].

High precision semileptonic $B \to D^*\ell\nu$: The decay $B \to D^*$, rather than $B \to D$, promises to provide a much more precise value for $|V_{cb}|$. The first lattice calculation of the decay $B \to D^*$ at nonzero recoil was completed by USQCD members [6].

Direct CP violation in $K^0 \to \pi\pi$ decay: Results from a second, physical mass calculation of the direct CP violation parameter ϵ' [7] and a companion calculation the $\pi\pi$ scattering phase shifts in the $I = 0$ and 2 channels have been published [8]. These calculations are substantial improvements over earlier 2015 results [361] with additional $\pi\pi$ interpolating operators and nearly four times the statistics. The standard model result for $\mathrm{Re}(\epsilon'/\epsilon) = 21.7(8.4) \times 10^{-4}$ agrees with experiment, $16.6(2.3) \times 10^{-4}$. (The exploratory calculation which developed the methods and produced the first results were all performed using USQCD resources.)

Given the importance of this quantity, a second calculation of ϵ' has been undertaken using periodic instead of G-parity boundary conditions and first results published [9, 10]. This new direction provides quantitative information about finite-volume effects, a foundation for future inclusion of electromagnetic effects and, by not requiring bespoke G-parity gauge ensembles, will allow the reuse of a substantial archive of eigenvectors and distillation data saved from earlier projects as this calculaton moves on to 48^3 and 64^3 lattice volumes. All of these first studies with periodic boundary conditions were carried out using USQCD resources.

K_L-K_S mass difference (ΔM_K): The first calculation of ΔM_K with physical, up, down, strange and charm quark masses was completed including a scaling study in which the dependence on the lattice spacing was studied by examining larger lattice spacings and corresponding smaller lilghter quark masses [11]. The long-distance corrections to the indirect CP violation also come from K^0-$\overline{K}^0$ mixing amplitudes and exploratory results for these effects from unphysical quark masses have been

published [12].

Including the light-quark mass difference and electromagnetism: A new method has been developed [362] to remove power-law finite-volume errors in the calculation of E&M effects in light-quark physics and successfully applied to compute the π^+-π^0 mass difference at 1.5% accuracy [13] as well as other quantities [14, 15]. (This method was developed and the mass difference calculation performed using USQCD resources.) Techniques have also been developed to calculate the E&M corrections to $\pi_{\ell 2}$ and $K_{\ell 2}$ decays with exponentially small finite-volume errors [16] as well as for $K_{\ell 3}$ decay [16, 17].

Standard model prediction for $K_L \to \mu^+\mu^-$: A comparison of the standard model prediction for the second-order-weak, neutral-current decay $K_L \to \mu^+\mu^-$ with the accurate experimental decay rate requires a first principle result for the competitive third-order electroweak process which is mediated by two photons. In a series of calculations on increasingly challenging related decays, method have been developed and demonstrated which make this calculation possible. These include the calculation of $\pi^0 \to e^+e^-$ [18], $K_L \to \gamma\gamma$ [19] and most recently the quark-line-connected contribution to two-photon-mediated $K_L \to \mu^+\mu^-$ decay itself [20].

3.1.2 Plans

High precision semileptonic B decays: With the now nearly complete all-HISQ dataset for B decays, coupled with high-statistics experimental results, we expect significant improvements in the determination of several CKM matrix elements, the $R(D)$ ratio, and in our understanding of the current theoretical/experimental discrepancies in rare decays such as $B \to K\ell^+\ell^-$, $B \to K^*\ell^+\ell^-$, and $B_s \to \phi\ell^+\ell^-$. In the meantime, a companion analysis of semileptonic B decays to light mesons from an existing older dataset with HISQ light quarks and "Fermilab" heavy quarks is in progress [21]. Finally, calculations of B semileptonic decays with DWF light quarks and relativistic heavy quarks are "warming up" with a calculation of D meson decays.

High-precision $B \to D^*\ell\nu$: Members of USQCD are determining form factors for the decay $B \to D^*\ell\nu$ using a new, improved heavy-quark OK action that promises a higher-precision value for $|V_{cb}|$ [22]. An independent study with HISQ light quarks and a "Fermilab" b quark is also planned. Finally, an all-HISQ project has been started on USQCD clusters [23].

Radiative decays of pseudoscalar mesons: Following methods developed in Ref. [409], members of USQCD are studying radiative decays of pseudoscalar mesons in the DWF formulation.

Inclusive B decays from the lattice: The simulation of inclusive decays on the lattice has been a long-standing challenge. Recent proposals [410, 411] show promise that such simulations can be done. Although members of USQCD have been applying the method first to neutrinoless double-β decay [24], the methods can also be applied to inclusive B decays.

Bottom-baryon decays: Calculations of semileptonic decays Λ_b and Ξ_c are important for constraining $|V_{ub}/V_{cb}|$ from Λ_b decay measurements at LHCb and for lepton flavor universality in light of tensions observed in $R(D^{(*)})$. Recent measurements of Ξ_c decays has motivated a need for precise lattice calculations of the relevant form factors. Improved calculations will be carried out over the proposal period [25, 26] in step with improved measurements from LHCb.

Semileptonic B decays to two resonant mesons: Collaborative calculations of the form factors for $B \to \pi\pi\ell\nu$ and $B \to K\pi\ell^+\ell^-$ will continue [412].

B-$\bar{B}$ and K-$\bar{K}$ mixing: Lattice precision still lags measurements from e^+e^- (for B) and hadron (for B_s) colliders. Members of USQCD are preparing a new study of B-$\bar{B}$ mixing with new methodologies. Results from the DWF and relativistic heavy-quark action are expected in the near future.

Direct CP violation in $K^0 \to \pi\pi$ decay: Large-scale calculations are currently underway to extending the G-parity studies to $40^3 \times 64$ and $48^3 \times 64$ ensembles with the inverse lattice spacing increased from 1.38 GeV to 1.73 GeV and 2.1 GeV to allow a continuum extrapolation. The calculations with periodic boundaries will be extended from a $24^3 \times 64$ to a $32^3 \times 64$ volume at fixed lattice spacing as well as $1/a$ increased from 1.02 GeV to 1.38 GeV to study both finite-volume and finite-lattice spacing effects. Large-scale future calculations with periodic boundaries and inverse lattice spacings of 1.73 GeV and 2.38 GeV are being explored which will reuse data computed in earlier $g_\mu - 2$ studies. Substantial effort will be devoted to computing the E&M corrections to ϵ' [363][27] (with first calculations expected to begin this year) and to replacing all perturbative Wilson coefficient calculations at or below the charm scale with non-perturbative lattice QCD results [364].

K_L-K_S mass difference (ΔM_K): Large-scale $64^3 \times 128$ calculations with $1/a = 2.3$ GeV are expected to begin this year to obtain the first physical-quark-mass results for the long distance contribution to ϵ_K, these will be followed with calculations on larger lattice volumes and inverse lattice spacings of 2.77 GeV and 3.5 GeV. Past scaling studies suggest these finer lattices will allow a reliable continuum limit with a goal of total errors below 10% for ΔM_K and the LD part of ϵ_K.

Including the light-quark mass difference and electromagnetism: The new developments in computing E&M effects described above are now being exploited in a calculation of these correction for $\pi\ell2$ and $K\ell2$ decays. These results when combined with current high-precision lattice results for f_π and f_K should allow the determination of V_{ud} and V_{us} to accuracies approaching 0.1%.

Standard model prediction for $K_L \to \mu^+\mu^-$: The next step is the calculation of the disconnected contributions to the two-photon-mediated contribution to this decay on a small coarse lattice ($1/a =$ 1.02 GeV). This will be followed with better-controlled calculations on $48^3 \times 96$, $1/a = 1.73$ GeV and $64^3 \times 128$, $1/a = 2.38$ GeV ensembles to a continuum limit with errors below 10%.

3.2 Lepton flavor physics

The muon anomalous magnetic moment, $a_\mu = (g-2)_\mu/2$, or anomaly, represents one of the most important HEP efforts of USQCD members and the world-wide lattice community. Fermilab's E989 experiment has now measured the anomaly to 0.2 ppm [413] and should reduce this uncertainty by another factor of two after the final three runs are analyzed. A final result from E989 is expected in 2025, and it remains one of the lattice community's highest priorities to match their precision goal for the hadronic vacuum polarization (HVP) and light-by-light (HLbL) contributions which dominate the total theory uncertainty [414].

The world-wide HEP community involved in the theory calculation of a_μ comprises the Muon g-2 Theory Initiative (TI) which was started by USQCD members. Since the early 2000's a discrepancy between (data-driven, or R-ratio) theory and experiment has persisted. Taking the TI whitepaper value for the SM [414], it is now more than 5σ. But the BMW collaboration result from 2021 with comparable (sub-percent) errors is consistent with experiment. Further, a recent high-statistics R-Ratio based value from the CMD-3 experiment is consistent with experiment and disagrees significantly with previous R-ratio values. Sorting out these discrepancies is a high priority for the lattice and wider communities.

The next significant muon experiment coming up at Fermilab is Mu2e which will begin data taking in the Fall of 2026. Mu2e will improve the sensitivity for detecting muon to electron conversion in a nucleus by four orders of magnitude. Since the conversion rate in the SM is so small, a detection would immediately signal a discovery of new physics. To interpret the results requires precise knowledge of the light and strange quark content of the nucleon, parameterized as the so-called nucleon-sigma terms. These matrix elements of scalar densities can be calculated in lattice QCD. In fact a whole set of form factors is needed to fully describe the matrix elements of the relevant weak effective theory (WET) coefficients [415]. Unlike five years ago, now most information comes from the lattice. The derivatives of the form factors at zero momentum transfer are also important, and the lattice

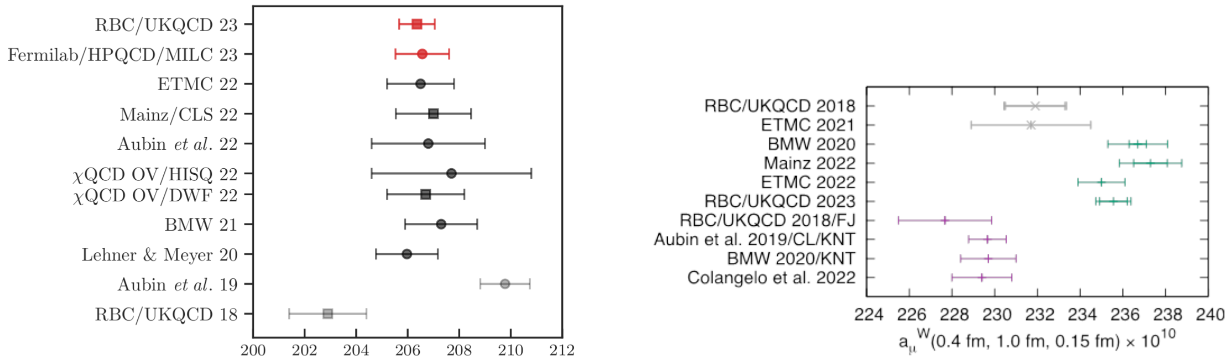


Figure 2: Intermediate window part of the muon anomaly, $(g-2)/2$. From u, d quarks (left) and total (right), including heavy quarks, disconnected diagrams, and isospin breaking compared to data-driven determinations (lower-left four). The most precise values are from USQCD members.

is essential here since one needs the split between quark and gluon contributions. It turns out the same matrix elements and form factors are needed for DM direct detection experiments as well. A discussion of accomplishments and plans is given in Sec. 3.9.

3.2.1 Accomplishments

Muon g-2: Since 2019 USQCD members have made indispensable contributions to the accuracy and precision of the value of $(g-2)_\mu$ in the Standard Model. The so-called "intermediate window" (about 30% of the total, a_μ^{HVP} = short+intermediate+long distance) has been computed using both domain wall and staggered fermions, yielding the most precise values of this quantity to date [28, 29] (see Fig. 2). The window method was proposed by USQCD members [30] and the first indication of a discrepancy between lattice and data-driven (R-ratio) results also came from the collaboration [31]. It is now used by the entire lattice community and shows a more than 4σ discrepancy with the R-ratio value [416] and even more for the light-quark connected contribution alone [417].The short distance window contributes a small amount to the total. It has been calculated by several groups [418][8][419] and is in reasonable agreement with the R-ratio value [416].

