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QUANTUM COMPUTING FOR THEORETICAL NUCLEAR PHYSICS

A White Paper prepared for the U.S. Department of Energy, Office of Science, Office of Nuclear Physics

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Executive Summary

Tremendous excitement exists among quantum computing enthusiasts as we witness the rapid evolution of quantum computing devices toward early practical implementation. Importantly, algorithm developments suggest that qubit devices have the potential to solve quantum many-body and quantum field theory problems of relevance to various research directions within the Department of Energy Office of Science and National Science Foundation. While exascale platforms represent the current horizon of excellence in computing, quantum computing provides the technology that lies beyond this horizon and opens the door to new vistas of theoretical endeavor.

During a recent workshop at the Institute for Nuclear Theory, a group of 39 scientists from academia, government, national laboratories, and industry gathered to discuss the future of quantum computing for nuclear physics. Researchers described the basic scientific challenges in quantum chromodynamics and quantum many-body problems that could be addressed utilizing the power of quantum computing in the future. The group also discussed mechanisms for developing quantum-computing algorithms specifically for nuclear physics applications. This White Paper provides a synopsis of the workshop discussions, and suggests possible activities that might be supported as part of a vibrant pilot program of nuclear physics research in this area.

Introduction

For decades, scientists have known that devices to store and manipulate information in quantum physical systems such as atoms, photons or superconductors, could provide radical new capabilities in computing [**1**]. As existing computing technologies approach fundamental limits to continued scalability, quantum computing (QC) has emerged as a profoundly different and potentially more powerful way of computing. By exploiting the novel laws of quantum physics, QC promises to open new scientific and industrial frontiers by transforming some computationally hard conventional computing problems into tractable and scalable forms. However, the development of practical QC technologies is a grand challenge requiring significant advances in material science, device physics, hardware and system engineering, computer science and algorithm development.

Quantum bits (qubits) are the basic physical building blocks of any future quantum computer or coprocessor. QC requires many qubits that can be initialized into predefined quantum states, manipulated to process quantum information (QI), and measured to extract computational results. In addition, qubits must reliably store the prepared quantum state between successive operations. The effectiveness of a qubit for these tasks depends on the fundamental physical interactions between the qubit and its local environment, particularly the electric, magnetic, and phonon environments. Despite progress in minimizing unwanted interactions, current state-of-the-art efforts cannot measure, model, or predict the qubit environment with sufficient accuracy to enable the large-scale fabrication of the high-fidelity qubits needed for mission-scale QC. The state-of-the-art in QC hardware during the next few years, coinciding with the exascale era in conventional computing, will involve intermediate scale systems with at most a few hundred qubits without error correction capabilities. This era, recently dubbed NISQ for *Noisy Intermediate-Scale Quantum,* is upon us [**2**].

Open questions exist regarding how to effectively use qubits as computational resources. As basic units of information, qubits obey logical rules that are very different from those governing conventional bits and are often nonintuitive. Consequently, nascent quantum programming models differ from traditional ones, and are not nearly as well understood. Moreover, some core quantum algorithms show significant promise for computational speedups in physical science applications, such as many-body quantum chemistry, but to date these algorithms have only been developed for a small set of problems of practical interest. Near-term, real-world applications do not yet illustrate the interplay between quantum and traditional computation; a broader understanding of quantum and traditional programming models, as well as quantum and conventional computing hardware, is currently lacking. In chemistry, variational calculations of atomic orbital configurations of complex molecules are currently the ``killer app'' for QC, e.g., Refs. [**3**] [**4**] [**5**] [**6**]. The anticipated improvements in the determination of the energy levels of such molecules, and the capability to scale to larger molecules than are accessible to conventional computational resources, will have important societal implications.

The conventional computing resources that will be required to meet the scientific objectives of the nuclear physics (NP) research program during the next several years were established in the 2017 Exascale Requirements Review [**7**]. Because of the nature of quantum many-body systems and quantum chromodynamics (QCD), the range of relevant lengths scales spanning from subatomic to astrophysical, and the emergent nature of nuclear systems, computing resources at exascale and beyond are required to address many of the Grand Challenges facing nuclear physics. The need for these large-scale computing requirements follows from the exponential growth in the number of quantum states required

to describe nuclear physics systems as the number of particles increases, and the complex nature of the sum over paths required to evolve quantum states in time. Even with exascale conventional computing resources, there are systems and environments that cannot be explored with the desired accuracy using current theoretical formulations and algorithms; this is schematically illustrated in Figure 1.

