Lattice QCD for Cold Nuclear Physics

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CONTENTS

I. EXECUTIVE SUMMARY

Quantum chromodynamics (QCD) is the theory of the strong interactions which, along with the electroweak interactions, underpins all of nuclear physics and the vast array of phenomena, from the microscopic to the cosmological, that nuclear physics impacts. This document summarizes the current status of the application of Lattice QCD to the calculation of quantities that are of central importance to science, including the structure of the nucleon, the spectrum of the mesons and baryons, the interactions between nucleons, the spectrum and structure of the light-nuclei, and probes of fundamental symmetries in nuclear physics. The planned programs, along with the anticipated computational resource requirements, are outlined in each of these areas, and the connections between the nuclear physics experimental program and the *Nuclear Science Advisory Committee* (NSAC) Performance Measures[1] are highlighted.

It is anticipated that the next five years of research in this area will include the first (Lattice) QCD calculations of low-energy nuclear physics quantities of central importance to the field at the physical light-quark masses and with fully quantified uncertainties, thereby fundamentally changing the field of nuclear physics. This transformative change to the field is predicated on Moore's Law growth in available computational resources. Indeed, such has been the remarkable progress made by USQCD during the preceding five years that this new and emerging methodology could exploit resources growing faster than Moore's law to accelerate still further our understanding of nuclear physics.

II. INTRODUCTION

The strong interaction is responsible for a diverse range of physical phenomena, including binding gluons and the lightest quarks into pions, protons, and neutrons. Through its manifestation as the strong nuclear force, it then binds neutrons and protons together to form the elements of the periodic table. The strong nuclear force plays a central role in the fusion of light nuclei, which occurs within the sun's core. Within certain heavy nuclei, the strong nuclear force, in a delicate balance with the electromagnetic interaction, is responsible for the process of fission that is exploited, for instance, in nuclear power stations.

A key issue is the phenomenon of confinement that is a well-established outcome of QCD, but the exact nature of confinement and all of its consequences are still a mystery. Thus, how does QCD give us the particular mesons and baryons we observe, and how are gluons manifest in the spectrum? In nucleons, how do quarks and gluons interacting through QCD produce their observed mass, size, and spin? Similar questions remain unanswered about the exact nature of the strong nuclear force and its lineage from QCD. For example, what is the nature and origin of the nuclear spin-orbit interaction? How does the three-neutron force emerge from QCD? Even partial answers to these questions will help illuminate long-standing issues in nuclear physics and ultimately provide a deeper understanding of how protons and neutrons combine to form nuclei, and therefore the elements germane to everyday life.

The breadth of these open issues does not represent a lack of progress in understanding nature in these environments. Rather, computational resources are now reaching a point where answers to many of these questions are within the realm of possibility over the next five years. Already, substantial progress has been made in using available computational resources to investigate these questions. As computational research in these areas matures, we expect still further progress in exploiting the increasingly powerful computational resources that will be available.

Accomplishments over the last five years have established the methodology and the groundwork for lattice investigations of hadron structure, spectroscopy, and the structure of the lightest nuclei and their interactions. Calculations have been performed of the strong-interaction effects needed to unveil the fundamental symmetries of the Standard Model from precision nuclear-physics experiments. An impressive range of calculations has been performed at decreasingly smaller values of the light-quark masses. However, present day computational-resource limitations restrict the mass of the pion input into those calculations to one exceeding that of nature.

The next five years will be a transformational period for nuclear physics. The 12 GeV upgrade of Jefferson Laboratory will explore the role of gluonic excitations in the QCD spectrum, provide a three-dimensional tomographic view of the proton, and through parity-violating electron scattering explore the fundamental symmetries of the Standard Model. Experiments at RHIC-spin will probe the gluon and antiquark contributions to the spin of the proton, and experiments at JLab will explore the contribution of orbital angular momentum. The construction of the *Facility for Rare Isotope Beams* will enable the exploration of multi-nucleon interactions from neutron-rich nuclei. Provided sufficient computational resources are made available, precision first-principles calculations of the spectrum, structure and interactions of the building blocks of all the visible matter in our universe will be performed with fully quantified uncertainties.

The centrality of computational physics in providing new understandings of, and predictive capabilities for, nuclear physics was recognised in a recommendation of the NRC decadal review of nuclear physics *Nuclear Physics: Exploring the Heart of Matter*[2]:

> *A plan should be developed within the theoretical community and enabled by the appropriate sponsors that permits forefront computing resources to be deployed by nuclear science researchers and establishes the infrastructure and collaborations needed to take advantage of exascale capabilities as they become available.*

Not only will this provide the first reliable connection between QCD and low-energy nuclear physics, but it will also provide the tools to explore and ultimately understand the fine-tunings that, in some sense, define matter.

In the remainder of this paper, we begin by outlining the computational resources available to the USQCD collaboration, the essential rôle of software development facilitated through SciDAC, and our assumptions about growth in computational resources over the next five years. We will then describe the opportunities for Lattice QCD to advance our understanding across four key campaigns in hadronic and nuclear physics before concluding with a summary.

III. COMPUTATIONAL RESOURCES FOR LATTICE QCD

At present, members of USQCD are making use of dedicated hardware funded by the DOE through the LQCD-ext Computing Project, as well as a Cray XE/XK computer, and IBM Blue Gene/Q and Blue Gene/P computers, made available by the DOE's INCITE Program. During 2013, USQCD, as a whole, expects to attain approximately 300 Tflops-years on these machines. USQCD has a PRAC grant for the development of code for the NSF's petascale computing facility, Blue Waters, and expects to obtain a significant allocation on this computer during 2013. Subgroups within USQCD also have allocations at the DOE's National Energy Research Scientific Computing Center (NERSC) and through the NSF's XSEDE Program, access to dedicated Blue Gene/Q computers at Brookhaven National Laboratory and the University of Edinburgh, access to the Blue Gene/Q computers at Forschungszentrum JÜlich, and access to computers at LLNL.

For some time, the resources we have obtained have grown with a doubling time of approximately 1.5 years, consistent with Moore's law, and this growth rate will need to continue if we are to meet our scientific objectives. The software developed by USQCD under our SciDAC grant enables us to use a wide variety of architectures with very high efficiency, and it is critical that our software efforts continue at their current pace. Notably, many of the calculations we outline below were *enabled* through our ability to exploit GPUs on the USQCD clusters for the most demanding parts of the calculations. Over time, the development of new algorithms has had at least as important an impact on our field as advances in hardware, and we expect this trend to continue, although the rate of algorithmic advances is not as smooth or easy to predict as that of hardware.

IV. HADRON STRUCTURE

A. Motivations and Achievements

One of the great challenges posed by QCD is understanding how protons and neutrons, the basic building blocks of most of the observed matter in the universe, are made from quarks and glue. Just as calculating the structure of atoms was a cornerstone of quantum mechanics, a cornerstone of contemporary nuclear physics is to achieve a quantitative, predictive understanding of the structure of nucleons and other hadrons using lattice QCD.

One goal in hadron structure is precision calculation of fundamental quantities characterizing the nucleon, including form factors, moments of parton density, helicity, and transversity distributions, moments of generalized parton distributions (GPDs) and transverse momentum distributions. Hadronic observables calculated from first principles are directly relevant to the experimental programs at JLab and RHIC-spin, for experimental data from SLAC and FNAL, and will have significant impact on future experiments at the JLab 12 GeV upgrade and at a planned electron-ion collider. Another essential goal is obtaining insight into how QCD works. How does the spin of the nucleon arise from the helicity and orbital angular momentum of quarks and of gluons? What is the fundamental mechanism for confinement and what is the role of diquarks and instantons in hadrons? How does hadron structure change as one varies parameters that cannot be varied experimentally, such as the number of colors, the number of flavors, the quark masses, or the gauge group? Finally, once lattice calculations are validated by extensive comparison with directly comparable experiments, one can exploit lattice QCD to make predictions relevant to planned experiments, to the resolution of experimental controversies, and to other areas of physics as discussed below.

Recent work has laid the groundwork for a broad range of important hadron structure calculations, subject to limitations in computational resources. Calculations have focused on the dominant connected diagram contributions to matrix elements since the sub-dominant disconnected contributions are much more computationally expensive. Fortunately, disconnected contributions vanish for isovector quantities. Since the cost of lattice QCD calculations in a volume large enough to contain a pion grows rapidly with the inverse pion mass, past calculations have been performed for a series of pion masses that have gradually approached the physical mass and then been extrapolated to the physical mass using chiral perturbation theory. Due to uncertainty in the convergence of chiral perturbation theory, extrapolations from pion masses 300 MeV and above give rise to presently unquantified systematic uncertainties. Also, calculations for low pion masses are susceptible to contamination by excited states that can cause apparent disagreement with experiment [3]. A recent calculation including the nearly physical pion mass and using a method to reduce the contribution of excited states yielded agreement with experiment within statistical uncertainties for several key isovector observables [4].

Electromagnetic form factors reveal the distribution of charge and current and how constituents interact to recoil together at high momentum transfer. Calculations[4–8] have shown the emergence of the pion cloud at the periphery of the nucleon as the pion mass is lowered. Calculations [4] at a pion mass of 149 MeV yield agreement with experiment for the isovector charge radius, magnetization radius, and magnetic moment. The statistical error for the charge radius is comparable to the discrepancy between electron scattering and Lamb shift measurements, so future high precision calculations will be important in helping resolve this discrepancy.