Though it is one loop higher order in the fine structure constant α, the HLbL contribution contributes significantly to the total hadronic uncertainty in $(g-2)_\mu$. USQCD members produced the first value from the lattice for this quantity with all errors controlled [32], and it was included in the TI white-paper average [414]. Since then the most precise value, including data-driven and model values, comes from USQCD [33].

It is important to note that the first, pioneering, works for these quantities [365, 366] were accomplished on precursor USQCD and USQCD machines funded by the DOE by USQCD scientists.

3.2.2 Plans

Muon g-2: Members' plans have now turned to the more challenging long-distance window. To tackle this part, USQCD theorists have developed and/or innovated several methods to dramatically increase computational efficiency that are now used widely by the community. These include all-mode-averaging (AMA) [367, 368], low-mode-averaging (LMA) [30] [420–424], and the improved bounding method [34][425]. The latter is based on a generalized eigenvector problem (GEVP) solution for the exclusive state reconstruction of the long distance pion-pion tail of the electromagnetic correlation function. Using these techniques, several USQCD groups expect to reach sub-percent precision in 2024 and the final goal of 1-2 per mille in 2025, or soon after. Even though the dominant HVP contribution comes from the connected light quark part of the correlation function, improved disconnected (two quark loops), isospin breaking (QED and non-degenerate quarks), and heavier flavor contributions are necessary to reach our goal. These calculations are underway as well, some of them on USQCD resources. We note that the same isospin contributions needed for a_μ^{HVP} can be used to correct tau decays which can then be used in the data driven method [369] which may help illuminate the current discrepancies between lattice and data driven results.

3.3 Neutrino physics

Neutrino physics addresses many issues, from physics beyond the Standard Model to nuclear structure and is, thus, of interest to both HEP and NP. In quark- and charged-lepton-flavor physics (Secs. 3.1 and 3.2, respectively) hadronic physics can be factored (at least in the sense of convolution) from electroweak and BSM physics. Neutrino scattering experiments, which test the three-generation paradigm of neutrino mixing and masses including the search for leptonic CP violation, are the cornerstone of the P5 science driver "Elucidate the Mysteries of Neutrinos". Neutrinoless double-beta ($0\nu\beta\beta$) decay searches, which test the Majorana nature of neutrinos, not only address this driver and "Pursue Quantum Imprints of New Phenomena" but also are a key component of the NP experimental program directed at (violations of) fundamental symmetries. In both, lattice QCD will have to be combined with nuclear many-body theory (NMBT) in order to gain an adequate theoretical understanding. NMBT often starts with the "impulse approximation", factoring the amplitude or cross section for νA interactions into a nucleon-level process embedded in a nuclear wavefunction. This setup then requires form factors and other quantities familiar from flavor physics, albeit now for nucleons instead of mesons. NMBT also requires two- and three-body interactions and one- and two-body currents. In the modern "*ab initio*" setting, these ingredients are described by a chiral effective field theory (χEFT) of pions and nucleons. Lattice-QCD calculations of reasonably small nuclei ($A \leq 6$) can be used to constrain the parameters of the χEFT.

It is worth noting that USQCD has played a central role in drawing attention to the role of lattice QCD in understanding neutrino-nuclear interactions, starting with the lattice-QCD working group of the Project X Physics Study. The framework was further developed in white papers from USQCD [35] and from the community with USQCD members' participation [426, 427] and coordination [428]. Original research by USQCD members in collaboration with others is beginning to explore this interface [36–39]. The rest of this section covers the connection between LQCD and neutrino-scattering experiments; Sec. 3.9 covers $0\nu\beta\beta$.

3.3.1 Accomplishments

Nucleon axial-vector form factor: Combining LQCD and NMBT is simplest for charged-current quasielastic scattering, where the relevant quantities are the isovector form factors of the electroweak transition matrix elements for $\nu_\ell n \to p\ell^-$ and $\bar{\nu}_\ell p \to n\ell^+$. The form factors of the vector current can be obtained via isospin symmetry from eN scattering (N is n or p), thereby providing a cross-check for lattice-QCD calculations. The form factors of the axial-vector current are not easily accessed via experiment: possibilities include neutrino-neutron scattering off deuterons in a deuterium target and antineutrino-proton scattering [429] off hydrogen in a hydrocarbon target [430]. Many groups around the world are carrying out LQCD calculations of the axial form factor, both USQCD members [40–43] and others [431–434]. See Ref. [44] for a review (including references to earlier work) and a discussion

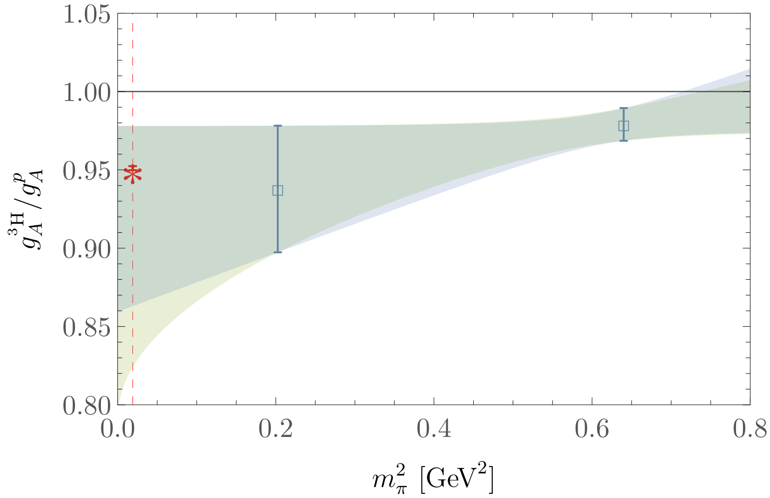


Figure 3: Axial-current matrix element governing the triton β decay rate calculated in LQCD [372] [48] for two unphysically large quark mass values with simple extrapolations to the physical point. Reproduced from Ref. [48].

of how these calculations pertain to the neutron lifetime puzzle. Note that USQCD has played a special role in identifying [370, 371] and resolving [42] challenges of excited-state contributions of $N\pi$ and $N\pi\pi$ states [435].

Constructing $N\pi$ and $N\pi\pi$ states in LQCD: Recent studies have highlighted the need for precise predictions of $N \to \Delta$ transition form factors at energies relevant to DUNE [37]. Because the $\Delta(1232)$ resonance lies above the $N\pi$ and $N\pi\pi$ thresholds, $N \to N\pi$ and $N \to N\pi\pi$ amplitudes must be explicitly computed in order to disentangle resonant and non-resonant effects and determine $N \to \Delta$ transition form factors. The first LQCD study of $N\pi\pi$ correlation functions was recently published [45]. This study was enabled by the quark field "sparsening" algorithm for approximating all-to-all propagators developed in Ref. [46]. Efficient GPU implementations for the tensor contractions of sparsened quark propagators required to construct $N\pi$ and $N\pi\pi$ correlation functions were developed with USQCD resources.

Two-body axial currents from LQCD: Two-body currents can have significant effects on neutrino-nucleus cross sections in the energy region relevant for DUNE. USQCD members are exploring opportunities for LQCD to provide constraints on two-body axial currents in nuclear effective theories, as reviewed in Ref. [47]. To reduce computational requirements, early calculations of two-body axial currents in two- and three-nucleon systems have unphysically large quark masses, corresponding to $m_\pi \approx 800$ MeV [372–375]. More recently with $m_\pi \approx 450$ MeV, the triton β-decay rate was calculated [48]. Although several systematic uncertainties have not yet been quantified, extrapolations of these LQCD results to physical quark masses are encouragingly consistent with precise results obtained from triton decay-rate measurements as shown in Fig. 3.

PDFs for neutrino-nucleus scattering from LQCD: Analogs of the "EMC effect" describing how isoscalar nuclear PDFs differ from deuteron PDFs are expected to arise in the isovector PDFs relevant to charged-current neutrino-nucleus scattering but have not been determined experimentally. A USQCD group performed the first LQCD calculation of moments of these isovector quark PDFs in ^{3}He nuclei [49]. Although the calculations use unphysically large quark masses, the results provide a proof-of-principle demonstration that LQCD results can improve constraints on the two-body current operators describing the isovector EMC effect in pionless EFT and eventually improve global fits of nuclear PDFs.

Variational studies of two-nucleon systems: As with the axial-vector form factors, variational methods via the generalized eigenvalue problem [436] are needed to explicitly remove excited-state contamination. USQCD members recently performed detailed variational studies of the energy spectrum of two-nucleon systems using the largest set of interpolating operators in a LQCD study of these systems to date [50, 51]. This study was enabled by quark field sparsening, efficient codes, and group theory formalism from USQCD members [46]. By comparing with previous two-nucleon studies using the same gauge field ensemble [376–378], the variational study clearly demonstrated that excited-state effects on determinations of two-nucleon energies were larger than previously expected.

3.3.2 Plans

Nucleon axial-vector form factor: With total uncertainties on the axial-vector form factor at the 10% level, the next steps are to reduce the uncertainty to 5% or even 1%. Per-cent-level uncertainties are estimated to require ten times the computing devoted to the problem so far [44]. Given the developing understanding of excited-state contributions, this goal will require midscale cluster computing to develop ideas and leadership-class computing to gain high statistics on fine lattices. An example of the former is the synergy between calculations of nucleon elastic axial form factors and calculations of pion-production amplitudes. The most important systematic uncertainty that remains to be quantified in detail in current LQCD calculations of nucleon elastic axial form factors is contamination from $N\pi$ excited states [42] [371] [431]. The same LQCD calculations used to disentangle $N \to N\pi$ and $N \to \Delta$ transition form factors can be used to quantify and remove the contamination from $N\pi$ excited states on $N \to N$ axial form factors. This will provide an important test of the systematic uncertainties in current LQCD calculations, which show 2–3σ tension with phenomenological determinations of nucleon elastic axial form factors based on 1970s-80s deuterium bubble chamber measurements.

Pion production and $N \to \Delta$ transitions: The construction of $N\pi$ and $N\pi\pi$ correlation functions mentioned above will be extended to calculate electroweak pion-production amplitdues. Using quark field sparsening techniques, correlation functions involving vector and axial currents can be described using tensor contractions and matrix multiplication operations that can be performed efficiently using GPUs and generalizations of the methods in Ref. [45]. Calculations will be performed using approximately physical quark masses and a large set of interpolating operators including not only single-hadron N and Δ operators but also multi-hadron $N\pi$, $N\pi\pi$, and $N\sigma$ operators. These operators will be projected to finite-volume analogs of partial waves using group theory formalism being developed to generalize the Lellouch-Lüscher formula [437]. Strategies for directly matching nuclear effective theories appearing in nuclear many-body calculations to finite-volume LQCD results for resonant and non-resonant pion production will be carried out and collaboration with nuclear many-body theorists is planned.

Deuteron axial form factors: Direct calculations of deuteron axial form factors are needed to shed light on the current tension between phenomenological determinations of nucleon elastic axial form factors using deuterium bubble chamber experiments [429] and current LQCD results for the same nucleon form factors [42] [371] [431]. These calculations will target a precision of 10% at $Q^2 \sim 0.7$ GeV^2 in order to reach the level of systematic uncertainties from nuclear effects estimated in Ref. [429] and test whether these nuclear effects account for the 3σ discrepancy between LQCD and deuterium bubble chamber results at this momentum transfer. Calculations with light quarks are conceptually simplest because one bound state, the deuteron, is known to exist from experiment. Variational studies of two-nucleon systems with a range of quark masses will be carried out to resolve the quark-mass dependence of nucleon-nucleon energy levels. The optimal operators will then be used to obtain the deuteron form factors at non-zero Q^2.