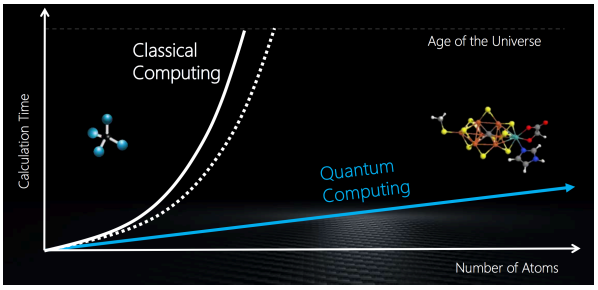

Figure 1: A schematic of the scaling of required computation times with increasing particle number in simulations of large molecules. [This image is reproduced with permission from David Wecker (Microsoft Research)].

Technology companies such as Google [**8**], IBM [**9**], Intel [**10**] and Microsoft [**11**] expect to have programmable quantum computers with circa 50-qubits (without error correction) available during 2018. IBM announced an operational 50-qubit QC near the end of 2017, and currently has a 20-qubit QC, a 16-qubit QC and two 5-qubit QCs available to users through the **IBM Q Experience** web-interface, which is an upgrade from the 5-qubit QC that was available during 2016. The architectures of these QCs encompass superconducting qubits (IBM, Google and Intel) and topological qubits (Microsoft). D-wave [**12**] constructs quantum computers that use quantum annealing to address minimization problems. A growing number of smaller technology companies are also moving toward building programmable QCs, such as Rigetti [**13**], IonQ [**14**] and others. These technologies have typically emerged from, and have ongoing ties with, university-based research groups funded by the Department of Defense (DOD), the Department of Energy (DOE) and the National Science Foundation (NSF). In addition, some university-based groups are making significant progress in quantum simulation, with recent results announced in quantum many-body systems obtained with programmable quantum simulators using more than 50 cold trapped ions as qubits [**15**] [**16**].

Within the DOE Office of Science, the Office of Advanced Scientific Computing Research (ASCR) has been increasing its engagement with the scientific community in the areas of quantum computation and information since 2014. Awards have been made through the **Quantum Testbed Pathfinder** program ``*to provide decision support for future investments in QC hardware and increase both breadth and depth of expertise in QC hardware in the DOE community*'', and also through **Quantum Algorithms Teams** ``*to stimulate early investigations of quantum simulation and machine learning algorithms by focusing on key topics of research with relevance to problems of interest to SC*''. Within the NSF, programs have been established in quantum computing and quantum information that support ``*theoretical and experimental proposals that explore quantum applications to new computing paradigms or that foster interactions between physicists, mathematicians, and computer scientists that push the frontiers of quantum-based information, transmission, and manipulation.*''

There is little expectation that QC will soon replace conventional computing in addressing the "Grand Challenge" problems facing nuclear physics. However, the NISQ systems that are expected in the near future could be of benefit to nuclear physics research as stand-alone systems, or through integration into exascale or post-exascale computing hardware (in analogy with GPUs), complementing conventional high-performance computing (HPC) systems. The algorithms that are required to formulate problems on QCs, exploiting their massive quantum parallelism, will be significantly different from, and are expected to influence, those employed on conventional computers. The development of algorithms appropriate for emerging QC architectures, and the evolution of

nuclear physics research to take advantage of these new computing platforms, will require establishing a workforce that is trained in nuclear physics, conventional HPC and QC. Development of this workforce is expected to benefit from close collaboration between universities, national laboratories and technology companies, in addition to possible collaboration between Offices within DOE, such as ASCR, High Energy Physics (HEP), Basic Energy Sciences (BES) and NP.