The axial charge, g_A, governing neutron β-decay, is the value of the axial form factor at zero momentum transfer. Chiral extrapolations of calculations of g_A at heavy quark masses agree with experiment[5, 9, 10] with statistical uncertainties as low as 7%. However, calculations closer to the physical pion mass with presently affordable spatial volumes, temporal extents, and excited state suppression are inconsistent with experiment[3, 4, 9]. Precision calculations at a fraction of a percent will impact the proton-proton fusion rate central to solar models and constrain the weak matrix element $|V_{ud}|$. The scalar and tensor charges, g_S and g_T, corresponding to the scalar and tensor form factors at zero momentum transfer, are being calculated[11, 12] and are essential in searching for physics beyond the standard model in ultra-cold neutron Beta-decay experiments at LANL. A precise prediction of the tensor charge will be particularly significant prior to a major experimental program to measure it at the JLab 12 GeV upgrade. The precise knowledge of the strangeness content of the nucleon through the calculation of the strange quark scalar matrix element has implications for the interactions of certain dark matter candidates with ordinary matter[13].

Quark parton distributions have been studied in deep-inelastic scattering experiments around the world and yield detailed data specifying quark density, spin, and transversity distributions as functions of the momentum fraction, x, of the struck quark. The moments of

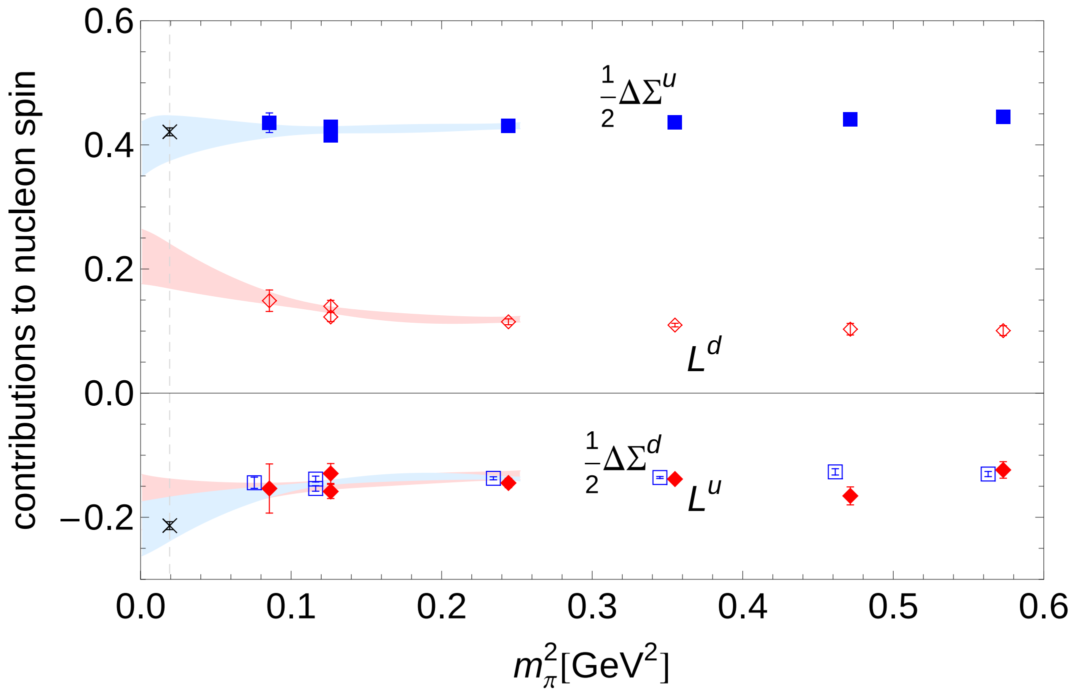

FIG. 1. Contributions of quark spin $\Delta\Sigma^{u,d}/2$ (blue error bars) and orbital angular momentum $L^{u,d}$ (red error bars) to the spin 1/2 of the proton for up and down quarks [5]. Chiral extrapolations (shaded error bands) agree with HERMES data (crosses).

these distributions can be calculated with lattice QCD and to date, the dominant connected diagram contributions to the lowest three moments of each have been calculated[5, 14–16]. When connected and disconnected contributions have been calculated to high precision, the combination of a finite number of moments and experimental measurements over part of the range of x will determine these distributions better than either lattice calculations or experiment can alone.

The so-called nucleon spin crisis refers to the fact that whereas in the naive quark model, all of the spin of the nucleon comes from the spins of the three quarks, experimentally only a small fraction arises from quark spin. This issue is addressed by the lowest moment of the spin distribution, $\Delta\Sigma$, which specifies the fraction of the nucleon's spin arising from the spin of the quarks. As shown in Figure 1, chiral extrapolations of the calculations in Ref. [5] agree with deep inelastic scattering results from HERMES[17] and show that only 30% of the nucleon spin comes from quark spin. Thus, we see directly from solving QCD through lattice calculations that the simple quark model is indeed quite naive.

The first moment of the quark density distribution, $\langle x \rangle$, specifies the fraction of the nucleon momentum carried by quarks, and is well measured in deep inelastic scattering. The lattice QCD calculations of the isovector combination $\langle x \rangle_{u-d}$ have no disconnected contributions and thus, when compared with experiment, provide an unambiguous test of current lattice calculations. Figure 2 shows a chiral fit to a lattice calculation[4] down to a pion mass of 149 MeV that is in excellent agreement with the CTEQ6 analysis of deep inelastic scattering[98]. Here one observes that the 149 MeV point highly constrains the fit so that extrapolation

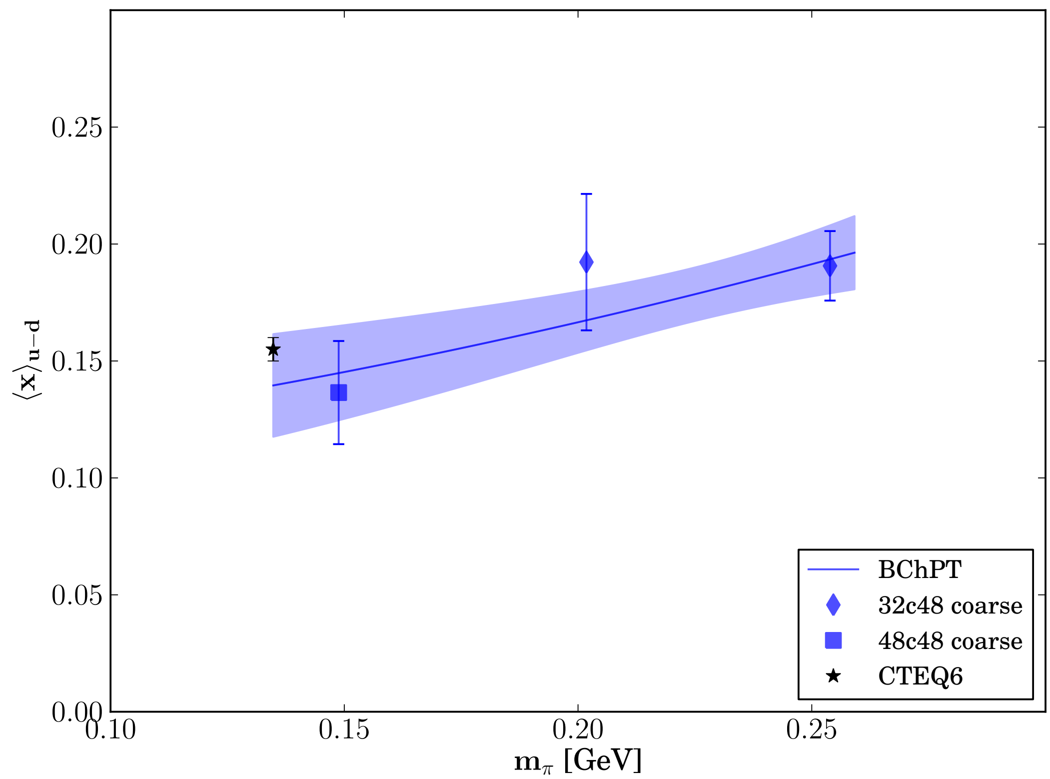

FIG. 2. The isovector quark momentum fraction $\langle x \rangle_{u-d}$ [4] and the chiral fit (shaded error band) agrees with the CTEQ6 result[98].

uncertainties are negligible.

Generalized Parton Distributions (GPD's) specify quark density, spin, and transversity as functions of both the longitudinal momentum fraction x and the transverse position, and if known completely would enable us to calculate a 3-dimensional picture of the nucleon. Their moments in x have been calculated on the lattice[5, 19] and are in qualitative agreement with phenomenology[20]. The combination of these moments with convolutions of GPDs measured at JLab and elsewhere will provide a more complete understanding than either effort could obtain separately.

Of particular interest and relevance to the DOE nuclear physics experimental program is the fact that one combination of moments of GPD's specifies the total angular momentum of quarks in the nucleon[5, 14, 18, 19, 21], so combined with the quark spin contribution above, the lattice provides a complete determination of quark spin and orbital contributions to the total spin 1/2 of the nucleon. The results [5] from the dominant connected diagrams shown in Figure 1 are striking. In addition to the fact mentioned above that only about 30% comes from quark spin, the substantial orbital contributions of up and down quarks cancel yielding a negligible orbital contribution, so that the remaining 70% must come from sea quarks and gluons. This is of great interest experimentally and a major focus of RHIC-spin and a future electron-ion collider is measuring the contribution of gluons to the nucleon spin. Direct calculation of the gluon contribution to the nucleon spin is clearly desirable. An important initial step was taken by calculating the contribution of gluons to the momentum fraction $\langle x \rangle$ of the pion[22] and obtaining a result which when added to the quark contribution yields 100% within uncertainties. A calculation of the gluon contribution to nucleon momentum and angular momentum has been made using a gluon energy-momentum tensor operator derived from the overlap operator, in the expectation of reduced ultraviolet fluctuations[23].

Transverse momentum distributions show the quark momentum distribution, and initial calculations in a nucleon[24, 25] have opened the way for future results relevant to semi-inclusive deep inelastic and single-spin asymmetry experiments at COMPASS, Hermes, JLab, and a future electron-ion collider. Also, the spin-isospin excitation of the nucleon, the $\Delta(1232)$, has been shown to be deformed, consistent with phenomenology, by calculating its quark transverse charge densities[26] and the transition form factors to it from the nucleon[27].