Hadron tensor for the shallow-inelastic region The DUNE neutrino energy spectrum is broad, substantially overlapping the "shallow" inelastic scattering region. In this region, there are too many pions to usefully speak of resonances but the energy is not yet high enough to apply the factorization of perturbative QCD. In any region, the object of interest is the hadron tensor $W^{\mu\nu} = \langle H|J^\mu J^\nu|H\rangle$ where H is the struck hadron, where J^μ is an electroweak current. In principle, H is a nucleus of the detector material, but the problem can be approximated with a convolution of a spectral function and a nucleon hadron tensor. As pointed out in Ref. [35], LQCD provides a first-principles approach to compute the nucleon hadron tensor in this difficult region. Earlier and recent work already investigated the hadron tensor in the quasielastic [379] and deep-inelastic regions [52, 52]. An interesting development is a demonstration that a certain smeared version of the inverse problem admits mathematically rigorous error bounds [53].

3.4 Strongly coupled quantum field theories beyond the Standard Model

As the experimental search for new physics beyond the Standard Model (BSM) continues, the absence of clear new-physics signals from the LHC and other experiments motivates to cast a wide net from a theoretical perspective, thus improving our understanding of the full breadth of possibilities for new physics. Many possible BSM models involve strongly coupled gauge theories, which limits the effectiveness of perturbative methods; lattice field theory calculations of such "beyond QCD" theories can give crucial quantitative and qualitative insights.

Since QCD is the only strongly-coupled gauge theory that is experimentally accessible so far, lattice calculations can provide a numerical laboratory for exploring how the physics changes with the number of colors, number of light fermions, fermion gauge representation, and many more parameters. This allows access to specific theories that match phenomenological models such as composite Higgs or composite dark matter scenarios. More broadly, lattice studies allow us to learn qualitative features of the broad space of strongly coupled theories as these parameters are varied. Calculations focused on specific models are thus doubly useful as explorations of the broader space of strongly coupled quantum field theories. Even more broadly, observation of emergent phenomena at strong coupling, e. g. conformal symmetry [438] or symmetric mass generation [439], deepens our overall understanding of field theory and may lead to completely novel proposals for models of new physics in the future, as well as connections to other disciplines such as condensed matter physics.

3.4.1 Accomplishments

Composite Higgs phenomenology: Detailed study was done by USQCD members [380] of a concrete composite Higgs model based on SU(4) gauge theory with fermions in two different gauge representations [440]. New results included a key matrix element relevant for the top-quark mass [54, 55] and radiative contributions to the Higgs potential [56]; based on the results, the simplest version of the theory was effectively ruled out. More recent studies have varied the number of light fermions, studying the β function to search for a more promising variant on the model [57]. Results show that SU(4) gauge with four sextet and four fundamental fermions are within the conformal window. In addition, the anomalous dimension of the chimera baryon is too small to make this system a candidate for partial composite mass generation.

Emergence of a light scalar: Lattice calculations of SU(3) gauge with $N_f = 8$ fermions in the fundamental representation [381][58] identified a scalar σ boson that is lighter and well-separated from the ρ and heavier resonances. The σ mass is close enough to the Goldstone pion that these systems require dilaton EFT analyses [441][59]. Investigations of the SU(3) gauge theory with two flavors of sextet representation fermions, another candidate technicolor-like system, have also been reported by USQCD members [60].

Supersymmetric theories at strong coupling: For a review of recent progress in supersymmetric gauge theories on the lattice, see [442]. Recent results from USQCD members include [382, 383]. In the first work, the duality between three-dimensional super-Yang-Mills theory and a stack of black branes was considered. The second work investigated the emergence of holography from lattice $\mathcal{N} = 4$ super Yang-Mills.

Large-N_c scaling: USQCD results studying the large-N_c expansion with dynamical fermions for topological susceptibility [61], finite-temperature phase transition [62, 63], and chiral limit properties [64, 65] have appeared in the previous period. Qualitative consistency with the large-N_c prediction is seen, but lattice results allow quantitative use by providing coefficients in large-N_c scaling formulas.

Radial quantization of lattice field theories: New developments in theory and methods have begun to enable the simulation of quantum field theories on curved spacetime lattices [66–75]. This enables a variety of interesting calculations, including the study of conformal theories on $\mathbb{R} \times S^{d-1}$ (radial quantization), which can allow access to exponentially larger scale separations compared to study on standard uniform hypercubic lattices.

Conformal phase of gauge-fermion theories: Identifying the opening of the conformal window is important for theoretical understanding of conformal systems and for Composite Higgs models. USQCD groups developed new methods to predict the continuous renormalization group β function [76, 77]. In the last two years, important improvements to the method have been developed to overcome limitations that plagued prior lattice calculations. The inclusion of heavy non-physical Pauli-Villars (PV) regulator fields has been particularly successful. The PV improved gauge action pushes unphysical bulk phase transitions to strong coupling, opening up the parameter space where lattice systems can be investigated [78, 79]. The use of extended gradient flow transformations provides a new consistency check in the calculation of the RG beta function and the running anomalous dimension of various operators [80, 57].

Renormalization group properties of gauge-fermion systems: The nonperturbative methods developed for near-conformal and conformal systems to determine the renormalization group β function and anomalous dimensions can also be used in QCD. USQCD collaborations have determined the Λ parameter of the pure-gauge SU(3) Yang Mills system [81, 77, 80, 82], and a novel, fully nonperturbative renormalization scheme was suggested in Ref. [83].

Symmetric mass generation: Recent works in both the condensed matter and high-energy physics communities have shown that in certain theories fermions can acquire mass due to nonperturbative dynamics without breaking chiral symmetries. This phenomenon is termed *symmetric mass generation* (SMG)[443, 439]. SMG phases have been identified in 4-dimensional lattice Higgs-Yukawa and gauge models with staggered fermions [384][84, 85, 84, 86]. Several recent publications suggest that in the SMG phase fermions with given chirality can be kept massless, while their mirror partners could be gapped. This opens the possibility of using staggered or domain wall fermions as a route to chiral lattice gauge theories [87, 88][385].

3.4.2 Plans

Radial quantization of lattice field theories: Continued development of methods and numerical studies will be critical, especially the inclusion of dynamical fermions and scaling up to $d = 4$, with the eventual goal of application to the conformal phase in QCD-like theories.

Renormalization group properties of gauge-fermion systems: USQCD groups are working to complete calculations of the RG β function with $N_q = 2$, 3, and 4 massless flavors. These calculations will predict α_{strong} with higher precision than presently available methods. The new fully nonperturbative renormalization scheme has been studied with $N_f = 2$ domain wall fermions. An extension to 4 flavors, either with staggered or with domain wall fermion formulations is being proposed.

Symmetric mass generation: Perhaps the most important question for lattice studies is to identify systems where the SMG phase is separated from the weak coupling (most likely conformal) phase by a continuous phase transition, where an infinite cutoff continuum limit can be defined. There are ongoing calculations to determine the order of the phase transition in the SU(3) gauge $N_f = 8$ system with staggered fermions, in SU(2) gauge with $N_f = 4$ and 8 staggered fermions, and Sp(4) gauge with $N_f = 2$ and 4 flavors. If necessary, these systems could be extended with a 4-fermion interaction that protects all the symmetries. In addition to the phase structure, calculations of the hadron spectrum and the Dirac eigenvalue spectrum are also considered for several of the above models. These observables will guide future composite Higgs models and possible chiral fermion formulations.

3.5 Dark matter and the cosmic frontier

Dark matter is an extremely well-motivated target for searches for new physics, as the astrophysical and cosmological evidence for dark matter at many different length scales is overwhelming. While there is still a wide range of theoretical possibilities for particle dark matter, lattice calculations can provide key inputs to several aspects of dark matter physics. In direct detection experiments searching for nuclear recoil from dark matter particles, knowledge of the corresponding nuclear matrix elements is crucial to bounding the dark matter-Standard Model couplings. The same comments about the importance of lattice calculations of form factors as made at the end of Sec. 3.2 apply here as well. The QCD axion can also serve as a potential dark matter candidate [444]; because of its role in solving the strong CP problem, the properties of the axion are tied closely to the QCD topological susceptibility and its temperature dependence, which has been calculated using lattice methods [445–447][386].

Moving away from QCD, composite dark matter is an intriguing class of models in which dark baryons (or mesons, or glueballs, or nuclei) arising from a confining hidden sector act as the dark matter. Such dark matter candidates can naturally arise in a variety of models, and they can naturally be cosmically stable with highly suppressed interactions with the Standard Model. Composite dark matter may also provide a compelling explanation for astrophysical hints of dark matter self-interactions, e.g. [448]. Because these models are generally strongly coupled, reliable prediction of their properties and detection prospects requires input from non-perturbative methods such as lattice calculations.

3.5.1 Accomplishments

Dark confinement and gravitational waves: If a composite dark matter sector exists, it may have a first-order confinement transition in the early universe, which can give rise to a gravitational wave signal. Recent studies of "stealth dark matter" (SU(4) gauge theory with four massive fermions) at finite temperature [89] show evidence of a first-order transition in part of the parameter space.

Composite dark matter: Although not focused on dark matter specifically, generic results for gauge theories at large N_c can be broadly useful inputs for model builders. See Sec. 3.4 above and Sec. 3.7 below for more details on this work.

3.5.2 Plans

Dark matter direct detection: The scalar current nucleon matrix elements $\sigma_{\pi N}$ and σ_s are key inputs for dark matter that interacts with nuclei e.g. through Higgs exchange; these the scalar matrix elements in the proton are known fairly precisely from lattice QCD, but there are lingering tensions with experiment-based estimates that should be understood. In addition, nuclear many-body effects are particularly important for scalar interactions [47], and previous lattice calculations have indicated potentially large discrepancies from naive expectations in small nuclei, albeit at heavy pion mass [375]. These studies should be extended and continued closer to the physical point, and combined with many-body models in order to gain a deeper and more precise understanding of the physics.

Dark baryon scattering: Calculations of baryon scattering lengths away from QCD can provide insight into whether composite dark matter models can be compatible with astrophysical hints for dark matter self-interactions; this has been done in the past for SU(2) [387]. Recent preliminary work [90] on methods for spectroscopy in SU(4) theory lays the groundwork for SU(4) baryon scattering calculations.

Dark confinement and gravitational waves: Further finite-temperature studies of non-QCD systems can shed light on the possible gravitational wave signals from composite dark sectors. New USQCD studies of SU(4) with one flavor, a variation on the original stealth dark matter model, are underway [91]. Once first-order transitions are located, further lattice calculations of properties of the phase transition such as the latent heat will provide critical inputs for predicting gravitational wave spectra. Applying new methodology based on direct calculation of the density of states [449, 450] will be explored in this context.

Spectroscopy and matrix elements: In general, spectroscopy and vacuum matrix elements for a wide range of theories besides QCD are useful for model-builders. This includes further work on glueballs in pure-gauge theories, and study of large-N_c expansions. Undertaking a more systematic survey of theories as N_c and N_f are varied will provide a valuable foundation for future dark matter models.

3.6 Hadron structure

Understanding the structure and dynamics of hadrons in terms of their constituents, quarks, and gluons is paramount to unraveling the mysteries of the strong force and providing crucial insights into the behavior of matter at its most fundamental level. Lattice Quantum Chromodynamics (LQCD) is a powerful computational tool to explore the nonperturbative regime of QCD, allowing us to investigate the properties of hadrons directly from the underlying theory of strong interactions, with controlled and quantifiable uncertainties. The exploration of hadronic structure has been for many years a central component of the USQCD project. Basic questions about hadronic structure such as how the charge and current are distributed in the nucleon as described by the electromagnetic form factors have been studied for years and recently have reached high precision. Computations of distributions of mass and pressure in the nucleon as derived from gravitational form factors also achieved important milestones recently. Finally, the implementation of novel techniques for obtaining Parton Distribution Functions (PDFs), Generalized Parton Distributions (GPDs), and Transverse Momentum Distribution (TMDs) have allowed a glimpse to the 3D structure of the nucleon for the first time.

These calculations are directly relevant to the DOE experimental program at US facilities, such as FNAL, JLab and BNL (future EIC). First computations of nucleon form factors are essential theoretical input to neutrino experiments such NOvA, MINERvA, DUNE, and MicroBooNE where the nucleon form factors are required input for calculations of the neutrino-nucleous cross-section. Parton distribution functions play a central role in searches for new physics at LHC. The study of GPDs and TMDs are essential for the JLab 12 GeV program where the 3D structure of the nucleon is studied and lattice QCD results will play essential role in the analysis of experimental results.