A program to develop QC algorithms and program current QC architectures to solve nuclear many-body problems and quantum field theories was recently initiated within the Institute for Nuclear Theory (INT) (see, for example, Ref. [**17**]). In this program, fellows, postdoctoral researchers and graduate students are collaborating with researchers at Oak Ridge National Laboratory (ORNL), Los Alamos National Laboratory (LANL), Microsoft Research and the Institute for Quantum Information and Matter at Caltech [**18**]. These collaborations integrate well with the INT's core mission to introduce and disseminate new ideas, theoretical frameworks and technologies into the nuclear physics community, through its local research activities, workshops, programs and summer schools. At ORNL, the Physics Division and the Computational Sciences and Engineering Division participate in an effort in QC connected to ASCR projects, which is supported through the **Quantum Testbed Pathfinder** and **Quantum Algorithms Teams** described previously. The Theoretical Division at Los Alamos also has a strong effort in quantum computing, and the nuclear theory group at LANL is collaborating with their condensed matter colleagues in this area.

This White Paper on Quantum Computing in Nuclear Physics has been prepared at the request of the DOE Office of Science, Office of Nuclear Physics. It represents an extension of discussions and material presented at the workshop ***Quantum Computing for Nuclear Physics,*** which was held at the INT during Nov. 14-15 2017 [**19**], which brought together experts in quantum and conventional computing, the computing industry, quantum information, computational physics, condensed matter experiment, high-energy physics and nuclear theory. Here we will focus on opportunities to develop and apply QC specifically to nuclear physics; we note that within the Office of Science, ASCR, BES, and HEP are individually pursuing aspects of QC relevant to their respective missions. There is a clear opportunity for NP to develop relevant QC algorithms and applications through partnerships with these DOE Offices.

Principles of Quantum Computing

The fundamental principles of QC stem from the theory of quantum mechanics. Quantum mechanics was developed in the early 20th century to explain the behavior of a wide variety of physical systems including nuclei, atoms, electrons, and photons, as well as novel condensed matter and macromolecular systems. Among the many essential quantum concepts that impact QC are superposition, entanglement, and the uncertainty principle, i.e., the statistical nature of quantum mechanical measurements. The application of those ideas to the theory of information led to the development of QI theory, from which QC originates, as well as other potential application areas such as quantum communication and quantum sensing.

In QI theory, the principle of superposition is used to construct new representations of information. Conventional computing is formulated using a binary representation of data and instructions, in which a register element r stores a bit b that may take on either of two values, b_0 or b_1. By comparison, QC also requires a physical element r to store information, but the quantum register element may now take on a value q allowed for a quantum bit, or qubit, q. The qubit q represents a superposition of binary states, e.g., value(r) = $q = \alpha b_0 + \beta b_1$, in which the basis states b_0 and b_1 represent the quantum two-level system, and α and β are complex numbers. For example, the quantum state of an electron prepared in a well-defined superposition of the orthogonal spin-up and spin-down basis states represents a qubit, while the electron itself represents the register. Formally, the qubit is a superposition over a complex 2-dimensional (2D) vector space with normalized coefficients, i.e., $|\alpha|^2 + |\beta|^2 = 1$. This leads to a diagrammatic representation for the possible values of a qubit as points on the surface of the unit sphere, the Bloch sphere. As shown in Figure 2 [**20**], the opposing north and south poles of the sphere are analogous to the two possible states of a classical bit, b_0 identified with 0 and b_1 identified with 1, respectively, while *every* point on the surface corresponds to a possible qubit value q.

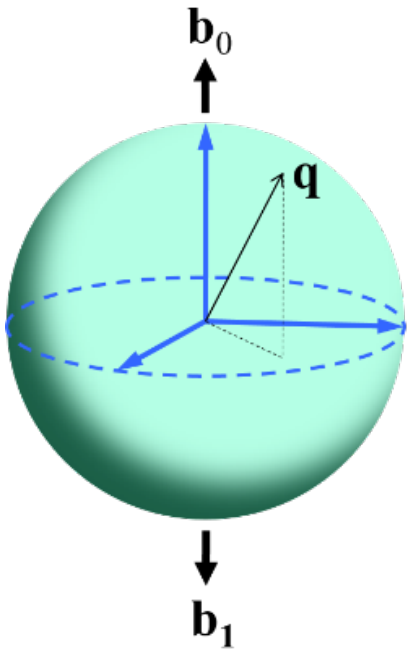

Figure 2: The Bloch sphere illustrates the infinite set of possible values for a qubit q on the unit sphere, while opposing poles of the sphere identify the classical limits of binary values, b_0 with *0 and* b_1 with *1*. A qubit can be realized by preparing a superposition of the quantum states of a two-level system, such as a linear combination of the spin-up and spin-down states of an electron.