B. Future Program and Resource Requirements

Current computer resources and algorithms coupled with their expected improvements over the next five years provide exciting opportunities for definitive precision computation of presently calculable observables as well as exploration of new observables and theoretical issues.

- *Precision computation of presently calculable observables*

  During the next five years, a major focus of the program will be precision computation of form factors, moments of quark parton distributions, and moments of quark GPDs at the physical pion mass with control of systematic uncertainties associated with finite lattice spacing, spatial volume, temporal extent and excited state contaminants. These calculations are explicitly required to meet the **2014 NSAC Performance Measure HP9**, which states "*Perform lattice calculations in full QCD of nucleon form factors, low moments of nucleon structure functions and low moments of generalized parton distributions including flavor and spin dependence*", and to address experimental measurements mandated by six of the other nine Performance Measures. These lattice calculations are essential for realizing the full physics potential of experiments at the JLab 12 GeV upgrade, RHIC-spin, and a planned electron-ion collider.

  The methodology for calculating connected diagrams and removing excited state contaminants is now sufficiently well-developed to enable estimation of the computational cost for calculating these observables at the physical pion mass. Because of the exponentially small signal-to-noise ratio at large times for measurements of nucleon observables at the physical pion mass, the computational cost of the required number of measurements on a configuration is much larger than the cost of generating the configuration itself. Useful estimates can be obtained by taking present results very close to the physical pion mass, scaling the cost to the physical pion mass and appropriate spatial volume, time extent, and parameters to reduce excited state contamination, and increasing the number of measurements to reduce the statistical error to the desired precision. Cost estimates are given in Table I.

  Disconnected diagrams, which describe processes in which the operator being calculated excites a quark-antiquark pair that in turn interacts with one of the quarks in the nucleon, are computationally much more difficult and expensive to calculate than connected diagrams, but they are essential for precision calculations of the properties of protons and neutrons separately, and thereby to resolving the contributions of the individual quark flavors to hadron structure. Although they have been calculated for a few operators, where their contributions are found to be smaller than those of the corresponding connected contributions, they have never been calculated for the full suite of form factors, moments of quark parton distributions, and moments of quark GPDs. Hence, it will be necessary to study the effectiveness of alternative dilution techniques and truncation methods to find the most efficient set of algorithms for a full calculation. In addition, it is necessary to compute the mixing of gluons with quark disconnected diagrams in order to calculate flavor singlet matrix elements. This entails a significant effort in developing an optimal gluon operator and calculating the necessary renormalization factors and mixing coefficients. The ultimate computational cost of calculating disconnected diagrams and the associated gluon mixing is presently unknown, but is expected to be more than an order of magnitude greater than that of connected diagrams.

- *New Observables and Theoretical Issues*

  Much of the intellectual vitality and excitement of the field centers on new theoretical developments and ideas for calculating important physical quantities that are presently inaccessible. Some of the key problems that are important for further understanding the quark-gluon structure of the nucleon are described below.

  Form factors at high momentum transfer: At sufficiently high momentum transfer q, asymptotic scaling sets in and the electric form factor falls off as q^{-4} and other form factors fall off with other known powers. To determine this scale for asymptotic scaling, form factor calculations must be extended to high momentum transfer where new techniques[28] need to be explored and applied in large volumes at the physical pion mass.

  Higher moments of quark structure functions: Because the hypercubic group of the lattice has less symmetry than the continuum, unphysical operator mixing can occur in lattice QCD and current lattice QCD calculations only eliminate this mixing for the lowest three moments of these distributions. To reconstruct quark distributions as fully as possible and to constrain phenomenological models, it is necessary to explore new algorithms for calculating higher moments, such as introducing a heavy quark field [29], and using extended operators at sufficiently fine lattice spacings[30], and to exploit them at the physical pion mass.

  Gluon contributions: Our understanding of nucleon structure will remain fundamentally incomplete until we learn to directly calculate gluon contributions to the nucleon mass, momentum, and angular momentum. Given the focus on measuring the gluon contribution to the nucleon spin at RHIC-spin and a future electron-ion collider, this will have great impact on the experimental program. Since the fluctuations in gluon fields grow strongly as the lattice spacing is decreased, extracting the continuum limit for gluon observables will require a combination of theoretical ideas, new algorithms, and techniques for obtaining extremely high statistics.

  Transverse momentum distributions: It is important to relate lattice calculations of transverse momentum distributions quantitatively to experimental measurements of semi-inclusive deep inelastic scattering and Drell-Yan processes. This requires accessing the regime in which QCD factorization applies, which in turn requires developing techniques to treat high nucleon momentum. Because of the rapid decrease of the signal-to-noise ratio with momentum, extremely high statistics will be required for these calculations as well.

TABLE I. Resources, in Tflops-years (TF-yrs), required to calculate the connected diagrams for a complete set of form factors and the lowest three moments of structure functions and generalized parton distributions for the nucleon at the physical pion mass. Lattice Generation is the cost of 10^4 trajectories, Measurements A reduce the error for g_A to 3 % , and Measurements B reduce the error for $\langle x \rangle$ to 3 %. The actions used are Wilson-clover fermions (W) and Domain-wall fermions (DW); measurements for both use the EigCG algorithm[32], and for the latter we also employ low-mode averaging[31].

$N_s^3 \times N_t$	Action	a_s (fm)	$m_\pi L$	$m_\pi T$	Lattice Generation (TF-yrs)	Measurements A (TF-yrs)	Measurements B (TF-yrs)
$64^3 \times 128$	W	0.11	5.0	10.0	45	120	1800
	DW	0.11	5.2	10.3	700	100	1400
$96^3 \times 192$	W	0.09	6.1	12.3	380	210	3100
	DW	0.09	5.9	11.8	4000	390	5100
$128^3 \times 256$	W	0.06	5.4	10.9	1940	340	5000
	DW	0.07	5.9	11.8	20000	1000	13000

The resources required for calculating connected diagrams for a complete set of form factors and the lowest three moments of structure functions and generalized parton distributions for the nucleon at the physical pion mass are shown in Table I. Of the observables g_A, the charge radius, the magnetization radius, the magnetic moment, and $\langle x \rangle$, g_A is the least expensive to calculate to 3 % accuracy and $\langle x \rangle$ is the most expensive. Measurements A shows the cost of a set of calculations in which g_A is computed to 3 % accuracy and the other observables are less accurate and Measurements B shows the cost of a set of calculations in which $\langle x \rangle$, is computed to 3 % accuracy and the other observables are more accurate. Both Wilson-clover and domain wall actions have been used extensively in nucleon structure calculations, so we show the costs using each action. Obtaining consistent results using both actions will strengthen the credibility of lattice results, and each action has advantages for specific calculations. The costs of the disconnected and gluonic contributions to enable the flavor-separated hadron structure are not known sufficiently reliably to include in the table.

V. HADRON SPECTROSCOPY

A. Motivations and Achievements

The calculation of the bound state spectrum of QCD encapsulates our ability to describe the strong interactions, and the confrontation of high-precision calculations with experimental measurements is a vital test of the theoretical framework. The precise calculation of the masses of the lowest-lying meson and baryon states in the spectrum represents an important milestone in our ability to solve QCD[33]. The calculation of the excited-state spectrum provides an opportunity to explore in detail the dynamics of QCD, and further refine our knowledge of the theory.

The experimental investigation of the excited states of QCD has undergone a resurgence: the observation of new states in the Charmonium system at Belle and at BaBar, the search for the so-called missing baryon resonances of the quark model at CLAS at JLab@6GeV, and the flagship search for so-called exotic mesons at GlueX at the upgraded JLab@12GeV. How do the apparent collective degrees of freedom arise that describe the spectrum arise, and can we identify them? What role do gluons play in the spectrum, and how are they manifest? The work proposed here will facilitate those calculations both to describe the existing experimental data, and to *predict* the outcomes of future experiments.

In contrast to electromagnetism, the “field-lines” between a quark and antiquark in QCD do not diffuse over large distances, but rather are confined to compact “flux tubes” connecting them. A quark-antiquark pair connected by a flux tube is the simplest picture of a meson. A quark-antiquark pair with relative orbital angular momentum can only possess certain allowed values of J^{PC}, and mesons having quantum numbers outside those allowed values are known as “exotics” and must have a richer structure. The hybrid hypothesis is that these exotic quantum numbers arise from the addition of an excited gluon field, and thus exotic states have attained the status of a “smoking gun” for gluonic degrees of freedom. A recent calculation of the isovector meson spectrum including those of high spin and exotic quantum numbers, suggests that the presence of exotics in a regime accessible to GlueX[34, 35], illustrated in Figure 3, and furthermore the existence of both exotic and non-exotic “hybrids”. Calculations in the isoscalar sector revealed the hidden flavor-mixing angles describing the admixtures of their light- and strange-quark components[36, 37], and suggested the presence of isoscalar exotics at a mass comparable to their isovector cousins[37].