3.6.1 Accomplishments

Electromagnetic and Axial Form Factors: In recent years, members of the USQCD collaboration have produced the world's most precise determinations of the nucleon electromagnetic and axial form factors. This includes detailed studies of both axial vector and vector form factors of the nucleon using the USQCD 2+1 flavor clover ensembles [41, 42]. Members of USQCD, with collaborators, have also published studies of the vector and axial vector form factors utilizing the twisted-mass fermion ensembles [92, 43]. The axial form factors are of particular interest for future neutrino experiments in the US and LQCD calculations have now reached 10% accuracy and are consistent with the recent experimental results from the MINEvA experiment.

Gravitational Form Factors: The gravitational form factors of a hadron, which are defined in terms of matrix elements of the energy-momentum tensor, encode information about the mechanical properties of the hadron, such as pressure and stress, energy, and momentum distributions. In addition, they are related to the contributions to the spin of the hadron by its constituents. Recent experimental extractions of the pressure inside the proton [451] sparked renewed interest in LQCD calculations. Using the USQCD 2+1 flavor ensembles, collaboration members published calculations of the gravitational form factors of the nucleon [93, 94]. Furthermore, computations of the trace anomaly [95] have been performed on the USQCD domain wall fermion ensembles in a range of quark masses to shed light on the dynamical generation of hadronic masses.

Parton Distribution Functions: Since the emergence of methods that allow Euclidean Lattice QCD calculations to determine the momentum fraction x-dependence of the parton distribution functions [452–457], the USQCD collaboration has performed a series of calculations implementing these ideas. The ongoing efforts have achieved significant results, indicating that LQCD methods can achieve ab initio computations of parton distribution functions in the large-x region. The continuum limit of the nucleon unpolarized PDFs with 2 flavors of clover-Wilson quarks was recently explored by members of USQCD [96]. In this work, a novel method of Bayesian data analysis technique was introduced to obtain the desired PDFs and the contaminating factors stemming from lattice spacing errors and higher twist effects. Furthermore, the so-called distillation technique for constructing nucleon interpolating fields was implemented and used to extract parton distribution functions of the nucleon, including helicity and transversity distributions [97–101] using the 2+1 flavor clover fermion USQCD ensembles. Using the USQCD HISQ fermion action ensembles, collaboration members have computed parton distribution functions on super-fine lattices utilizing the LAMET approach. Finally, the continuum limit of parton distributions has been explored using twisted-mass dynamical fermion ensembles both in the LAMET and short-distance-factorization (SDF) schemes [102–104].

Generalized Parton Distributions: Generalized parton distribution functions (GPDs), expressed as functions of (x, ξ, t) where x is the momentum fraction of the parton, ξ is the longitudinal momentum transfer, and t is the magnitude of the total momentum transfer, encapsulate the 3D structure of the nucleon. Experimental information on GPDs is obtained through processes such as Deeply Virtual Compton Scattering (DVCS), and Deeply Virtual Meson Production (DVMP), flagship targets of experimental programs at the 12 GeV Jefferson Lab upgrade and the future EIC. However, experiment can only provide 2D projections of such 3D objects resulting in an ill-defined inverse problem. Here LQCD calculations have particular potential in that they do provide three-dimensional information that can guide or complement information from experimental analyses. Many methodological as well as exploratory computations of GPDs in LQCD have been performed in recent years by members of the USQCD collaborations [105–107].

Transverse Momentum Distributions: Transverse Momentum-dependent parton Distribution Functions (TMDs) provide valuable insights into the three-dimensional structure of hadrons. Unlike conventional Parton Distribution Functions (PDFs), TMDs capture the longitudinal momentum distribution of partons within hadrons while also accounting for their transverse momentum, offering a more complete picture of the hadron's partonic structure. Understanding TMDs is essential for interpreting experimental data from processes sensitive to transverse momentum, such as semi-inclusive deep inelastic scattering and Drell-Yan production, thereby bridging theoretical predictions with experimental observations in QCD dynamics. Moreover, TMDs play a vital role in probing the spin and orbital angular momentum contributions of quarks and gluons inside hadrons, contributing significantly to our understanding of the nucleon's internal structure and the dynamics of strong interactions. Members of USQCD have performed pioneering computations of TMDs with LQCD [388–391]. Recently completed lattice computations of TMDs have shed light on quark orbital momentum contribution to the spin of the nucleon [108]. An important non-perturbative quantity in the physics of TMDs is the Collins-Soper (CS) kernel responsible for the evolution of TMDs in rapidity. Members of the USQCD collaboration have computed the quark CS kernel directly from QCD, thus reducing the theoretical uncertainty in analyzing experimental data where TMDs are important [109–116].

3.6.2 Plans

In future years, members of the USQCD collaboration will continue this vigorous program of investigating hadronic structure as it emerges from the fundamental theory of strong interactions. The goal is both to obtain results from purely theoretical means, as well as to aid phenomenology in better determining hadronic structure from experiment [117–120]. The collaboration will aim to improve precision of the calculations of Form Factors, PDFs, GPDs and TMDs, to control the relevant systematic errors arising from lattice spacing, finite volume, and quark masses. For that reason, we will continue to support the generation of state-of-the-art gauge ensembles.

Nucleon Form Factors: The computation of nucleon form factors will continue to be pursued to achieve control of all systematic errors. Accuracy, of a few percent is expected to be achieved in vector and axial vector form factors providing better understanding of nucleon elastic scattering cross-sections. Furthermore, improvements in computations of Gravitational Form factors (GFFs) is central in understanding the mass an presure distributions inside the nucleon and help understand the contribution of the parton spin and orbital angular momentum to the total spin of the nucleon. Furthermore, GFFs can provide constraints in the extraction of GPDs both from experiment and from lattice QCD.

Parton Distribution Functions: The computational methods for determining the full x-dependence of PDFs are well understood. Computations at smaller lattice spacings are ongoing and will continue to be pursued to probe the nucleon at shorter distance scales and at higher momenta, allowing for improved reach in the accessible range of the momentum fraction x. Furthermore, these new studies will enable control of the higher twist contamination that is present in Euclidean lattice computations of twist-2 PDFs.

Generalized Parton Distributions: As detailed above, GPDs have recently become accessible to LQCD computations. In the next cycle of the USQCD project, these calculations will be refined, and systematic errors will be controlled, aiming toward proving the much-needed theoretical input for extracting GPDs from experiments. As shown in [458], the so-called shadow GPDs represent a real challenge for extracting GPDs from experiments. Thus LQCD calculations are expected to play a central role in analyses of future experiments at the JLab 12GeV facility and the EIC.

Transverse Momentum Distributions: In the next five years, Lattice QCD is poised to make significant strides in advancing our understanding of TMDs. Calculations will continue to improve in precision and accuracy, allowing for more reliable determinations of TMDs. In particular, refined computations of the Collins-Soper kernel will be an important non-perturbative input to phenomenology. Future computations of these TMD quantities are planned at smaller lattice spacings and with larger hadron momenta, which will allow better control of the determination of the partonic spin and orbital angular momentum contributions to the nucleon spin.

3.7 Hadronic and Nuclear Spectroscopy and Interactions

Hadron and nuclear spectroscopy is critical to understanding the masses and excitations of hadrons and nuclei as well as to learning about hadronic and nuclear interactions. LQCD can be used to determine the finite-volume energies for a given set of quantum numbers; for stable particles this determines their mass (up to exponentially-small volume effects), while for unstable particles and scattering channels, the extracted energies can be used to determine scattering phase-shifts and resonance parameters. These calculations are relevant to the experimental programs at JLab [459, 460], the EIC [461] and FRIB [462], as well as to nuclear astrophysics. Exotic and heavy quark spectroscopy is a science driver for an upgrade of the JLab CEBAF accelerator [460], and a key area of investigation at LHCb, Belle-II and other HEP facilities [463–465]. Recent overviews of LQCD spectroscopy are presented in Refs. [121, 47, 122–125].

3.7.1 Accomplishments

In the previous five year period, USQCD researchers have made progress on many techniques and applications of spectroscopy.

Theoretical developments: USQCD members have made significant progress in expanding the scope of applicability of spectroscopic tools. In particular the Lüscher formalism [466] that is used to relate finite-volume energies determined in numerical LQCD calculations to scattering observables has been improved in its implementation in large-scale analyses [126–129] and extended to include the effects of electromagnetism [130, 131]. The three-particle version of this formalism has been extended to many different systems [132–140] including three-neutrons [141]. Additionally, theoretical progress has been made in connecting LQCD calculations to more complicated multi-particle quantities. These include multi-particle interactions with an external current [142, 143], two-photon production of $\pi\pi$ [144, 145], long distance electroweak interactions (for example, double β decay [146–149], see Sec. 3.9), and the form factors of resonances [150]. For nuclear systems, the matching of LQCD calculations to finite-volume pionless effective field theory has also been extended [151–153].

Significant work has been devoted to improving the technology needed for performing the Wick contractions required for multi-particle systems [154–156], through support of the NP SciDAC-5 LQCD project. First efforts to exploit quantum computing for determinations of scattering processes have also been made [157–162] (see Sec. 3.10).

Mesonic systems: Over the previous project period, USQCD researchers have turned studies of few meson systems into a precision tool. The two-pion system has been investigated extensively in all three isospin channels: $I = 0$ where the σ resonance is, $I = 1$ and the ρ resonance, and $I = 2$ [163–168, 8, 169, 170]. The relevance of $\pi\pi$-scattering for long-distance contributions to $(g-2)_\mu$ has also been investigated [171] (see Sec. 3.2). In associated work, the radiative decay of the ρ resonance has been investigated with relevance for heavy-flavor decays [172]. New work on the a_1 [173, 174] and b_1 [175] resonances has also appeared. Finally, two particle scattering in channels with strangeness including the $K^{(*)}$ resonance have seen renewed interest [176–178].

The frontier for mesonic studies has moved to three-particle systems and those that decay with three-body final states. With the refinement of the formalism needed to analyze these systems, these studies have begun to probe intricate details of the $\pi\pi\pi$, $\pi\pi K$, πKK and KKK systems both numerically [179–186], and through the expectations of chiral perturbation theory [187, 188]. Spectroscopic

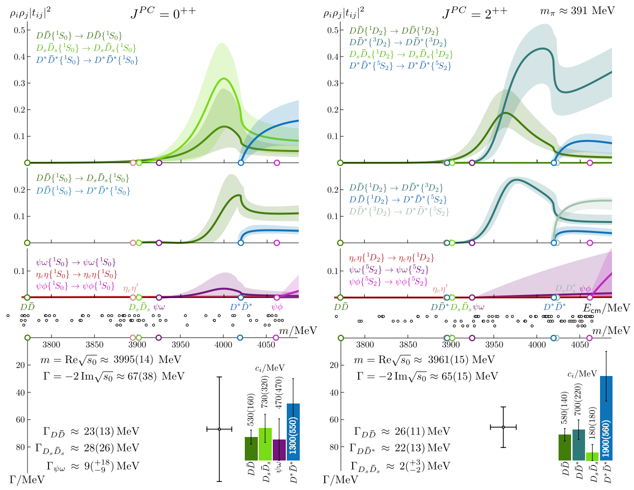


Figure 4: Scalar and tensor charmonium resonances seen in scattering phase shifts (from Ref. [213]). The top panels show the extracted phase-shifts and the bottom panels show the complex pole position of the resonance as well as information about their decay widths.

studies of $N > 3$ π^+ systems were also undertaken to investigate charged particle interactions [131] and large isospin-density [189]. The extraction of the full 3-body scattering amplitude for isospin $I = 3$ $\pi\pi\pi$ scattering, was recognized with a DOE Highlight For the First Time, Scientists Rigorously Calculate Three-Particle Scattering from Theory.