An immediate extension of the superposition principle is to the case of more than one quantum register element (qubit). The simplest example is a set of n independent qubits, for which each register element r_i stores a value q_i that is independent of the others. However, quantum mechanics permits another possibility in which multiple register elements may collectively store superpositions over multiple binary values. This phenomenon, known as "entanglement," is a form of information that has no classical analog. The qubit register elements must remain independently addressable, but the information that they store can no longer be expressed piecewise, i.e., value(r_1r_2) ≠ value(r_1) value(r_2). For example, two qubits may be entangled so that

they are both in the b_0 state, $b_0\ b_0$, or both in the b_1 state, $b_1\ b_1$, but exclude any possibility of anti-correlated values, $b_0\ b_1$ or $b_1\ b_0$. The implications of entanglement were central to the Einstein, Podolsky, and Rosen (EPR) paradox, which conjectured the incompleteness of quantum mechanics. EPR argued that the apparent non-local correlations between the properties of otherwise independent physical systems violated notions of locality and reality. However, Bell established experimental conditions to verify the existence of quantum mechanical entanglement, which have since been tested extensively, including in pioneering experimental works by Stuart Freedman and John Clauser [**21**], and by Alain Aspect [**22**]. This remarkable feature of quantum mechanics is central to the functioning and the capabilities of QCs.

Superposition and entanglement force a fundamental change in the interpretation of a register in a QC compared with a conventional computer. "Observing" a qubit by performing a measurement in the original $\{b_0, b_1\}$ basis results in a projection of the quantum state onto either the b_0 or b_1 basis states. This transition from a qubit to a bit corresponds to the "collapse of the wave function" that is induced by quantum measurement. The implication is that the qubit q is not a physical observable. Instead, a superposition state $q = \alpha b_0 + \beta b_1$ must be interpreted with respect to the probability of observing either b_0 to b_1, which are identified as $p_0 = |\alpha|^2$ and $p_1 = |\beta|^2$, respectively. Either of these two outcomes may be observed following measurement, and the exact measurement results cannot be predicted for any arbitrary qubit. Rather, the probabilities p_0 and p_1 provide the likelihood that a given outcome will be observed. Practitioners of QC have learned to use this statistical behavior to their advantage. For example, the collapse induced by measurement is useful for preparing register elements in well-defined initial states and reading out conventional values (for example, quantum expectation values) following a sequence of quantum operations.

Computing with qubits requires controlling the quantum mechanical interactions between register elements. Several computational models support the implementation of universal QC, and all use different methods to transform quantum registers. The first is the gate model of QC, which applies transformations called "gates" to the register elements. Formally, gates define fixed transformations of the quantum states by controlling the short-time dynamics of the register, and a gate may act on either a single or multiple register elements. When laid out as an ordered sequence, the gates define a circuit that can express higher functionality, such as addition, multiplication, and so on. In a laboratory setting, gates are implemented through Hamiltonian dynamics with sequences of externally applied fields. Alternatively, adiabatic QC continuously controls the register dynamics using gradual modifications of the interaction Hamiltonian. By slowly changing the Hamiltonian, the register value can be transformed from one equilibrium configuration to another, in which the initial and final configurations define the desired computation. A third model for quantum computation is topological QC, which implements computational transformations by controlling the topological order of register elements. The basis for this approach is the non-Abelian exchange statistics obeyed by anyonic quasi-particles. Anyonic quasi-particles arise in 2D systems and possess spin-statistics that generalize those of boson and fermion systems. Exchanges of non-Abelian anyons induce non-trivial state transformations termed "braiding." Braiding represents permutations on register elements that are formed from pairs of anyonic quasi-particles. A key feature of this model is that the computation is stored in the degenerate ground state of the anyonic system, which offers intrinsic protection against erroneous transformations.