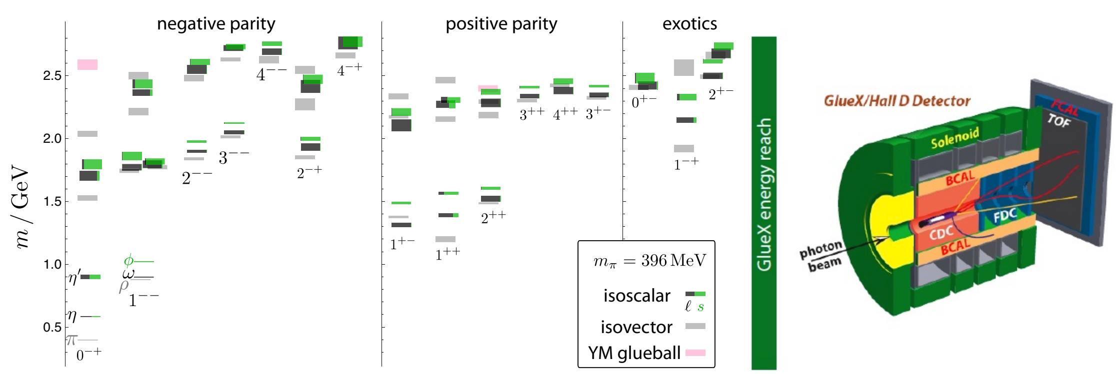

FIG. 3. The spectrum of states of exotic quantum numbers for both isovectors and isoscalars, for quark masses corresponding to those of a pion of mass 396 MeV[37]. *These results suggest the presence of many exotics in a region accessible to the future GlueX experiment.*

Baryons, containing three quarks, are emblematic of the non-Abelian nature of QCD, and of SU(3). The search for so-called “missing resonances” focuses on whether the baryon

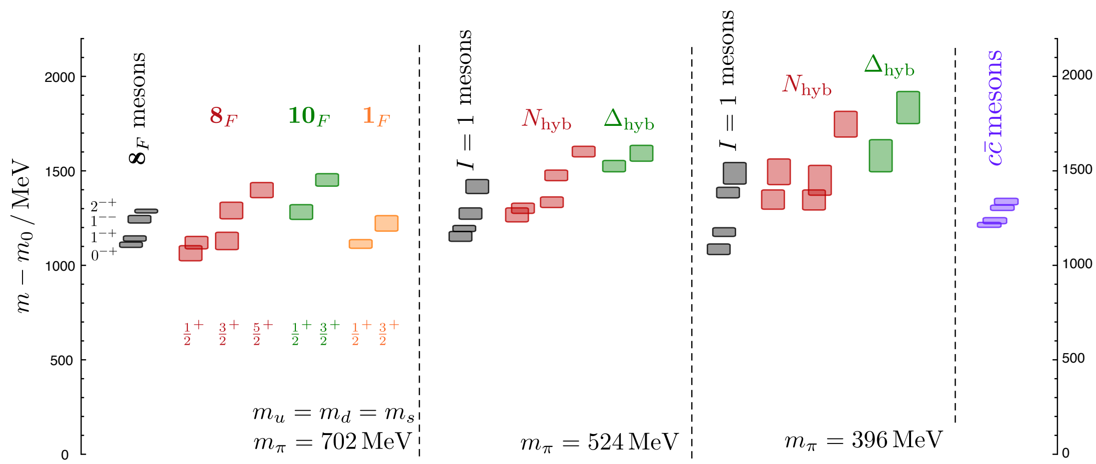

FIG. 4. The excitation spectrum of hybrid mesons and baryons at three values of the light-quark mass; for mesons we show $m - m_\rho$, while for baryons we show $m - m_N$.

spectrum can be well described by a quark model, or whether an effective theory with fewer degrees of freedom, such as a quark-diquark picture, provides a more faithful description. A recent calculation of the low-lying nucleon and Δ excited spectrum[38] exhibited a counting of levels consistent with the non-relativistic *qqq* constituent quark model and inconsistent with a quark-diquark picture of baryon structure. In contrast to mesons, there are no "exotic" quantum numbers for baryons that *demand* a richer structure than that of three quarks with relative orbital angular momentum. None-the-less, the N and Δ spectrum reveal the presence of "hybrid" baryons, in which, as in the case of mesons, the gluonic field plays a vital structure role. Remarkably, the mechanism giving rise to such gluonic excitations appears common to both mesons and baryons, as shown in Figure 4, where the excitation energy of both "hybrid" mesons and "hybrid" baryons is shown.

The excited-state spectrum of QCD is characterized by states that are resonances unstable under the strong interaction, and the spectrum is encapsulated within momentum-dependent phase shifts which may then be parametrised in terms of a mass and decay width. In Euclidean space QCD, shifts in the energy spectrum at finite volume can be related to infinite-volume phase shifts at the corresponding scattering momenta[39, 40]. Recently, the energy dependence of the ρ resonance in $\pi\pi$ elastic scattering has been mapped in unprecedented detail[43], using methods developed to extract the momentum-dependent phase shifts in non-resonance $I = 2$, $\pi\pi$ scattering[41, 42].

Finally, there has been significant insight into understanding the electromagnetic properties of the excited states in QCD, in an approximation in which they are treated as quasi-stable particles. The transition form factor from the nucleon to its lowest-lying excitation, the so-called Roper resonance[46], has been computed, complementing a vigorous experimental program in this area. The electromagnetic transition form factors between charmonium states, including to those of exotic quantum numbers[47], have been calculated, indicating a large partial width for the decay $\Gamma(\eta_{c1} \to J/\psi\gamma)$, and laying the groundwork for those between mesons composed of light quarks relevant for the 12GeV upgrade of Jefferson Laboratory.

The progress in our understanding of the spectrum of QCD has been contingent on theoretical advances, computational advances, and on the USQCD facilities that have enabled us to efficiently exploit those advances. Notably, USQCD has adopted a program to generate so-called anisotropic lattices[48, 49], with a finer temporal than spatial lattice spacing, that are designed to enable calculations of the excited-state spectrum at far less computational cost than would be possible using isotropic lattices with sufficiently fine resolution. A new method of constructing correlation functions, "distillation"[50], has enabled the large number of hadronic correlation functions needed to apply the variational method to be computed. Finally, the USQCD facilities project, including the provision of GPU-accelerated nodes, has provided a highly cost-optimized means of implementing the method, thereby facilitating calculations that would otherwise not have been feasible.

B. Future Program and Resource Requirements:

The next five years present an exciting opportunity for lattice QCD calculations of the spectrum to *predict* the outcomes of future experiments, with the first experiments at the 12GeV upgrade of Jefferson Laboratory expected in 2015, a proposed detector PANDA at the FAIR facility in Germany, and an on-going program at COMPASS at CERN. A vibrant program of lattice calculations is vital to capitalize on these experimental investments:

- *The spectrum of the low-lying meson resonances*

  Lattice calculations of the excited meson spectrum, albeit at unphysically large values of the u and d quark masses, already suggest the presence of hybrid states with masses around 1.3 GeV above that of the ρ. Computations at quark masses corresponding to the physical quark masses will enable the mass scale associated with hybrid mesons to be confidently calculated, thus enabling the confrontation of the calculation of the spectrum within QCD, and experimental extractions of states in the region of sensitivity of GlueX of 1.8 to 2.7 GeV.

  With decreasing pion mass, and with increasing excitation in the spectrum, the states of interest are resonances unstable under the strong interaction, and furthermore have multi-channel decay modes for which the methods detailed in ref. [39, 40] are not applicable, or require extensions. The development and application of methods to include coupled-channel that appear above the inelastic threshold[51–56] and multi-hadron final states, will be key to the implementation of this program.

  The lattice calculations of the spectrum of *isoscalar* mesons address the question of why some states are near ideally mixed, whilst others have a completely different admixture. Calculations at the physical quark masses will enable the mixing patterns to be discerned, notably for hybrid states, providing predictions for the decay modes that can be tested in experiment.

  These calculations will be key to capitalizing on the **2018 NSAC Performance Measure HP15** to complete the first results on the search for exotic mesons using photon beams.

- *Radiative transitions to excited mesons*

The *GlueX* experiment aims to photoproduce mesons and in particular those of exotic quantum numbers. The use of photons as a means to preferentially produce hybrid states is bolstered both by phenomenological calculations, and by lattice calculations in charmonium indicating the radiative couplings to hybrid mesons are not small. Calculations of the photocouplings for light quarks will inform the expected photoproduction rates in experiment.

- *The spectrum of excited baryon resonances*

  The excited-state spectrum of all the excited baryons that can be constructed from the u, d and s quarks will elucidate the role of quark flavor and mass in the spectrum of QCD. For the Ξ and Ω in particular, containing two and three s quarks respectively, our knowledge is very limited, with only a few states experimentally established and scant knowledge as to their properties; the production of such "very strange" baryons is proposed with both the CLAS12 and GlueX detectors at the 12 GeV upgrade of JLab. Precise calculations of the N^* spectrum at the physical pion masses will fully capitalize on the experimental baryon resonance program and the achievement of the **2009 NSAC Performance Measure HP3**. Finally, a knowledge of the decay modes and widths of excited states can address key questions that might guide experiment, such as whether the doubly strange Cascades are really narrower than baryons composed of the light quarks.

- *Electromagnetic properties of baryon resonances*

  Understanding the structure of the nucleon is not limited to mapping out the charge or momentum distributions of its constituents in its ground states; as the hydrogen atom has shown, and understanding of the structure of a bound state and of its resonances go hand-in-hand. Calculations of the $\gamma NN*$ electrocouplings at $Q^2 < 5$ GeV^2 will elucidate the important role of pionic degrees of freedom, whilst calculations at high Q^2 will explore the transition from the large-distance scales with confinement-dominated dynamics, to the short-distance scales with perturbative-dominated dynamics. Furthermore, a knowledge of the electromagnetic properties of excited states may provide insight as to the quark and gluon make up of such states.

The resources needed to compute the low-lying spectrum for both mesons and baryons, together with some of their electromagnetic properties at lower momentum transfers, is outlined in Table II. The calculations are performed on anisotropic clover lattices that have the fine temporal lattice spacing of $a_t = 0.035$ fm enabling the resolution of the many low-lying energy levels in the spectral function required; the longer-term approach for spectroscopy will be to use *isotropic* lattices with spacings at or below $a = 0.035$ fm.

VI. HADRONIC INTERACTIONS, NUCLEAR FORCES AND NUCLEI

A. Motivations and Achievements

The strong interactions among baryons are key to every aspect of our existence. The two- and higher-body interactions among protons and neutrons, along with the electroweak interactions, produce the spectrum of nuclei and the complex chains of nuclear reactions responsible

TABLE II. Resources, in Tflops-years (TF-yrs), required to calculate the low-lying excited-state spectrum for mesons and baryons, and the electromagnetic properties of the lowest-lying states, using an anisotropic clover action with a temporal lattice spacing of $a_t = 0.035$ fm.