Spectroscopic studies have also been pursued with different numbers of colors and flavors of quarks. With the goal on constraining scattering in the large-N_c limit, Refs. [190–192] investigated scattering calculations with $N_c = 3$–6. Similar calculations motivated by composite Higgs models were pursued with $N_c = 3$ and $N_f = 8$ in Ref. [193], and the spectrum of baryons and mesons was investigated with $N_c = 4$ in Ref. [90] as a putative model of strongly-interacting dark matter (see Sec. 3.4).

Baryonic systems: Systems of one or more baryons present additional computational challenges that are less significant in the mesonic sector; baryonic correlation functions are statistically noisy, and multi-baryon systems have particularly small energy gaps. Consequently, multi-baryon studies are less advanced and are not yet performed at the physical quark masses.

While the stable single-baryon spectrum has been well-determined for a number of years [392][467, 468], baryon resonances are an area of active study within USQCD. Both the Δ resonance in πN scattering [194–200] and the $\Lambda(1405)$ in $\Sigma\pi$–KN mixed-channel scattering [201–203] have seen detailed studies. In the former case, studies are being extended to $N\pi\pi$ systems [45] that are relevant in neutrino scattering experiments (see Sec. 3.3). Studies of isospin effects in baryon masses have also been undertaken [204].

For two baryons, there have been investigations of the NN [205–207, 50, 208], H-dibaryon [209–211] and full baryon octet-octet [51] scattering processes. A number of these works have explored more sophisticated interpolating opertor constructions and seen dependence on these choices and consequently the LQCD understanding of these systems is not yet complete. Nonetheless, first studies of the partonic and axial structure of ^{3}He have also progressed [48, 49, 47].

Heavy quarks and exotic systems: Investigations of heavy quark [212–214], hybrids [215], and exotic [216–218] systems and their decays [219] have continued. Recent progress in determination of charmonium resonance parameters illustrates the power of LQCD spectroscopy in this sector as shown in Fig. 4.

3.7.2 Plans

In the coming period, progress is expected on both the theoretical underpinnings of spectroscopy and on numerical studies using USQCD facilities. On the theoretical side, completion of the finite-volume spectrum formalism for arbitrary-spin two- and three particle systems, including couplings between two-three states, and left-hand cuts [141, 220] is anticipated, as is the formalism for studying structure of two-particle states with one current insertion and further long-range processes such as double-β decay (see Sec. 3.9).

New studies of resonant three body systems will be undertaken including in the a_1, generic $\pi\pi\pi$ and $DD\pi$ channels which will provide insights into the ω resonance, as well as the doubly-charmed tetraquark. Controlled $\pi\pi$ and πK scattering calculations will be relevant for heavy and light-quark flavor physics studies (see Ref, 3.1). Calculations of meson-baryon scattering and eg. $N\pi\pi$ are also expected to be fully developed and will advance towards physical quark masses and finer lattice spacings. This will lead to control over pion-nucleon scattering lengths, $\Delta(1232)$, Roper, and $\Lambda(1405)$ resonant structures, and axial transitions such as $N \to \Delta$. Calculations of nucleon-nucleon scattering amplitudes will be performed at physical values of the quark masses and studies of hyperon-nucleon and hyperon-hyperon interactions will progress. Continued work on coupling of two baryon systems to external currents is planned. Beyond two-baryon systems, renewed progress on NNN and $NN\Lambda$ interactions and light nuclear spectroscopy is planned

Heavy quark spectroscopy is a very active area of research with a rich spectrum of possible states suggested by experiments. LQCD is well suited to address the challenges in our understanding of such systems. Photoproduction is a tool for spectroscopy, and future calculations will compute the photo-decay couplings for heavy quark and possible exotic states enabling a comparison of their resonant structure with hadronic decay extractions. Exotic systems such as the partners of the π_1 and tetraquarks will be studied as well as excited-states in systems with the quantum numbers of the D_s and B_s mesons. New calculations of the latter with $J^P = 0^+$ and 1^+ B_s will inform phenomenology as these states have not yet been observed in experiments, leading to confusion in the phenomenology community.

3.8 QCD at nonzero temperature and densities

Understanding the properties and phase diagram of strongly interacting mater at high temperature and density is one of the major goals of contemporary nuclear physics research. Experimentally these questions being explored in heavy ion collisions at RHIC and LHC. Lattice QCD calculations provide valuable input for these experimental programs.

3.8.1 Accomplishments

In 2019-2024 the hot-dense QCD lattice efforts had three major thrust: study of QCD thermodynamics at nonzero baryon density, exploring the critical behavior of the chiral transition in the limit of vanishing light quark masses and the study of spectral functions related to heavy quark observables. The first and the second thrusts are related to the beam energy scan program at RHIC and the search for the critical end-point on the QCD phase diagram. The last thrust is important for the study of heavy flavor probes in heavy ion collisions that are used in STAR and sPHENIX experiments at RHIC as well as in the heavy ion program at LHC, such as quarkonia yields and spectrum of open heavy flavor hadrons.

The QCD thermodynamics has been studied using Taylor expansion of the QCD free energy up

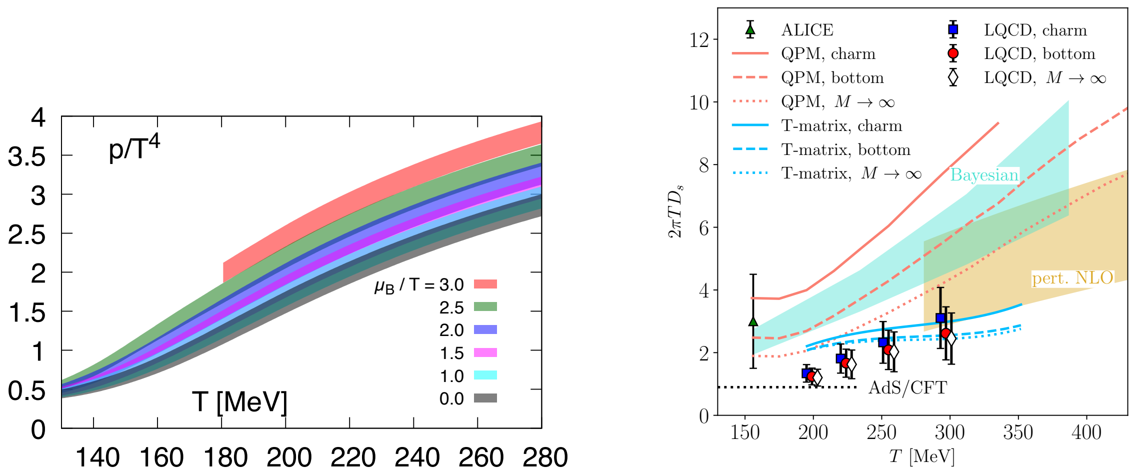


Figure 5: The QCD pressure as function of the temperature (T) for different values of the baryon chemical potential (μ_B) [221] (left). The heavy quark diffusion coefficient from lattice QCD calculations [222, 223] compared with NLO perturbative QCD predictions, from AdS/CFT and from various phenomenological models (right).

to eighth order [224, 225, 221, 226] [393]. The Taylor expansion coefficients are also related to the fluctuations of conserved charges that can be studied experimentally at RHIC. The fluctuations of Baryon number has been calculated as function of the chemical potential and compared to the RHIC data [224]. The pressure, energy density and the speed of sound have been obtained from the Taylor series [221]. The results are shown in Fig. 5 (left). Using Pade resummation of the Taylor series it was concluded that the Taylor expansion can be used up to $\mu_B/T = 2.5$ [226]. The study of the pole structure of the Pade revealed that there no singularities in μ_B close to the real axis for $T > 135$ MeV [226]. This implies that the critical point is likely located at $T < 135$ MeV. Similar conclusion was reached using exponential resummation of the Taylor series [227].

Using lattice calculations at three different temporal extent, N_τ, it was demonstrated that the properties of the chiral transition in 2+1 flavor QCD are consistent with the expected universal $O(4)$ scaling [228, 229]. Furthermore, the chiral phase transition temperature in for physical strange quark mass and vanishing light quark mass was determined to be $T_c = 132^{+3}_{-6}$ MeV [228]. Furthermore, the dependence of chiral phase transition temperature on the chemical potential has been studied at leading order in the Taylor expansion, and it was found that the leading order curvature coefficient of T_c is similar to the corresponding curvature coefficient of the chiral crossover temperature at physical light quark masses [230]. Together with the above value of T_c this implies that the temperature corresponding to the critical end point, T^{CEP} on the QCD phase adiagram in $T - \mu_B$ plane has to be smaller than 132 MeV [231]. This is consistent with the estimates for the location of the critical end-point based on the analysis of the Taylor expansion above. In Ref. [230] the magnetic equation of state— the dependence of the chiral condensate on the temperature and quark mass— was determined along with the non-universal scaling parameters, t_0 and h_0, that map QCD to the $O(4)$ model. These parameters play an important role in the analysis of the convergence of the Taylor expansion. Extending the scaling function into the complex place allows one to estimate the singularities of the QCD pressure in the complex plane μ_B plane [232].

The bottomonium in-medium mass shift and width have been estimated in Ref. [233–235]. Interestingly, no significant in-medium mass shift was observed. On the other hand, the thermal widths, which are related to the dissociation rate of bottomonia states, were found to be sizable [233, 234] Using spatial meson correlation function the melting temperature of the $\Upsilon(1S)$ has been estimated to be larger than 350 MeV (DOE NP Highlight: Getting to the Bottom of When the Smallest Meson Melts) [236]. For long quarkonium melting was thought to be related to the screening of the heavy quark anti-quark potential. The complex potential was estimated and, interestingly, it was found that the real part of the potential is not screened [237, 238]. The imaginary part of the potential, on the other hand, was found to be large and is the likely cause of the quarkonium dissociation [238]. The transverse momentum spectra and azimuthal anisotropies of the open heavy flavor production is believed to be related to the heavy quark diffusion coefficient. This quantity is also important for estimating the quarkonium regeneration rate in quark-gluon plasma (QGP). The heavy quark diffusion coefficient has been calculated on the lattice using lattices with temporal extents $N_\tau = 20 - 36$ and light quark masses that correspond to the pion mass of 320 MeV [222, 223]. The spatial heavy quark diffusion coefficient was found to be quite small close to the lower bound estimated for strongly coupled gauge theories using AdS/CFT, see Fig. 5. This means that the heavy quark thermalized quickly in QGP (DOE Highlight: Calculation Shows Why Heavy Quarks Get Caught Up in the Flow).

3.8.2 Plans

Calculations based on the Taylor expansions of the QCD pressure have, so far, provided some bounds on the location of the critical end-point: $T^{CEP} < 135$ MeV, $\mu_B^{\mathrm{CEP}}/T^{\mathrm{CEP}} > 2.5$. In future it will be important to refine the estimates of the location of the critical end-point on the QCD phase diagram. This can be done by performing calculations of the Taylor expansion coefficients of the QCD pressure at many values of the purely imaginary chemical potential, μ_I. One then can combine the information from Taylor expansion with the dependence on μ_I in a multi-point Pade approximation of the QCD pressure, which then allows a better estimate of the singularities of QCD pressure that can be related to the location of the critical end-point [469, 470]. We plan to perform such studies in the near future.

For reliable estimates of the thermal widths of different bottomonium states it will be important to extend the previous calculations to lattices with larger temporal extents. We plan to study bottomonium correlation functions at nonzero temperature using lattice with $N_\tau = 20 - 28$, and using these correlation functions improve the estimates of thermal mass shift and width. The calculation of the heavy quark diffusion coefficient was performed at nonphysical values of the light quark masses. The dependence of this quantity on the light quark mass is expected to be significant for temperatures close to the chiral crossover temperature. Therefore, it will be important in the future to extend the calculations of the heavy quark diffusion coefficient to the physical light quark masses.

3.9 Fundamental symmetries

A key area of research in both nuclear and high-energy physics is that of understanding the fundamental symmetries of nature and their violations. Symmetries have been central to the development of the Standard Model and to testing theories beyond it. Fundamental symmetry tests in the form of double β decay experiments are a high priority in the nuclear physics community long range plan [397].