The principles of QC arise prominently in developing applications for digital and analog quantum simulations. Although the revolutionary principles of quantum mechanics have led to

breakthroughs in our understanding of physics at subatomic length scales, systems described by these theories quickly grow in complexity with the number of degrees of freedom and can become unwieldy. Feynman offered the early QC insight that the quantum mechanical description of atoms, molecules, and photons may be more efficiently represented by using other quantum mechanical systems to carry out calculations of the properties of a given quantum system. There are currently two approaches to realizing Feynman's insight regarding a more efficient solution of the Schrödinger equation. The first is digital quantum simulation, which can solve the Schrödinger equation using a discretized approximation of the time-evolution operator. The approach of digital quantum simulation first makes use of efficient methods for constructing the system Hamiltonian and then efficiently decomposing the time-evolution operator into a sequence of well-defined instructions. These instructions are applied to the register in order to carry out a specific simulation sequence. Processors that support digital quantum simulation can, in principle, also support the execution of other quantum instruction sequences. By contrast, analog quantum simulation uses the interactions between register elements to simulate the continuous-time dynamics generated by a defined Hamiltonian. The efficiency of this method lies in the direct implementation of Schrödinger's equation. However, executing these instructions requires specific implementations of the Hamiltonian that may not suffice for general-purpose QC. For either digital or analog quantum simulation, the resulting computational state represents the many-body wavefunction characterizing the system of interest. Subsequent evaluations may then use the wavefunction to compute observables of the systems being simulated.

Quantum Computing in Nuclear Physics Applications

Quantum Chromodynamics and Quantum Field Theories

QCD is the quantum field theory formulated in terms of quarks and gluons that give rise to protons and neutrons (nucleons), the nuclear forces between them, and the nuclei that ultimately emerge. Decades of efforts by high-energy and nuclear experimentalists in partnership with theoretical efforts led to the formulation of QCD. In general, for high-energy processes occurring in small volumes of space-time, QCD is amenable to expansions in the strong interaction coupling constant, but these techniques become unreliable at lower energies and the longer length scales relevant to low-energy nuclear processes. The only theoretical technique for solving QCD that has proven reliable for describing low-energy structure and processes is **Lattice QCD** (LQCD), in which Euclidean space-time is discretized as a four-dimensional grid and the resulting lattice theory is solved numerically. Motivated by the expectation of exascale HPC resources, a well-planned LQCD research program is being carried out by computational nuclear theorists, in collaboration with high-energy theorists, computer scientists, applied mathematicians and statisticians, to precisely calculate the low-energy properties, structure and interactions of hadrons, including nucleons and light nuclei, and the equilibrium properties of matter under extreme conditions of temperature and density. Theoretical research in these areas complements experimental programs in the US and internationally, such as at RHIC at Brookhaven National Laboratory, CEBAF at Thomas Jefferson National Accelerator Facility and the Facility for Rare Isotope Beams (FRIB) at Michigan State University. LQCD calculations are also expected to play an essential role in a future electron-ion collider (EIC), and in studies of fundamental symmetries, such as in the search for lepton number violation through double-beta decay of nuclei, or in the search for time-reversal violation manifesting itself in electric dipole moments of particles and nuclei.

Dynamical and non-equilibrium properties of nucleons and nuclei, of matter under extreme conditions, and the equilibrium properties of dense matter, are significantly more difficult to determine with conventional computing. For finite-density systems, calculations in Euclidean space suffer from sign problems in the evaluation of the quantum mechanical path integral. In the absence of mitigating variable transformations, these typically require exponentially large conventional computing resources to furnish results with useful accuracies. Further, finite-density systems can require exponentially large numbers of quark contractions in order to correctly describe their underlying dynamics. QCD calculations associated with these systems provide important input into nuclear many-body calculations, as described in the next section.
Significantly, the real-time evolution of strongly interacting systems comprised of quarks and gluons cannot be reliably determined using currently available computational systems and algorithms.

Fragmentation functions, which describe how quarks and gluons that are produced in high-energy collisions ultimately transform into the hadrons that enter the detectors, are essential for the discovery of new physics at the energy frontier. Their analogues in finite-density systems are critical for understanding the quark-gluon plasma and low-viscosity liquid produced in heavy ion collisions and in the earliest moments of our universe. Exploration of matter

through such collisions is a major component of the nuclear physics research program in the United States. Also relevant for the study of matter under extreme conditions of density and pressure, such as occurs in core-collapse supernovae, is coherent real-time quantum evolution in neutrino propagation and oscillations. The nonlinearities present in such evolution, through neutrinos interacting coherently with other neutrinos, render these especially challenging systems to describe quantitatively using conventional computing [**7**].