$N_s^3 \times N_t$	a_s (fm)	a_t (fm)	m_π (MeV)	$m_\pi L$	$m_\pi T$	Trajectories	Lattice Generation (TF-yrs)	Measurements (TF-yrs)
$32^3 \times 512$	0.12	0.035	200	3.8	17.6	10^4	44	550
$48^3 \times 512$	0.12	0.035	200	7.7	17.6	10^4	592	1305
$48^3 \times 512$	0.12	0.035	140	4.0	12.3	10^4	411	1515
$64^3 \times 512$	0.12	0.035	140	5.4	12.3	10^4	1210	3270
$64^3 \times 512$	0.09	0.035	140	4.0	12.3	10^4	1210	3980
$96^3 \times 512$	0.09	0.035	140	6.0	12.3	10^4	5531	10510

for the production of the elements forming the periodic table at the earliest times of our universe, in the stellar environments that follow, and in reactors and our laboratories. Decades of experimental effort have led to the precise measurement of the nucleon-nucleon scattering cross sections over a wide range of energies, which have given rise to the modern nuclear forces. These experimentally determined two-body forces, encoded by modern nucleon-nucleon potentials such as the chiral potentials [57], when supplemented with three-body interactions, and implemented using the renormalization group [58], provide the cornerstone of our theoretical description of nuclei and their interactions. Coordinated efforts by the US nuclear physics community during the last several years to develop the computational technology to perform convergent nuclear structure calculations show that three-nucleon forces are required to determine the structure of light nuclei. Given the size of the three-nucleon and higher-body interactions, there is considerable uncertainty in their form, and hence in the predictions for systems for which there is little or no experimental guidance, such as arise in extreme nuclear environments [59] that can be found, for instance, in the interior of core-collapse supernova. One of the motivations for building FRIB (Facility for Rare Isotope Beams) is to better constrain the multi-neutron interactions from very neutron-rich nuclei.

As the standard model of particle physics is responsible for all nuclei and their interactions, Lattice QCD holds the promise of providing the long sought rigorous underpinnings of nuclear physics. We anticipate that nuclear interactions will be systematically refined by lattice QCD calculations, and the uncertainties associated with future predictions of nuclear processes will be fully quantified. Equally important, lattice QCD allows for the quark-mass dependence of nuclear structure and the nuclear forces to be precisely determined, thereby providing a detailed exploration of fine-tunings that define our universe (in addition to being necessary for a complete determination of the chiral nuclear forces). Serious efforts to determine the properties and interactions of the light nuclei, leading to nuclear forces which can be propagated throughout the periodic table, have been underway for nearly a decade. Significant progress has been made toward calculating the lowest lying states in s-shell nuclei and determining the scattering parameters in the two-baryon systems. These calculations have been performed with the clover action at one lattice spacing in the isospin limit and without electromagnetism by three different lattice collaborations. The deuteron binding energy has been determined at pion masses of $m_\pi \sim 400, 500$ and 800 MeV [60–66] with presently insufficient precision. Similar calculations have shown the di-neutron to be bound at these heavier pion masses, and all of the two-baryon octet channels contain a bound state at the SU(3) symmetry point. The deepest bound state at the heavier pion masses is the H-dibaryon [67–69], as conjectured in the 1970's. The form of chiral extrapolations is sufficiently uncertain so that a reliable prediction for the H-dibaryon cannot presently be made at the physical pion mass. After significant developments in algorithms to efficiently evaluate Wick contractions [70], correlation functions for systems $2 < A < 6$ can now be constructed, and have lead to the first calculations of ^{3}He, ^{4}He. Further developments have been possible for α-cluster nuclei. Such calculations have been extended to hypernuclei, and a first comprehensive study of s-shell nuclei and hypernuclei has recently been performed [65]. Figure 5 shows the lowest-lying levels in s-shell nuclei and hypernuclei at a pion mass of $m_\pi \sim 800$ MeV. The binding energy of the deuteron at the heavier pion masses indicates

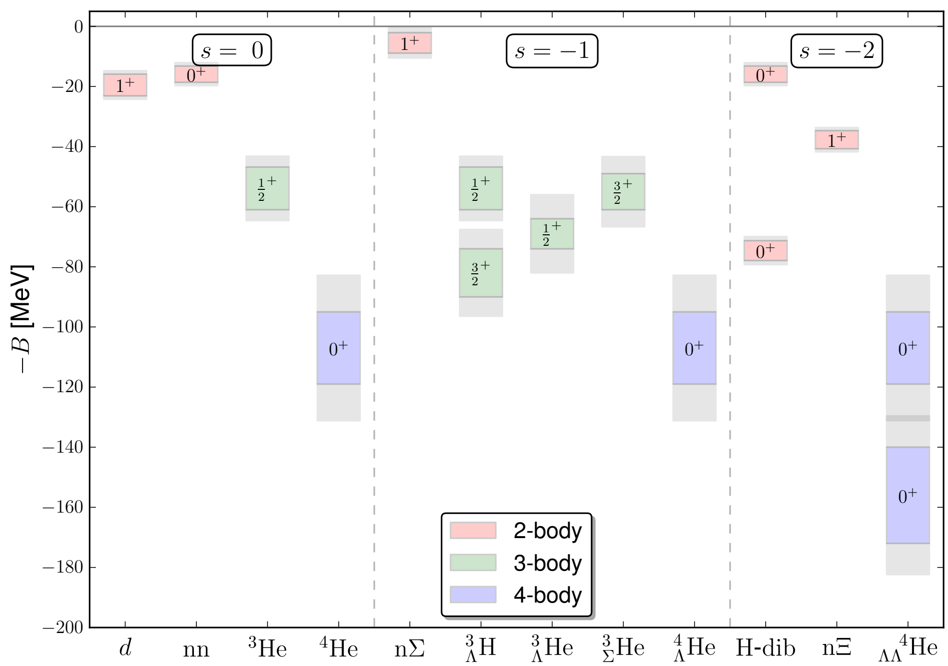

FIG. 5. The calculated low-lying spectrum of the lightest nuclei and hypernuclei at a pion mass of $m_\pi \sim 800$ MeV [65].

that the deuteron remains "unnatural" away from the physical pion mass as its binding momentum is much smaller than the inverse range of the nuclear force. In addition to interactions of the lowest-lying octet of baryons, a calculation of the $\Omega^-\Omega^-$ interactions has been recently performed [71], where small scattering lengths are found. Analogous calculations at a smaller lattice spacing, so that the lattice spacing dependence can be parametrically reduced, are planned. Further, calculations at lighter pion masses are planned to be able to make first post-dictions of the binding of nuclei at the physical light-quark masses, and also to further refine the light-quark mass-dependence of nuclear observables. These post-dictions will verify the Lattice QCD *technology*, and the uncertainties in the predictions for the structure of hypernuclei, and for the nuclear forces including the multi-neutron interactions, can be fully quantified.

The nucleon-nucleon scattering lengths in both spin-channels have been determined at these same heavier pion masses, but the precision of the calculations has not as yet allowed for extractions of the effective range, or higher terms in the effective range expansion. This situation is on the verge of changing, with the first calculations of the nucleon-nucleon scattering parameters expected in the near future at the SU(3) symmetric point. While the results presented by the HALQCD collaboration provide a reliable determination of the phase-shifts at the energies of the states in the lattice calculation, they are unreliable away from these energies, and hence the potentials [62–64] that they extract cannot be used in many-body calculations to provide reliable results.

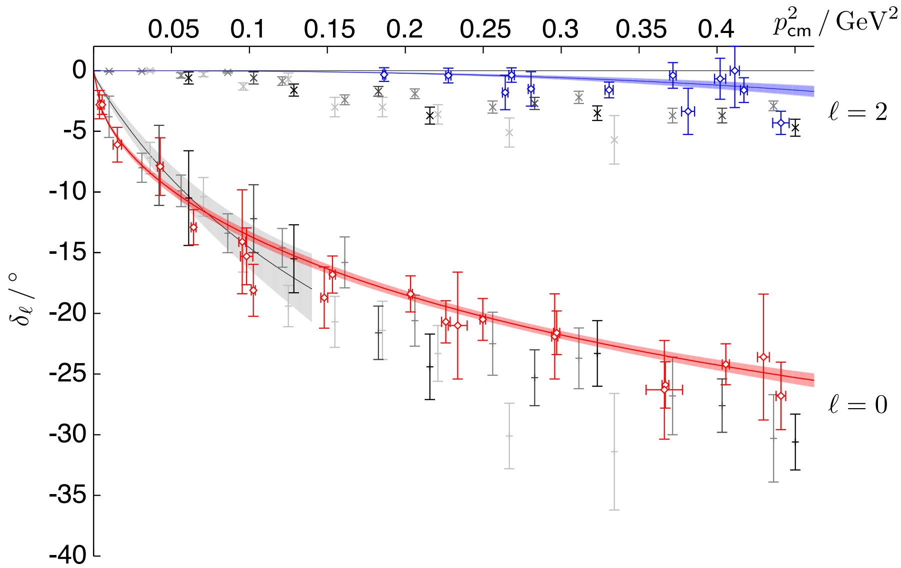

FIG. 6. The $I = 2$ $\pi^+\pi^+$ elastic $l = 0$ (red) and $l = 2$ (blue) phase shifts as a function of squared momentum at a pion mass of $m_\pi = 396$ MeV. The experimental data are shown in grey, and the constrained analysis using the Roy equations is shown as the black line and grey band. For the lattice calculation at this pion mass the entire region is elastic, while for the experimental data only $p^2_{\rm cm} < 0.058$ GeV is elastic [72].