3.9.1 Accomplishments

Electric dipole moments: If seen, an electric dipole moment (EDM) would provide evidence of time-reversal symmetry (T) violation [471, 472]. Such T violation can have many origins and LQCD calculations addressing EDMs arising from a QCD θ term, quark EDMs and the so called Weinberg operator have been pursued within the previous project period [239–246].

Precision beta decay: Experimental studies of the weak decay of the neutron [473, 474], $n \to pe\overline{\nu}_e$ have reached unprecedented precision in recent years, reaching comparable uncertainties in the extraction of the CKM matrix element $|V_{ud}|$ as found in super-allowed nuclear beta decays [475]. An important component in precision determinations is a re-evaluation of radiative corrections [476, 477] and electroweak box contributions where there has been important progress in LQCD calculations recently [247, 248] (related work also tackled the two-photon contributions to the muonic-hydrogen Lamb shift [15]). In comparison with LQCD calculations [249][394][398] of the ratio of axial and vector charges, g_A/g_V, these experiments offer the possibility of improved constraints on BSM right-handed currents as well as scalar and tensor interactions, provided new levels of precision can be reached. Direct LQCD calculations of scalar and tensor charges [250] have also been performed in recent years.

Baryon number violation: In the Standard Model, baryon number, B, is expected to be an almost exact symmetry (sphalerons induce B-violation but are exponentially suppressed below the electroweak phase transition) and searching for processes that violate this symmetry provides a window into BSM physics [478]. The most common processes that are looked for experimentally are proton decay, n–$\bar{n}$ oscillations and neutron decay to sterile mirror neutrons [478]. To convert any signal for such a process into constraints on BSM physics requires hadronic inputs in the form of QCD matrix elements of B-violating operators. In the past review period, matrix elements have been computed for both proton decay [251] and n–$\bar{n}$ oscillations [252].

Lepton flavor violation: Processes such as $\mu \to e\gamma$ violate the approximate Standard Model symmetries of electron number and muon number and so are sensitive to new physics contributions [479]. The Mu2e experiment, which searches for $\mu \to e$ decay in the background of the strong electric field of an aluminium nucleus, will soon beginning operation at Fermilab. One of the primary mechanisms for this process involves high-scale BSM physics that induces a scalar-current coupling of the decaying leptons to the quarks inside the nucleus and so this process is sensitive to the scalar charge, or σ-term, in nucleons and nuclei. In the past few years USQCD members have undertaken calculations of these matrix elements in the proton [253, 254] and explored calculations in ^{3}He nuclei [49].

Double beta decay: As with baryon number, lepton number, L, is a symmetry of the Standard Model (again, up to sphaleron effects), and searches for L-violation are ongoing. The most dramatic target for such searches is neutrinoless double-β decay ($0\nu\beta\beta$), a process that can occur through two weak interactions if neutrinos are their own antiparticles. Such decays are also possible if there are new L-violating interactions at high energies. If it occurs, $0\nu\beta\beta$ can only be observed in nuclei where regular β-decay is energetically forbidden. Nuclear models and effective field theory can be used to estimate the relevant nuclear matrix elements in the double weak-decay case, but have unquantified uncertainties. LQCD offers the prospect of constraining those uncertainties through calculations of $0\nu\beta\beta$ transitions in small nuclear systems. USQCD members have led multiple calculations in this direction, first addressing the sub-process $\pi^- \to \pi^+ ee$ [255–257] as well as the more phenomenologically relevant $nn \to ppee$ process [24]. A review of the prospects and opportunities in this area was also published [258] and the theoretical framework for connecting from LQCD to experimental constraints has been investigated [147–149].

3.9.2 Plans

Electric dipole moments: Since T-violating EDMs can have their origin in multiple BSM scenarios, understanding the mechanism responsible for a future observed EDM requires calculations of EDMs of various targets. While electron and neutron EDMs are the most well studied, new efforts plan for storage-ring measurements of the EDM of the proton and deuteron. Concurrent lattice calculations of operators relevant for T-violation will be required for all hadronic systems that are investigated experimentally (protons, neutrons, and light-ions) to realize the full potential of such searches. Additionally, for some sources of T-violation such as the Weinberg three-gluon operator and four-fermion operators, LQCD calculations are only at their earliest stages and more work is envisioned in the coming period.

Baryon and lepton number violation: New studies of baryon and/or lepton number violating processes are anticipated. With a range of experiments coming on line in the near term, there is renewed impetus for LQCD calculations in this area. With Hyper-K aiming for an order on magnitude increase in sensitivity for proton decay [480], a new set of LQCD calculation of the relevant matrix elements is planned and there is potential for extension of these calculations to small nuclei where there are interesting experimental prospects [481]. Similar improvement of calculations relevant for $\Delta B = 2$ $n\bar{n}$-oscillation searches are also likely. With the community endorsement of a new class of neutrinoless double-β searches in the 2023 Nuclear Science Long Range Plan, LQCD calculations that help to constrain nuclear models and thereby allow interpretation of observation or lifetime limits in terms of fundamental neutrino physics are critical. Given the results of the feasibility study [24] performed at unphysical quark masses, a clear goal for the coming period is a physical mass calculation of the $nn \to ppee$ process at multiple volumes, thereby allowing first constraints on the dominant low-energy constant in nuclear effective field theory.

Other processes: Given the success of first LQCD calculations of electroweak corrections in beta decay, further studies are planned to address systematic uncertainties in a more complete manner and first evaluations of similar γZ-box contributions in parity-violating deep-inelastic ep scattering are planned in preparation for the upcoming MOLLER and SoLID experiments. Work on $\Delta I = 2$ hadronic parity-violation, and improved calculations of axial, scalar and tensor charges of the nucleon are also planned.

3.10 Computational Tools and Architectures including ML and QIS

The computational cost of state-of-the-art lattice QCD calculations is formidable. USQCD's approach to meeting this challenge is at the forefront of high performance computing, with efforts advancing areas spanning hardware architecture design, applied mathematics, and software and workflow technologies, through to machine learning and quantum computing. Importantly, maintaining close links with industrial partners has enabled co-design and early adoption and exploitation of new hardware technologies. Examples include ACPMAPS, QCDSP, QCDOC, and IBM Blue Gene, which were designed or co-designed by lattice gauge theory teams, as well as the early adoption of GPUs and Intel Xeon Phis. As a result of continued efforts at this frontier, the USQCD collaboration is positioned to fully exploit exascale systems and beyond.

Simultaneously, the Collaboration continues to invest effort in preparation for future hardware. Recent trends in high performance computing have raised to prominence the rapidly developing areas of machine learning, big data analysis, and quantum computing. Deep learning has commercial applications that are influencing both hardware (e.g., in the development of Tensor Processing Units) as well as software approaches. While machine learning, and machine-learning-specific hardware, has not yet been applied at a large scale to lattice-QCD calculations, the approach has great potential in this context and applications are under active development within the collaboration. Similarly, although the use of quantum computing for production lattice-QCD calculations is many years away, the collaboration is working to be ready for its exploitation, developing the necessary computational frameworks and working with early quantum computing systems.

3.10.1 Accomplishments

Early hardware adoption and software readiness: Early adoption of new hardware by the Collaboration has been historically been key in enabling both immediate preparedness for Collaboration codebases to run efficiently at new generations of leadership-class facilities (LCFs), but also to enable the continued innovation that drives the USQCD science program forward.

Examples in the last reporting period include specific preparation for LCFs: JLab acquired AMD GPUs before Frontier, creating a system that was synergistic with the other test systems at the time e.g., those at Oak Ridge. For the past four years, members of USQCD have been working closely with Intel optimizing lattice QCD codes to exploit the Ponte Vecchio architecture and the SYCL programming model and are now contributing to the bring-up of Aurora. As a result, beyond the Collaboration's involvement in the U.S. Exascale Computing Project (ECP) which included efforts to prepare many elements of USQCD software for Frontier, the entire Collaboration was able to access this hardware early and prepare efficient workflows. The USQCD contribution to the ECP project has encompassed many areas including the improvement of gauge field generation, research in the areas of linear solver and related algorithms (e.g., eigensolvers, and trace estimation), a re-tooling of the software infrastructure paying special attention to upcoming architectures, modularization and layering of software components and their interoperability, novel computing languages, and new programming models to provide productivity and performance portability. Broadly, USQCD has coordinated member involvement in the full spectrum of Early Science Programs (ESP), spanning from the Argonne Leadership Computing Facility ESP, through the Center for Accelerated Application Readiness (CAAR) program at Oak Ridge, through the NERSC Science Acceleration Program (NESAP), ensuring application readiness at all relevant facilities.

Algorithm and software development: Within the last reporting period, the USQCD Collaboration has made considerable progress in both software and algorithm development. This spans the full pipeline from novel approaches developed and tested on USQCD hardware, through to broad participation in programs such as the DOE Scientific Discovery through Advanced Computing (SciDAC) program, preparing novel collaboration software to exploit the architectural diversity of currently available computing hardware.

On the algorithm side, recent progress includes specific work to improve and expand the applicability of multigrid techniques [259–261], the exploration of the multi-splitting algorithm as a preconditioner for Dirac inversions [262], investigation of gauge-fixed fourier acceleration of HMC [263], the development novel contraction algorithms [154–156], and advances in the area of inverse problem solving [53]. The collaboration has also exploited the Aurora Early Science Programs, including within the Data and Learning program where efforts include the development of novel machine learning approaches to lattice QCD algorithms (discussed separately below).

Machine Learning (ML): The Collaboration has made significant advances to define how ML techniques might be exploited to enable and accelerate lattice field theory calculations. This presents a number of challenges, in particular that ML methods must be re-designed from the ground up, rather than straightforwardly adapted from their use in other fields, to be effective in the lattice QCD context [264, 265]. In particular, ML implementations that incorporate the complex exact and approximate symmetries of lattice-QCD datasets must be developed, and rigorous methods of uncertainty quantification and error propagation must be investigated.

Within the last reporting period, the collaboration has made rapid progress in exploring how this new class of approaches can be used to accelerate all aspects of the lattice QCD workflow. For example, in the generation of lattice QCD gauge fields approaches have been developed that show promise to overcome critical slowing down in HMC as the lattice spacing is decreased [266–278], including various approaches to this task. Similarly, efforts have explored parameter optimization [395], and the acceleration of sparse matrix inversions [279], which are a significant cost in lattice QCD calculations. Various approaches to reducing statistical uncertainties through correlator optimization [280–282], and sign-problem mitigation through manifold deformation [283–286], have also been explored.

Quantum Information Science (QIS) and Quantum Computing (QC): On the frontier of QIS and QC, the last reporting period has seen a phase transition in defining the potential utility and application of these methods in lattice field theory research in the future. In particular, the objectives of the program have been identified [287–289, 287] [482, 483], and can be summarized as enabling first-principles simulations of matter in regimes where sign and signal-to-noise problems challenge the Monte-Carlo based computations of gauge theories. These involve finite-density systems (ranging from studies of nuclei to phase diagram of matter under extreme conditions, such as in the interior of neutron stars), real-time dynamics of matter in early universe and in high-energy particle collider, including its thermalization and hadronization mechanism, hadron and nuclear structure and reaction properties including dynamical response functions for neutrino-nucleus scattering and parton distribution functions for the LHC and EIC.

The practical developments to date by the USQCD members involve theory, algorithm, and implementation and co-design efforts. Many Hamiltonian formalisms have been developed for several lattice quantum field theories [290–305], and have been put to work in both numerical studies and in quantum-simulation algorithms and implementations. Time-digitization algorithms have been applied to almost all field-theory studies, including U(1), SU(2), and SU(3) gauge theories, and their associated errors have been analyzed in detail [306–316, 304]. State preparation, including preparation of interacting vacua, hadronic states, hadronic wave packets for scattering, and thermal states have been analyzed [160, 161, 317–321, 306, 322–325], although all demonstrations are still limited to 1+1 and 2+1 dimensions in small systems. Quantum algorithms to access a range of physics observables and entanglement properties exist. Spectroscopy, scattering amplitudes, hadron structure functions and other non-perturbative functions of relevance to collider physics, transport coefficients, probes of static and dynamical phases and phase transitions, and of thermalization, are among these observables, although demonstrations, if any, have been limited to small system sizes and/or simpler models [326, 327, 157, 328–332]. Finally, theoretical, algorithmic, and hardware errors have been partly or fully analyzed in various contexts [333, 334, 303, 304, 291, 159, 335–341]. All this progress has been accompanied by implementations on state-of-the-art platforms, although still not at a scale that enables simulation of Standard-Model theories, due to the limitations of the hardware technology today.