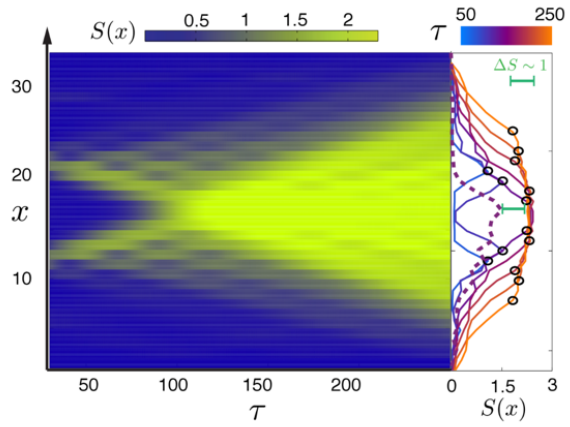

Figure 3: Entanglement entropy in the scattering of two mesons in the Schwinger model calculated using tensor networks [**23**].

Quantum computing offers the promise of radically changing how the physical systems described previously may be addressed computationally. Real-time Minkowski-space evolution of systems that are plagued by a sign-problem, or a signal-to-noise problem, in conventional computations may be free from such limitations when studied with quantum computation. The parallel nature of QC, along with the retention of quantum phase information, suggests that QC can address physical systems described by QCD and by the Standard Model of electroweak interactions that conventional computers, exascale and beyond, will be unable to effectively simulate. As an example, studying the real-time evolution of entropy in scattering processes, as has recently been explored with tensor-network methods in the Schwinger model (see Figure 3), may become possible for larger systems with QC and provide new insights into nuclear interactions and forces.

Only a handful of papers exist that consider QFTs in the light of QC, and only simple calculations in one-dimensional QFTs have actually been performed on present-day QCs. Seminal papers have been written on techniques for, and scaling of, scalar field theories, e.g. Refs. [**24**] [**20**] [**25**] [**26**] [**27**], and lattice gauge theories in the Hamiltonian formulation, e.g. Refs. [**28**] [**29**] [**30**] [**31**] [**32**] [**33**] [**34**] [**35**] [**36**]. Present estimates suggest that 10^5 -10^6 qubits may be required for realistic QCD simulations in spatial volumes comparable to those of present-day simulations using conventional computing resources. A goal for the next few years may be to develop the understanding, formalism and algorithms needed to perform calculations in a well-chosen subset of QFTs, including non-Abelian gauge theories and theories with fermions. Current algorithms mapping the field theories onto the registers of a QC are somewhat cumbersome, and a focused effort in algorithm development in this area is expected to be of great benefit. Studies of low-dimensional scalar field theories, working toward the dynamics of $\lambda\Phi^4$ theory in various dimensions, would provide first inroads for quantum field theory calculations. Low-dimensional gauge theories, such as the Schwinger model in (1+1) dimensions and non-Abelian gauge theories in various dimensions, would provide important insight into more complicated theories in (3+1) dimensions, complementing the understanding gained from the studies of scalar field theories. Calculating the properties of particles and their dynamics in low-dimensional gauge-theories using QC, such as the Schwinger model (where progress has already been made outside the nuclear physics

community, e.g. Refs. [**37**] [**38**] [**39**] [**40**] [**41**] [**42**]), and the associated studies of the scaling of the required number of qubits and gate, will be valuable. Such studies would provide important insights and algorithmic developments that will be necessary to simulate QCD with QC.

It is premature to assert that such disruptive changes to the nuclear physics computational programs in QCD will achieve quantum supremacy on a predetermined timescale. Presently, the lack of understanding about mapping QCD onto quantum computers, about the structure and properties of future quantum algorithms, and about the underlying architectures of QC, precludes such estimates. However, there is a compelling case for beginning to explore what could be accomplished with QC, and with heterogeneous (hybrid) QC-conventional computing systems, that would impact nuclear physics research, and how that might be achieved.