The $\pi^+\pi^+$ system is the simplest with which to explore hadronic interactions due to the ease of calculability of mesonic systems compared to baryonic systems. There have been a number of precise studies of the s-wave scattering length in this system, but recently calculations have been extended, with advances in algorithms and in source structures, to phase shifts below the inelastic threshold [41, 42, 72, 73]. Figure 6 shows the results of calculations of the $l = 0$ and $l = 2$ phase shifts calculated by the JLab group [72]. Extrapolation from the heavy pion masses of the calculations to the physical pion mass predict phase shifts that are consistent with experiment and are more precise for much of the kinematic regime [42]. As excited hadronic states are resonances in channels of two or more hadrons, the ability to determine phase-shifts from the lattice energy eigenvalues is critical in the isolation of such states, and for theoretical predictions of the excited hadron spectrum.

The low-energy interactions between hyperons and neutrons dictates the onset of strangeness in dense matter such as that which may be created in core-collapse supernova. With sufficiently attractive interactions, the strange mesons and baryons become energetically favored in the dense medium. Recent calculations of the $n\Sigma^-$ interactions at unphysical quark masses have been extrapolated to the physical point using effective field theory. Diagonalization of the effective field theory Hamiltonian in the finite lattice volume provided a direct comparison with the results of Lüscher's method, and agreement was found between the two methods within uncertainties. Weinberg's power counting was used to perform the quark mass extrapolation. The predicted phase-shifts agree with those determined from the available experimental data. It is projected that the next generation of Lattice QCD calculations will produce results with smaller uncertainties than those obtained from experiment, leading to a quantitative improvement of theoretical predictions in these extreme astrophysical environments.

Lattice QCD calculations of Bose-Einstein condensates have been extended to systems comprised of order eighty mesons [74–77]. Analysis of these systems, when combined with the precision two-meson calculations, have led to a determination of the three-meson interaction [74]. A surprising result is that tree-level χPT describes these systems even at the heavy light-quark masses, and hence tree-level χPT should provide reasonable estimates of the properties of a kaon-condensed phase that may form in dense matter. Recursion algorithms have been developed to allow for the Wick contractions contributing to a system with N mesons to be related to those for a system with $N-1$ mesons, requiring only a small number of operations [78].

With the exception of the threshold meson scattering parameters, all of the calculations of nuclear interactions have been performed at a single lattice spacing, and at light-quark masses that produce a pion with a mass greater than $m_\pi \sim 250$ MeV. This has been dictated by the computational resources that have been available to the program to date. Calculations involving nucleons are more complex than calculations involving mesons, such as those relevant to particle physics, and face different numerical challenges. While removing the systematic uncertainty introduced by a finite lattice spacing is crucial, valuable information about the nuclear forces can be extracted from calculations away from the physical pion mass, such as quantifying the fine-tunings that permeate nuclear physics, and the differentiation of various mesonic contributions to interactions and their subsequent contribution to inelastic processes. The calculations that have been performed to date indicate that the two-nucleon systems remain unnatural away from the physical values of the light-quark masses, a somewhat surprising result.

B. Future Program and Resource Requirements

The connection between nuclear physics and the underlying theory of fundamental forces will be solidified during the next decade using Lattice QCD. Technology will be developed to reliably calculate the properties and interactions of light nuclei and to quantify, and systematically remove, the uncertainties in such calculations. It is this rationale that underpins the **2014 NSAC Performance Measure HP10**. Fundamental questions regarding the dependence of nuclei and their interactions on the fundamental parameters of nature, and the fine-tunings in nuclear physics, will be answered along the way. Simultaneously, the behavior of exotic matter, such as kaon-condensed matter or hyperonic matter, that is extremely difficult, or impossible, to access in the laboratory but may play an important role in extreme environments, will be quantified. It is exciting to note that the upcoming experimental programs at J-PARC [96], FAIR [79], the Thomas Jefferson laboratory, and the relativistic heavy ion experiments at BNL and CERN, may be able to observe or constrain the simplest exotic systems.

A suite of baryon-baryon, multi-baryon and multi-meson calculations must be performed at the physical light-quark masses, and with a range of volumes and lattice spacings in order to quantify the systematic uncertainties associated with using a finite space-time grid. This will provide the first calculations of nuclear forces from QCD that can be compared directly with those of nature, which can then used to make reliable predictions for nuclear systems, though without electromagnetism or isospin breaking. The substantial hierarchy of energy-scales contributing to the correlation functions that are used to extract energy-levels and S-matrix elements continues to present a challenge to the Lattice QCD calculations and requires further algorithmic developments. The ongoing efforts to extend the range of calculations to multi-nucleon systems, for instance to p-shell nuclei, requires developments in the algorithms used to calculate Wick-contractions. Once the energy-levels of these multi-hadron systems can be determined with precision, the matrix elements of electroweak operators between such states can be calculated. Further, Lattice QCD will be used to make predictions for the interactions between strange baryons and nucleons, and the structure of the lightest hypernuclei, that may be tested in the upcoming experimental programs.

The key research drivers in this area of research are:

- *Nucleon-Nucleon Interactions and the Deuteron*

  The nucleon-nucleon scattering phase-shifts at low- and intermediate-energies will be calculated over a range the light-quark masses. This will provide a verification of the Lattice QCD technique for the nuclear forces and the associated deployed technology. It will also isolate and refine the chiral nuclear potentials that are used in nuclear many-body calculations, providing a rigorous underpinning to nuclear many-body calculations and allowing for the fully quantification of the uncertainties of such calculations. The complete decomposition of the chiral nuclear forces requires calculations at unphysical light-quark masses. In addition, calculations at unphysical pion masses will also quantify the fundamental parameter range that generates a finely-tuned nuclear physics. While the deuteron is the simplest nucleus, it is also the most challenging to generate at the physical light-quark masses due to its shallow binding. First post-dictions of the deuteron binding energy will be made during the next five years. One of the challenging issues to be faced as the pion mass is reduced toward its physical value is the approach of the scattering lengths to very large values in both channels, but particularly in the spin-singlet channel. This is shown explicitly in Figure 8, along with currently allowed effective-field-theory extrapolations of the Lattice QCD calculations [60]. The calculations at $m_\pi \sim 200$ MeV will be crucial in determining the form of the chiral extrapolation to the physical light-quark masses.

- *Hyperon-Nucleon Interactions and the Core of Neutron Stars*

  The composition of nuclear matter at densities somewhat above that found in the center of nuclei is uncertain, and this uncertainty limits our present ability to predict the evolution of explosive stellar systems, such as core-collapse supernova. Reducing

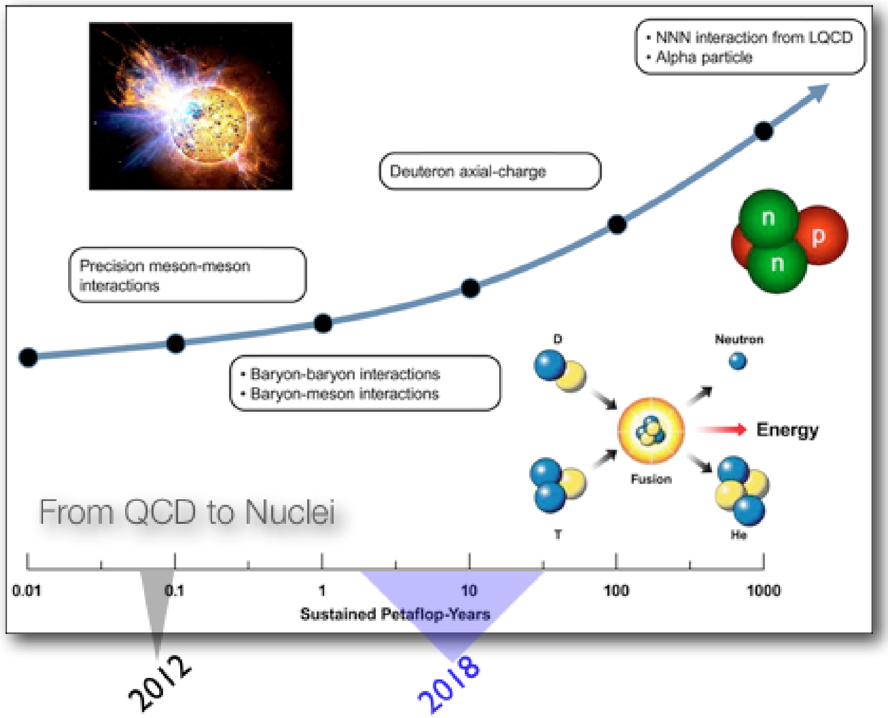

FIG. 7. Estimates of the resources required to accomplish calculations of importance to the nuclear physics program. The 2018 "effective" estimate is based upon Moore's law increases from present resources, with a range estimated from possible algorithmic advances - the left most corresponds to no algorithmic improvements while the right most corresponds to an extrapolation from present day advances.

the presently significant uncertainty in the forces between hyperons and nucleons, and also amongst hyperons, will greatly improve our predictive capabilities in such environments. With verification of the technology in the nucleon-nucleon sector, the predictions for the hyperon-nucleon forces will have fully quantified uncertainties.