3.10.2 Plans

Early hardware adoption and software readiness: Over the next reporting period further development of GPU lines e.g., the evolution of AMD's MI300/MI400 line and Nvidia's Blackwell B100/B200 line is to be expected. Continued efforts will be required to maintain USQCD software readiness for new facilities including OLCF-6 and NERSC-10. It can be expected that current trends will continue as compute nodes become more dense and powerful, inter-node communication bandwidth relative to node performance is reduced, and memory hierarchies deepen, demanding further adaptation and continued research into algorithms that can reduce or avoid communications to achieve the twin goals of optimal performance and energy efficiency.

As ML approaches to lattice field theory continue to advance, it will also be important for the collaboration to maintain flexibility in the hardware program to adopt other novel processor technologies when they become relevant. For example, recent substantial performance gains coming from the use of Tensor Processing Units (TPUs) through optimized GEMM routines can be more broadly exploited in USQCD software. It may also be appropriate to consider quantum hardware if the science case for such a testbed evolves (see further discussion below).

Algorithm and software development: Specific goals include further efforts to develop efficient contraction codes, and continued development of multi-grid solvers in gauge generation, including for domain wall fermions. Several interesting research avenues are to attempt to reduce the cost of subspace creation, for example by using an adaptive process. The strong scaling challenges can also be tackled for example using domain-decomposed preconditioners and communication avoiding solvers. Higher raw performance may potentially be obtained by working with multi-grid algorithms in a block-solver mode solving several systems at once. This will be especially important as larger physical volumes are studied and the exploding storage requirements of the now very successful eigenvector-driven deflation schemes become untenable. Fitting this block solver approach into an HMC algorithm still requires additional research.

Critical slowing down of the generation of gauge ensembles as the lattice spacing decreases is an increasingly important difficulty that substantially increases the computational cost of exploring the continuum limit and threatens the ergodicity of large-scale calculations. Research on this topic will receive continued high-priority attention with SciDAC-5 support, including production-scale, full-QCD studies of both gauge-symmetry-aware Fourier acceleration techniques and HMC evolution using Wilson-flow-transformed gauge variables. This algorithmic challenge is also addressed by the new efforts that exploit ML described below.

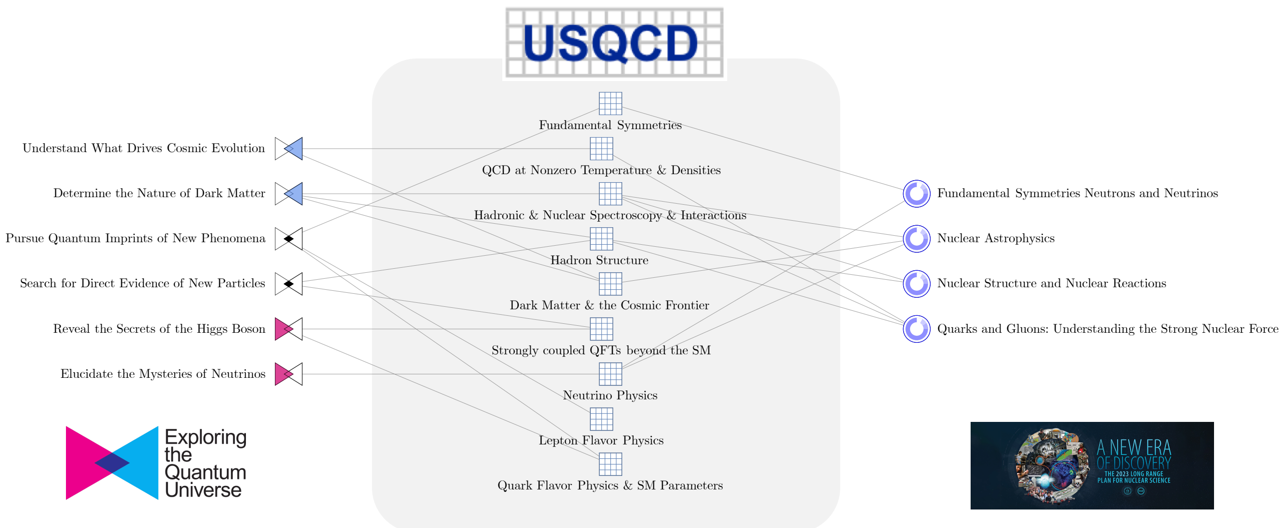
Machine Learning (ML): The Collaboration is well-situated both to continue to develop novel ML approaches to lattice field theory problems, and to support the scaling of these approaches such that they may be deployed in state-of-the-art applications for the first time. Specifically, within the next reporting period approaches that have been developed to gauge field generation, parameter optimization, propagator inversion, and sign-problem mitigation, will be scaled as their application is tested in settings growing from toy examples to QCD applications at a moderate scale.

The USQCD hardware program will allow the Collaboration to continue to be responsive as needs on this frontier develop. Immediate planned GPU hardware purchases support current ML approaches, and enable this important developmental work. In the future, the purchase of ML-specific hardware for development and testing can be considered, if it becomes appropriate to collaboration needs over the next 5 years.

Quantum Information Science (QIS) and Quantum Computing (QC): USQCD established a committee in 2019 to perform ongoing evaluations of QIS and QC as they relate to quantum field theory and quantum chromodynamics. This committee is expected to provide regular updates to the USQCD Executive Committee, creating a structure that enables the collaboration to effectively pivot as appropriate to exploit these new technologies as they continue to develop.

Key goals for the collaboration over the next reporting period will include continued work to understand how to map given quantum field theories onto a variety of analog quantum simulators, including atomic, molecular, optical, and solid-state systems, each with distinct intrinsic degrees of freedom, native interactions, and connectivity properties, and to co-develop along with hardware developers enhanced modalities and advanced quantum-control capabilities to facilitate simulating complex field theories of nature. It will be particularly important to conduct careful studies to determine whether industry-developed quantum hardware satisfies the needs of the HEP/NP community or if special-purpose hardware may need to be co-designed, following the development and application of special-purpose HPC hardware/software in the lattice-QCD research in the past. Simultaneously, it will remain important to exploit both QIS and current advancements on classical computation of field theories by developing strategies of augmenting classical computing with quantum-computing routines.

4 Relevance to HEP and NP priorities



The broad physics program of the USQCD collaboration impacts many aspects of high-energy and nuclear physics that are central to the long range plans of the broader communities. USQCD collaboration members were deeply invested in the recent Snowmass process in HEP, being involved in about 50 whitepapers. Similarly, USQCD input was critical to the community planning process in nuclear scince, with USQCD helping to organize a town hall meeting on Computational Nuclear Physics. USQCD members C. Monahahn and J. Dudek were members of P5 and the NSAC LRP writing committee, respectively.

In the above figure, the connections between USQCD science goals and the science drivers of the 2023 P5 report and NSAC LRP that are described in Sec. 3 are shown explicitly. The science accomplishments and plans discussed above also align with many of the facilities supported by DOE HEP and NP.

In HEP, LQCD calculations of neutrino-nucleus interactions (Sec. 3.3) are critical theory input for the science driver of "Elucidating the Mysteries of Neutrinos". Hadronic matrix elements in quark and lepton flavor physics (Secs. 3.1 and 3.2) are central components of the drivers "Pursue Quantum Imprints of New Phenomena" and "Reveal the Secrets of the Higgs Boson". LQCD constraints on parton distributions (Sec. 3.6) and understanding of strongly interacting QFTs (Sec.!3.4) are both important for the "Search for Direct Evidence of New Particles". Additionally, lattice studies of QCD matrix elements (Secs. 3.6 and 3.7), thermodynamics and phase transitions (Sec. 3.8), and models of strongly-interacting QFTs (Sec. 3.5) provide input into the drivers to "Determine the Nature of Dark Matter" and "Understand What Drives Cosmic Evolution". For nuclear physics, LQCD calculations of hadron structure and spectroscopy (Secs. 3.6 and 3.7) are critical to the driver to "Understand the Strong Nuclear Force" and to the interpretation of the results of the experimental programs at Jefferson Lab and the future EIC. Studies of QCD in extreme conditions (Sec. 3.8) are vital for the heavy-ion experimental programs at RHIC and the LHC. Calculations of hadronic contributions to rare or forbidden processes (Sec. 3.9) those involving neutrinos (Sec. 3.3) underpin searches and precision test in the driver of "Fundamental Symmetries, Neutrons and Neutrinos" and will be important for ton-scale $\beta\beta$-decay experiments. Finally LQCD inputs on hadronic and nuclear interactions and structure are becoming increasingly relevant to science drivers in the areas of "Nuclear Astrophysics" and "Nuclear Structure and Nuclear Reactions" and experiments at the Facility for Rare Isotope Beams.

5 Need for LQCD facilities

With uncertain access to leadership-class supercomputers, the continuity and accessibility of USQCD hardware ensure that important projects can persist over time, even in the face of unforeseen challenges. This stability is crucial for sustaining long-term research efforts and fostering collaborations that span multiple years. For example, USQCD resources have contributed significantly to the large multiyear lattice QCD studies on hadronic-vacuum-polarization [342, 31] and hadronic light-by-light [32] contributions to the muon's anomalous magnetic moment, hadron structure [343–348, 106], and QCD thermodynamics [393][349, 224], resulting in high-impact publications between 2019-24.

Alongside the large multiyear lattice QCD studies, many significant physics problems in lattice QCD can be effectively addressed using small-scale dedicated hardware, particularly when combined with community-wide gauge configurations generated on larger supercomputers. USQCD's hardware provides an ideal platform for leveraging these resources, allowing researchers to tackle a wide range of research questions efficiently and effectively.

USQCD hardware is instrumental in supporting exploratory research projects. Due to their lack of well-defined deliverables, these exploratory studies are not suitable for INCITE or ALCC awards on supercomputers. But often these exploratory lattice QCD studies serve as the foundation for future larger-scale endeavors. In many cases, these projects, initiated with the support of USQCD resources, have evolved into groundbreaking lattice studies.

USQCD resources, particularly the CPU-based machines, offer low-barrier platforms for the rapid development and testing of new algorithms and software implementations.

USQCD hardware has served as invaluable testbeds for developing codes and applications for future leadership-class machines. Time and again, USQCD has provided a platform for researchers to explore and optimize algorithms on emerging architectures before they become available in larger supercomputers. For instance, USQCD has been instrumental in testing and refining codes for IBM Bluegene Q, NVIDIA GPU, Intel KNL, and AMD and Intel GPU-based architectures, giving the lattice QCD community a significant advantage in adapting to these technologies. This proactive approach has enabled researchers to gain a head start on understanding and harnessing these architectures, ultimately positioning them as leading users of future leadership-class machines based on similar or evolved architectures.

In addition to its other crucial roles, USQCD hardware also serves as a vital resource for workforce development within the lattice QCD community. By providing opportunities for graduate students, and postdocs to lead small-scale projects, USQCD cultivates talent and nurtures future leaders in the field. Furthermore, the support offered by USQCD enables early-career faculty members to develop innovative ideas and secure prestigious awards from organizations such as the DOE or NSF.

6 Setting collaboration priorities

This proposal sets the the overall priorities for the LQCD Computing Initiatives, and the stewards for the research program are the Executive Committee (EC) and the Scientific Program Committee (SPC) of USQCD. (For current membership, see Appendix A.) Individual collaborations submit proposals requesting leadership scale computing resources directly to Leadership Computing Facilities (LCF). As noted in the introduction, most of these projects also require cluster computing to turn the LCF outputs (for example, millions of files containing hadron correlation functions) into physics results.

In addition to supporting LCF workflows, the SPC receives and supports dozens of proposals for research limited to small and medium sized lattices that the clusters can capably process. The SPC evaluates the proposals in light of the scientific priorities of USQCD and allocates time on the USQCD clusters at BNL, FNAL, and Jlab according to computational needs.