Nuclear Quantum Many-Body Problems

Nuclear properties that can be directly observed include ground-state and excited-state binding energies, spins, parities, and transition branching ratios between nuclear states, and various nuclear decay modes. Equally important are hadron, electron and neutrino scattering processes. Experimental information comes from increasingly sophisticated accelerators and detectors that continue to push into regions previously unexplored. QC holds the promise of systematically exploring the dynamics of strong and electroweak scattering of atomic nuclei, crucial to the nuclear physics experimental program. Because of their connection to nucleosynthesis, the current experimental emphasis focuses on weakly bound, neutron rich nuclei. FRIB will provide tremendous new capabilities for exploring these nuclei.

Over the years, nuclear theorists have used experimental data to refine models of the nuclear forces between protons and neutrons, and to suggest new experiments that may shed a better light on the details of that force. Nuclear theorists seek to develop and provide a theory that can be used to reliably predict, with quantified uncertainties, the properties and interactions of nuclei. Ultimately, this theoretical description of nuclei will connect directly to QCD. The theoretical underpinnings involve development of both adequate quantum many-body techniques and an accurate description of the interactions among nucleons, and their electroweak interactions with photons, electrons, and neutrinos. Significant progress has been made by focusing efforts on effective field theory (EFT) descriptions of the nuclear force and electroweak currents. EFTs incorporate the global symmetries of QCD, and provide a systematic approach to deriving terms in the nuclear force.

Parameters of the nuclear forces are based on experimental nucleon-nucleon scattering data and the properties of the deuteron. Because nucleons have an underlying structure, most descriptions of nuclear properties also include three-body interactions in addition to nucleon-nucleon interactions. Solution to nuclear quantum many-body problems require the application of sophisticated many-body techniques, such as Greens Function Monte Carlo (GFMC), Auxiliary Field Diffusion Monte Carlo (AFDMC), coupled-cluster theory, and Hamiltonian diagonalization. In applications of these methods, the challenges are to provide an accurate description of nuclei, with quantifiable uncertainties, and to utilize increasingly powerful computational platforms to enable accurate descriptions. The nuclear theory community continues to be at the forefront of developing such capabilities, working hand in hand with applied mathematicians and computer scientists to create efficient computational software to tackle problems of relevance to the

DOE Office of Science. Using modern conventional computational hardware, such as the Oak Ridge Leadership Computing Facility (OLCF) and Argonne Leadership Computing Facility (ALCF) platforms, and increasingly sophisticated algorithms, nuclear theorists have been able to accurately model nuclear systems comprised of up to approximately 100 nucleons, whereas most current calculations typically range from a few to approximately 40 nucleons. It is the proliferation in the number of quantum states in these systems and the dramatically increasing number of operations required to properly include multi-body interactions that presently limits the size of systems that can be studied with useful numerical accuracy.

The development of QC capabilities designed to address nuclear many-body problems have not been systematically attempted in the past. In order to begin an assessment of the applicability of QC to nuclear many-body problems, an ASCR **Quantum Algorithms Team** of nuclear theory experts of proven experience has been assembled by scientists at ORNL to work together with applied math colleagues in order to develop appropriate QC algorithms to tackle aspects of the problems. These algorithms, once formulated, are ported and prepared to run on near-term hardware by a **Quantum Testbed Pathfinder** team at the same institution. The nuclear force contains a central component, which induces proton-proton, neutron-neutron and proton-neutron pairing, spin-spin interactions among nucleons and spin-orbit and tensor interactions. Only the very simplest pairing interactions among particles have been addressed previously [**43**]. One important objective is to develop algorithms that span all aspects of the nuclear interactions.

Solutions to these problems could be obtained by deriving sets of operations that manipulate a QC to tackle each of the components of the nuclear interaction, first individually and then as a full interaction. An efficient way to perform a mapping from the nuclear Hamiltonian to a QC system could be investigated, both in terms of the number of qubit resources required to perform an operation and in terms of the required non-locality of the interaction. Once the appropriate quantum algorithm has been developed, qubit hardware to implement the developed mapping could be identified. Using a Trotter expansion of the time-evolution, an estimate could be made of the number of gates required to achieve a predetermined accuracy. As a final step, an exploration of how a derived nuclear QC algorithm could address Grand Challenge problems would be performed.