- *S-Shell Nuclei and Hypernuclei, and their Interactions*

  First calculations of S-shell nuclei and hypernuclei, *albeit* at unphysical pion masses, have recently been performed. These nuclei will be determined at smaller lattice spacings and over a range of light-quark masses down to the physical pion mass. These calculations will enable the construction of effective interactions, including multi-nucleon forces, that can be used to calculate processes the greatly extend the range of the Lattice QCD calculations themselves. While extracting the ground states have proved possible through algorithmic advances, the excited states have significantly larger uncertainties and isolating them from excitations of continuum states in the lattice volume remains a challenge. It is these continuum states that will yield the interactions of clusters of these nuclei, and so further developments in source structures are required to isolate scattering states, in addition to the formal developments that are beginning

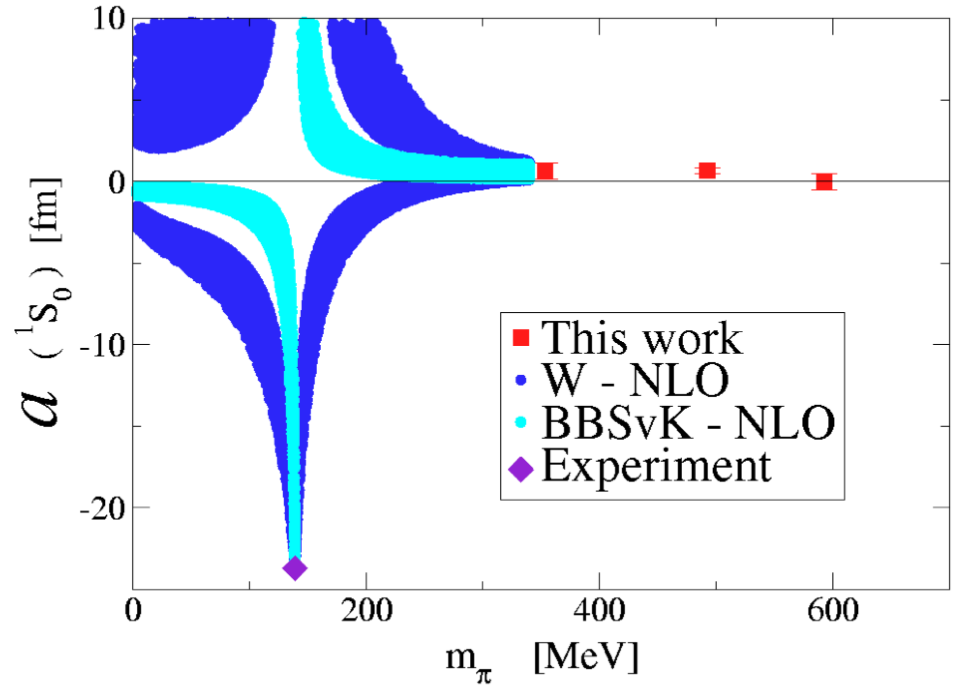

FIG. 8. The behavior of the nucleon-nucleon scattering length in the spin-singlet channel as a function of the pion mass [60] (in the isospin limit and without electromagnetic interactions). W-NLO denotes effective field theory with Weinberg's power counting, while BBSvK denotes that with BBSvK's power counting. "This work" denotes the calculations of Ref. [60], which are the only calculations within the range of validity of the effective field theory to date, and the lightest pion mass may also be too large for convergence of the effective field theory.

to be addressed.

- *P-Shell Nuclei and Hypernuclei*

  Lattice QCD calculations of p-shell nuclei have not been accomplished yet, limited by contraction algorithm developments. Algorithms are currently under development to extend calculations into the p-shell in the near future. First calculations of such nuclei are planned in the near future, and will be extended in parallel with those of the s-shell nuclei.

- *α-Cluster Nuclei, ^{12}C and the Hoyle State*

  An algorithm has been recently developed [70] to calculate lattice QCD correlation functions for α-cluster nuclei, and it has been applied to correlation functions for nuclei up to ^{28}Si. This technology will be developed and refined to calculate such nuclei, with a focus on ^{12}C and the finely-tuned Hoyle state, along with the analogous state in ^{16}O, that is responsible for producing sufficient carbon to permit life on our planet. This research thrust ties in closely with recent advances in nuclear many-body calculations of ^{12}C and the Hoyle State [80]. Presently, this is an exceptionally challenging problem for lattice QCD, and is secondary to the precision determination

TABLE III. Resources, in Tflops-years (TF-yrs), required to calculate the low-lying states in nuclei and hypernuclei at the physical pion mass with full quantification of uncertainties using the clover action. These estimates do not include strong isospin breaking or electromagnetism. A "*" indicates that the multigrid algorithm has been assumed in these resource requirements. Given the magnitude of these resource requirements, it is anticipated that only some of these calculations will be completed during the next five years.

$N_s^3 \times N_t$	b (fm)	m_π (MeV)	$m_\pi L$	$m_\pi T$	Trajectories	Lattice Generation (TF-yrs)	Measurements* (TF-yrs)
$64^3 \times 128$	0.09	200	5.8	11.7	10^4	43	90
$96^3 \times 128$	0.09	200	8.8	11.7	10^4	200	400
$96^3 \times 256$	0.06	200	5.8	15.6	10^4	560	1100
$128^3 \times 256$	0.06	200	7.8	15.6	10^4	1650	3300
$96^3 \times 192$	0.09	140	6.1	12.3	10^4	380	760
$128^3 \times 256$	0.09	140	8.2	16.4	10^4	1620	3200
$128^3 \times 256$	0.06	140	5.5	10.9	10^4	1940	3800
$192^3 \times 384$	0.06	140	8.2	16.4	10^4	14700	30000

of the chiral nuclear forces from the nucleon-nucleon interaction, s-shell nuclei and lighter p-shell nuclei.

Previously acquired resources have been used to generate gauge-field configurations using the isotropic clover action at one lattice spacing, two pion masses and in three volumes at the SU(3) symmetric point, and to perform high-statistics calculations of nuclear correlation functions. The 2013 resources will be used to generate configurations and nuclear correlation functions at a pion mass of $m_\pi \sim 400$ MeV. Current estimates, as shown in Figure 7, make clear that Lattice QCD calculations that directly include isospin breaking and electromagnetism directly into the gauge field evolution cannot be accomplished without exa-scale computing resources. However, in nuclear physics, these effects can be approximately included *post facto* with peta-scale resources. During the next five years, if resources available to this area of research increase with Moore's Law, calculations of s-shell and p-shell nuclei will be performed at a pion mass of $m_\pi \sim 200$ MeV, as seen from Table III. This will allow for predictions of the periodic table of elements at this pion mass through matching to existing and developing nuclear many-body calculations through collaboration with the broader nuclear physics community. Further, using the effective field theory techniques that have been developed during the last two decades, extrapolation to the physical light-quark masses will be performed with the uncertainties introduced in the extrapolation quantified. While the chiral nuclear forces are expected to be perturbatively close to those of nature, predictions for the nucleon-nucleon scattering lengths will likely suffer from significant uncertainties as both two-nucleon systems are near unitarity at the physical light-quark masses. When used in nuclear many-body calculations of systems that are not finely-tuned, these forces are expected to produce results that can be extrapolated to the physical light quark masses with small and controlled uncertainties.

Were the available resources to scale faster than Moore's law, and if developments in algorithms continue at the present rate, we expect to perform the first calculations of nuclei at the physical point with two or more lattice spacings and in multiple volumes. The resources requirements to accomplish these objectives are shown in Table III; note that the cost of the lattice generation on the smaller lattice volume at each lattice spacing can be shared with those generated for hadron structure. These calculations will be sufficient to quantify all uncertainties associated with this technology, and the *post facto* inclusion of isospin breaking and electromagnetism, will allow for direct comparisons with experiment. Once the technology is verified, predictions of processes that are difficult, or impossible, to determine experimentally can be performed with a full quantification of uncertainties.

VII. FUNDAMENTAL SYMMETRIES

A. Motivations and Achievements

Research efforts to uncover particles and symmetries beyond those of the standard model of the strong and electroweak interactions are multi-pronged, and key parts not only of the nuclear-physics program but of the high-energy-physics effort; some of the topics below are discussed in further detail in the companion white paper *Lattice Gauge Theory for Physics on the Intensity Frontier.*

One of the approaches in this effort is to perform precision measurements of the properties of known particles and there is an ongoing experimental program focused on the magnetic moment of the muon. The E821 experiment at Brookhaven National Laboratory has measured the muon g-2 with an uncertainty of 0.7 ppm, which deviates from the theoretical calculation by $\gtrsim 3\sigma$. The approved E-989 experiment at Fermilab is designed to reduce the uncertainty in g-2 below 0.14 ppm, either verifying the discrepancy with theory or resolving it. A major uncertainty in the theoretical calculation arises from strong interactions through quantum loops. Exploratory Lattice QCD calculations of the muon $g-2$ are underway to understand how to calculate the strong interaction contributions[81–83], and the 2011 **Kenneth Wilson Prize** [95] was awarded to Dru Renner of the *European Twisted Mass Collaboration* [84] for calculations of the leading contributions to the magnetic moments of the leptons.

Nature is very nearly invariant under certain symmetry transformations, and the consequences of the slight non-invariance can have widespread implications. A well known example is CP-violation, where the combined operation of charge-conjugation, C, and spatial-inversion, P, is known to be slightly violated, and without CP-violation, the present-day matter and antimatter asymmetry of the universe would not exist. The nEDM collaboration is preparing to measure the electric dipole moment (edm) of the neutron [97], a quantity that vanishes in the absence of time-reversal, T, violation (equivalent to CP-violation when CPT-invariance is exact), with a precision of $\delta d_n \sim 3 \times 10^{-28}$ e cm at the Spallation Neutron Source (SNS) at Oak Ridge National Laboratory; the behavior is illustrated in Figure 9. There have been a number of efforts, part of the broader effort to support the **2020 NSAC Performance Measure FI15**, to calculate the neutron edm arising from the QCD θ-term using Lattice QCD [85, 86], but such calculations are found to be sensitive to the topological structure of the gluon fields.