One should anticipate that new goals will arise during the coming five years while some may decline in importance. For example, should independent two groups reach the target precision for a particular result, this topic may no longer require significant resources. If a major discovery is made, new topics may bubble up or existing ones may 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 LCF 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 [125, 228, 350, 35, 351–353]. Further, the DOE's annual review of the research program's technical milestones has always 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 and NP the opportunity to influence 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 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 breakdown of the SPC's allocation of cluster time for 2023–2024 is approximately 30:40:30 for HEP:both:NP topics.

The science priorities, reflected in allocations, also drive the hardware priorities. USQCD was an early adopter of GPUs, first using them as single compute units, then aggregating them into clusters, typically for propagator calculations and later for gauge field generation. Finally computations moved onto leadership resources featuring GPUs. Today the hardware acquisition committees, composed for each purchase, look at the needs and gaps in hardware support for the research programs, and respond with recommendations for acquisitions.

Applications of QIS, as described in Section 3.10, have novel computing requirements. GPU systems are well suited to Machine Learning which take advantage of the tensor core, low floating-point precision, and high memory bandwidth architecture. USQCD already is responding to these computational needs with the LQ2 NVIDIA-GPU cluster acquisition at FNAL. In the future there may be a compelling need to acquire even more dedicated systems, such as Tensor Processing Units (TPU-s).

The Emergent Technologies Committee was created by USQCD in 2019 to provide advice on new technologies, such as TPUs, and also Quantum Computing. In addition, several USQCD members are actively participating in Quantum Computing projects, evaluating their potential, and investigating reformulations of non-perturbative spin systems and field theories that take advantage of the capabilities provided by such innovative systems. USQCD members – Martin Savage and Yannick Meurice – are leaders in the community of scientists actively engaged in this topic. At this point in time, USQCD has not found a sufficiently compelling justification to invest in Quantum Computing hardware solutions. However, the collaboration is closely following the rapid developments and advice from the committee.

7 Management

Although this document focuses on the science case for funding the LQCD computing initiatives, the proposed research program cannot be completed without sound management. Full details concerning project management can be found in the Program Execution Plans submitted by FNAL and JLab, and further details on USQCD can be found in Appendix A and the website `https://www.usqcd.org`, particularly the USQCD Charter

Alan G. Prosser (Fermilab) will be the Program Manager (PM) for the HEP initiative and Amitoj Singh will be the Program Manager for the NP initative. The two Program Managers will coordinate their efforts. The FNAL Program Manager will be responsible for negotiating Memoranda of Understanding with FNAL and BNL, the participating institution receiving HEP funds, for access to their institutional clusters, deciding the optimal distribution of funds, and tracking the technical milestones in FWP FNAL 25-29. Alan Prosser is the key interface to the DOE/HEP for financial matters, reporting, reviews, will maintain documentation, tracking expenditures, and monitoring progress in achieving the FWP FNAL 25-29 milestones. Prosser is carrying the same role for LQCD-ext III. The NP Program Manager is the key interface to DOE/NP for financial matters, reporting, reviews, documentation, tracking expenditures, and monitoring progress in achieving the FWP NP 25-29 milestones. Singh has been carrying this role since he joined JLab under the NPPLC Initiative. USQCD is very fortunate to be supported by such talented, experienced, and dedicated project managers.

Each participating laboratory has a Site Manager, currently Kenneth Herner at FNAL, Zhihua Dong at BNL, and Amitoj Singh at JLab. In addition to their part of the roles listed above, they are the key personnel for user support. At JLab, BNL, Fermilab and JLab 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.

In the dedicated-cluster model, the host laboratories and LQCD managers have several roles: designing, procuring, building, and operating the clusters. The host labs work closely with the LQCD Computing Initiative Business Manager, the Site Manager, and the Site Architects, to devise a plan for the timeline, finances, and input for the procurement process. During the last year of LQCD-ext III, the management team and BNL are having a constructive relationship, in their deliberations for the BNL dedicated computing facility. Under NPPLCI, the JLab facility has procured several systems under the dedicated-cluster model. The deliberations, procurement and deployment of the system have proceeded very smoothly with constructive conversations with the LQCD and lab management teams. Currently, JLab is in the final stages of deploying its new '24s' system that was procured at the end of FY23.

The Chair of the USQCD Executive Committee, Robert Edwards (JLab), serves as the scientific Spokesperson for the effort; Thomas Blum (Connecticut) 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 Managers, and the Program Managers's progress reports to the Executive Committee. The Program Managers, and Scientific and Deputy Spokespersons meet by conference call with each other and the LQCD-ext III 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.

The Emergent Technologies Committee provides advice on new technologies as described in Section 6. Martin Savage has been the chair of the committee, and the USQCD Executive Committee Chair serves in an ex-officio role.

The Chair of the USQCD Committee on Diversity, Equity and Inclusion, William Detmold (MIT), serves as the spokesperson for the CDEI efforts. More description of the PIER plan and DEI activities are provided in Sec. B.

The Scientific Advisory Board provides advice on USQCD scientific goals, how we are meeting them, and evolution of the goals. Recently, the SAB gave advice on the Snowmass 2021 process and EIC developments to the Executive Committee. The Chair of the USQCD Executive Committee and the Deputy Chair coordinate activities, including soliciting input on whitepapers, proposals, and experimental priorities.

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 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 2023 and 2022 there were no changes, but in 2021 there were two changes. 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. 7. Members serve terms of 3–4 years. The current members are Peter Petreczky (BNL, Chair), James Simone (FNAL, deputy Chair), Martha Constantinou (Temple), George Fleming (FNAL), Christopher Kelly (BNL), Stefan Meinel (Arizona), and Sergey Syritsyn (Stony Brook).

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), Roy Briere (Carnegie Mellon, Belle II, BES III), Abhay Deshpande (Stony Brook, RHIC, EIC), Lawrence Gibbons (Cornell University, Mu2e), Kendall Mahn (Michigan State, T2K, DUNE), Krishna Rajagopal (MIT, theory), Matthew Shepherd (Indiana University, GlueX, BES III), and Jure Zupan (University of Cincinnati, theory).

The software created under the SciDAC and Exascale Computing Project (ECP) grants has greatly enhanced the effectiveness with which USQCD member use the hardware resources, whether leadership-class or clusters. ECP completed at the end of CY2023. Software development continues under SciDAC-5 (HEP and NP). All of the software developed under the SciDAC grants is publicly available, and can be found at `https://usqcd-software.github.io/`.

B PIER Plan

The USQCD collaboration is invested in promoting diversity of its membership and providing a research environment that is equitable and welcoming to all. Over the previous five years, the collaboration established a Committee on Diversity, Equity and Inclusion (CDEI) and enacted a number of efforts to bring new members into the collaboration, enable better access to resources for junior members and improve the climate at USQCD scientific meetings.

B.1 Collaboration Activities 2019-2024

- *Early career executive committee members*: the collaboration is mindful of the different experiences of members at different career stages. To make sure junior collaboration members are heard, the executive committee has included a junior member since 2016 who serves for 2 years and is elected by the collaboration. This position has been held by William Detmold, Christoph Lehner, Huey-Wen Lin and currently is held by Phiala Shanahan.
- *Early career computing access*: USQCD believes that it has a responsibility to support the development of junior members. As computational scientists, access to computing for graduate students and postdocs for independent projects can be difficult to obtain, particularly on high-performance systems set up for LQCD calculations. To support our junior members, the CDEI-recommendation of a "junior-member track" in the annual Call for Proposals was adopted in 2021, allowing the SPC to specifically weight proposals for junior members. Postdocs are able to submit independent projects and have done so in significant numbers. Graduate students can also submit proposals for their thesis research with their advisor as a mentor (thus far, only a few graduate students have taken advantage of this track, so more encouragement is needed).
- *Hackathons*: USQCD members have run hackathons to introduce new users to USQCD software for many years. These often take place around the annual Lattice conference, for example C. Lehner's Grid Python Toolkit tutorials at Lattice 2021 and 2022. USQCD member Joel Giedt has also run a computational science school each year from 2018 to 2023 at RPI with support for NSF that has been very successful in providing access to instruction on HPC topics to under-represented minorities. These two-week schools brought students from the very basics of programming to advanced topics in multiple areas of physics including lattice gauge theory.
- *HEP traineeship program*: under the guidance and encouragement of the CDEI and EC, USQCD member Huey-Wen Lin spearheaded a proposal from a group of USQCD participant universities (Michigan State, Colorado, Connecticut, Maryland, MIT and UIUC) to the DOE with the goal of building a USQCD-wide training network to help bring new students into the area of lattice gauge theory, particularly those from under-represented groups. The proposal was successful and the 4-year LGT4HEP project started in 2023. A cohort of 4 students at member institutions are currently starting taking classes in quantum field theory and HPC and plans for them to visit one of the national labs involved in the hardware project are beign developed. Further details are given on the program website https://lgt4hep.github.io.
- *USQCD in the broader context and community surveys*: USQCD is part of the broader lattice field theory research community and our DEI and outreach efforts are embedded in that environment. CDEI chair W. Detmold initiated the creation of the Lattice Diversity and Inclusion

Committee which represents the broader community and has been responsible for understanding our community through surveys [354, 355] and increasing the accessibility and inclusivity of the annual Lattice conference. Within USQCD, in 2022, a Pulse survey was undertaken to gauge feelings of inclusion and community.

- *Accessibility*: In the past, USQCD All Hands Meetings were held on a rotating basis between the three national labs that host USQCD hardware. At the start of the pandemic, these meetings were switched to online and have been hosted at universities. There is interest to returning these meetings to an in-person format, particularly in the context of welcoming new students and postdocs into collaboration activities. Costs and logistics of in-person events must also be considered and the host institutions will likely continue to be universities if events return to being in-person as they have less issues of accessibility.
- *Individual members' DEI and outreach efforts*: Many members of USQCD participate or lead a range of DEI and Outreach efforts, far too many to list. Some efforts benefit implicitly from the existence of the LQCD and NPPLCI projects, about which the USQCD collaboration forms. As an example, through their USQCD connectionss, many collaboration members have participated as mentors in the Remote Experience for Young Engineers and Scientists (REYES) program led by USQCD member Raúl Briceño.

B.2 Plans

As the LQCD and NPPLCI hardware projects do not fund scientific research staff (typically funded through separate research grants), the focus of the PIER plan for this project is on activities that are enabled by the coalescence of the USQCD collaboration around the hardware that LQCD and NPPLCI provide. Many of the efforts discussed above will continue, but specific tasks that will be focused on are as follows:

- *Access to computing hardware*: USQCD is committed to enabling access to computing for lattice field theory calculations for all members and will continue to encourage proposal submission from anyone interested in lattice field theory and associated fields. In order to support developing scientists in this area, **the project will facilitate training in the various USQCD software frameworks through tutorials**.
- *Training*: the hardware project will support the LGT4HEP traineeship program with access to HPC resources through the "junior investigator" proposal track and through facilitating mentoring connections outside the trainee's home institution as appropriate. USQCD sees great benefit in such traineeships and USQCD members will engage with the DOE Office of Nuclear Physics regarding expanding this project to also involve training in LQFT for nuclear physics applications building upon the insights gained from the LGT4HEP project. In addition, **we are requesting funding in this proposal to support visiting scholarships for USQCD graduate students (beyond those involved in the LGT4HEP program) to intern at one of the three LQCD project labs over the summer**. This will allow for additional mentorship of USQCD students and will help establish their careers in this field.
- *Coordinating DEI and outreach efforts across USQCD*: the hardware project will help strengthen the DEI and outreach efforts of the CDEI and individual USQCD collaboration members in

two specific ways. **In consultation with the CDEI, the project management team will perform annual surveys on aspects of the USQCD community at the same time as surveying satisfaction with the computing hardware and allocation process. The project management team will also construct and maintain a webpage that collects the DEI and outreach activities of USQCD members.** This will both highlight the importance of these efforts to USQCD as a whole and also make it easier for USQCD members to learn about the experiences of others and to connect and engage with existing successful efforts.

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