During 2010, the first Lattice QCD calculation of nuclear parity violation was performed at a pion mass of $m_\pi \sim 390$ MeV [87], in which the “connected diagrams” contributing to the

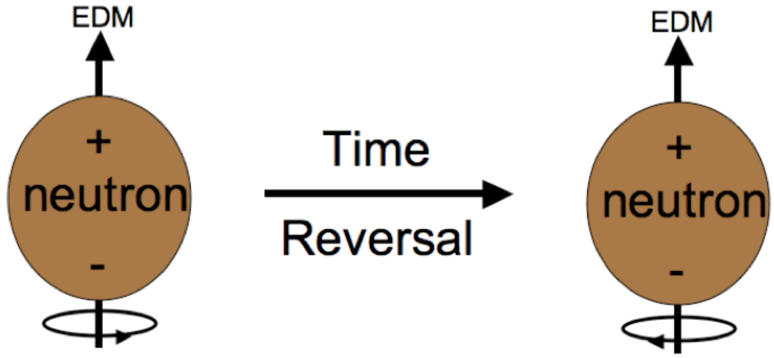

FIG. 9. A cartoon showing the behavior of the neutron electric dipole moment under time-reversal.

weak one-pion-nucleon vertex, $h^1_{\pi NN}$, were determined, illustrated in Figure 10. Its value at unphysically large light-quark masses was found to be consistent with the unnaturally small value extracted from theoretical analyses of a number of experimental measurements. An ongoing experimental effort by the NPDGamma Collaboration [88] at the SNS promises to greatly reduce the experimental uncertainties in the value of $h^1_{\pi NN}$, likely in a similar time-frame to the Lattice QCD calculations.

In anticipation of precise experimental constraints on the structure of the four-Fermi operators contributing to the β-decay of ultra-cold neutrons, lattice QCD calculations are underway to determine the strong interaction contributions to the matrix elements of such operators [89]. This is closely tied to the calculations of the structure of the nucleon, and provides constraints on physics beyond the standard model of electroweak interactions.

Observation of a transition of neutrons to antineutrons could provide distinct evidence for baryon number violation from beyond the Standard Model physics [90]. This hypothesized process, violating the baryon number by two units, can be observed through annihilation of the resulting antineutron. Prospects for its experimental detection include large scale proton decay and dark matter searches (in-nuclei oscillation), as well as free-neutron experiments [91]. For a wide range of grand unified theories (GUTs), the prediction for the oscillation period is between 10^9 and 10^{11} seconds [92]. These estimates include uncertainties from matrix elements of the effective six-quark operators between neutron and antineutron. Such matrix elements may be evaluated on a lattice, eliminating uncertainty from the oscillation period estimates and sensitivity of current and future experiments. Furthermore, they are free of contributions from so-called disconnected diagrams and hence of their associated uncertatinties. Some initial calculations have been performed to test the computational scheme [93].

B. Future Program and Resource Requirements

The currently exploratory calculations of nuclear parity violation, will be greatly refined with the inclusion of quark-loop contributions. While encouraging, the present calculations are far from conclusive even at the heavy pion mass. At lighter quark masses, with lowest-lying odd parity state unstable against pion decay, a different calculation strategy will be

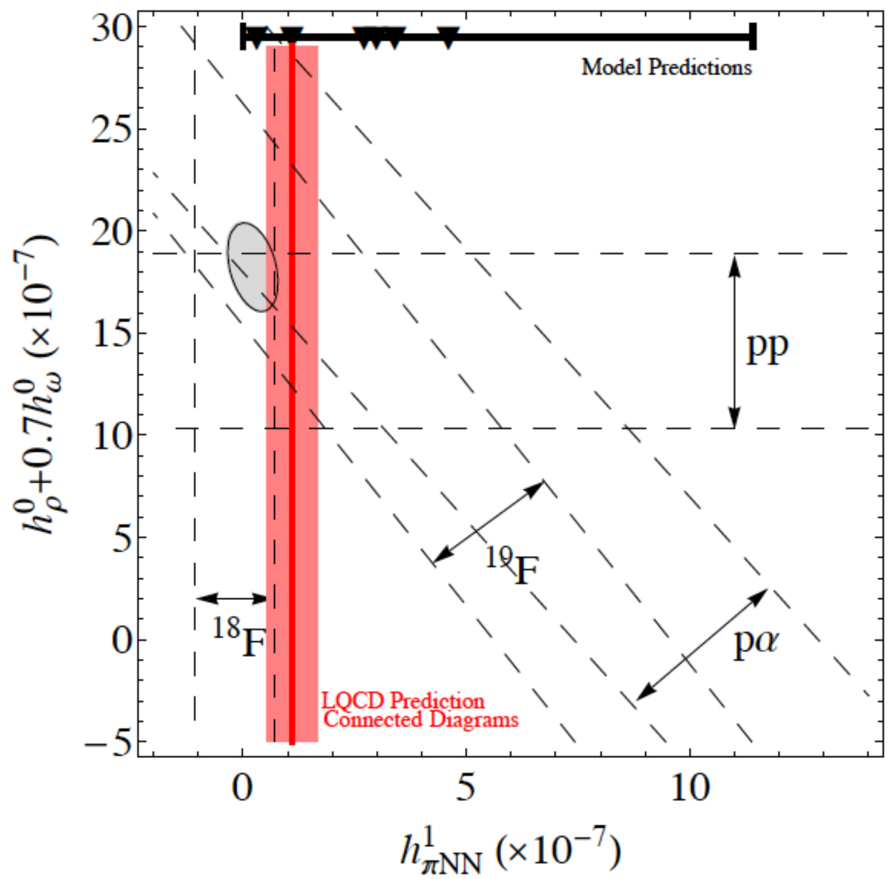

FIG. 10. Constraints on nuclear parity-violating interactions including the recent Lattice QCD result [87] (shaded (red) region), and the experimental 1σ uncertainty ellipse (gray).

required, likely along the lines of that described in Ref. [94]. A more complete program will involve direct calculations of parity violation in the multi-nucleon sector, and with the recent developments in the multi-nucleon sector (outlined previously in this document), such calculations are currently being planned.

- *Electric Dipole Moments of the Neutron, Proton and Deuteron*

  The neutron edm calculations will be performed at or near the physical quark masses. In addition to the contribution from the dimension-4 operator - the QCD θ-term, formally subleading contributions from dimension-5 operators will be evaluated as it may be the case that the θ-term is dynamically forced to vanish. The calculations will be extended to the proton and deuteron due to the experimental possibilities of measuring their edms at beam facilities.

- *Strong Interaction Contributions to the Muon Magnetic Moment*

  With the significant experimental program to more precisely measure the magnetic moment of the muon, the lattice community will be focusing on calculations to reduce the uncertainty in the contribution from the strong interactions. Efforts will be made to synchronize theoretical progress with that of the experimental program. The INT hosted a initial workshop on this matter in the recent past, and close connections between the lattice community, phenomenologists and experimentalists will be fostered going forward. This subject will also be a thrust in the *lattice QCD at the Intensity Frontier* area, as described in that Whitepaper.

Estimates of the computational resources required to accomplish the goals outlined in this section are shown in Figure 11.

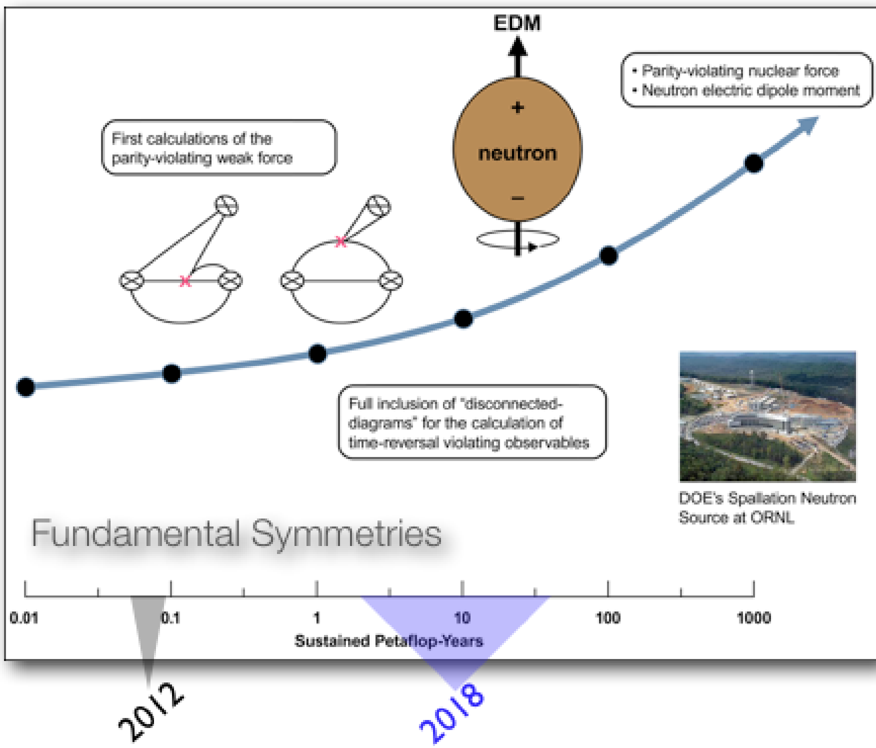

FIG. 11. Estimates of the resources required to accomplish calculations of importance to the Fundamental Symmetries program. The 2018 "effective" estimate is based upon Moore's law increases from present resources, with a range estimated from possible algorithmic advances - the left most corresponds to no algorithmic improvements while the right most corresponds to an extrapolation from present day advances.

VIII. SUMMARY

Lattice QCD, a technique to numerically evaluate the QCD path integral, is poised to transform the field of nuclear physics during the next five years. Not only will it provide a fundamental description of the nucleon, both its structure and its excitation spectrum, and the spectrum of exotics excitations of matter, it will also provide a first principles calculation of the spectrum and interactions of the light nuclei and hypernuclei. With sufficient computational resources, the first calculations of many quantities of importance for nuclear physics will be performed at the physical light-quark masses. In addition to providing a direct connection between QCD and low-energy nuclear physics, the results will be used to refine and constrain hadronic-level nuclear many-body calculations, effective field theories of mesons, baryons and multi-baryon systems, and also phenomenological descriptions of the structure of the mesons and baryons.

IX. ACKNOWLEDGMENTS

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