A logical approach to low-energy nuclear many-body problems would be to first simulate the lightest of nuclei, the deuteron and triton, and then to apply the lessons learned to studies of ^{4}He, ^{6}He and ^{8}He. This research could encompass both static properties but also dynamics of strong- and electroweak scattering and transitions. Starting from a leading-order nuclear force model, algorithms could be developed to systematically include the full complexity of the nuclear force in increasingly complex calculations of multi-nucleon systems. Impressively, in this path of development, the first QC calculation of the binding energy of the deuteron (using EFT) has recently been reported [**44**]. This research direction will lead to an understanding of how QC can be applied to a range of light nuclei, using QC hardware that is expected to be available during the next few years. The d+t nuclear fusion reaction and other electroweak transition rates in light nuclei could serve as important follow-on problems for the development of time-dependent QC algorithms. Understanding how new quantum algorithms scale to larger systems will be an important aspect of determining a roadmap for future QC applications.

Broader Impacts

Owing to the universal character of many-body expansions employed to describe nuclear structure, the development of efficient QC environments for configuration interaction, coupled cluster, equation-of-motion coupled cluster, and Green's function methodologies can also benefit other areas that require a detailed characterization of quantum many-body correlation effects. Over the last two decades, this universality has been demonstrated across energy and spatial scales. Applications of nuclear physics including nuclear medicine will be a long-term beneficiary of quantum computing. Related areas that will leverage QC to address outstanding quantum many-body problems are quantum chemistry and materials sciences where accurate and predictive descriptions of collective electronic effects is a prerequisite to understand ground and excited-state properties of molecules and materials and transformations. For example, accurate calculations including many-body effects are needed to model catalytic and photo-driven processes in molecules and materials, enzymatic reactions in proteins, electron transport in biological systems, ultrafast phenomena and spectroscopies to name a few. In this context, QCs may offer an opportunity to combine their capabilities with accurate, but compute-resource-expensive, formalisms that eliminate long-standing obstacles encountered in computational chemistry.

A Pilot Program

The rapid developments in QC and QI, and the potential for these areas to disruptively enhance nuclear physics research capabilities, suggest that a pilot nuclear theory program in QC and QI would now be beneficial. There is a current need to concentrate the efforts of nuclear theorists on developing algorithms and prototypical applications of QC and QI to problems in nuclear physics to better understand its potential for advancing nuclear physics research, both in the near-term and longer-term, and to estimate the resources required to optimally integrate these developments into the future nuclear physics research program. Such a pilot program should include a collaborative working environment that trains undergraduate students, graduate students and postdoctoral researchers on the use of QC and QI in nuclear physics, which will bring QC and QI into the "toolkit" of the computational nuclear physics workforce. During an initial phase, this program could identify research areas within nuclear physics in which rapid progress could most likely be achieved through the use of QC and QI. This would help identify longer-term research directions that may broadly impact nuclear physics. The pilot program would be expected to include the organization and coordination of summer schools (which could include a Nuclear Talent course [**45**]), workshops and other community outreach efforts.

Summary

Rapid advances in quantum computing and quantum information provide a near-term opportunity in nuclear physics research to identify and develop signature problems for which simulation on a quantum computer would provide new physical insights - well beyond the capabilities of conventional computing that is possible in the foreseeable future. Significant impact is anticipated in the areas of QCD and in relevant applications in nuclear structure and astrophysics, including nuclear reactions and nuclear and neutron matter dynamical evolution.

This White Paper outlines a possible pilot program of application development relevant to the Office of Nuclear Physics. A pilot program

funded at the level of $1.5M/year for three years to develop quantum algorithms enabling solution of aspects of QCD and of nuclear many-body problems would be of great benefit to the future of nuclear physics research. This scale of investment is consistent with the 2015 NSAC Long Range Plan [**46**] call for increased support in computational nuclear physics and represents a new and exciting path forward for our field. It also leverages initial investments from ASCR and possible new investments from BES as the Office of Science coordinates activities to address quantum many-body problems in materials science and chemistry.

Glossary of Terms

- Anyon: a quasi-particle obeying fractional statistics that exists (only) in 2-dimensional systems.
- Bloch sphere: a geometrical representation of the pure state space of a qubit (named after Felix Bloch).
- Entanglement: a phenomenon that occurs when particles are generated or interact in ways such that the quantum state of each particle is not independent of the others and cannot be separated from the others.
- Quantum chromodynamics: an asymptotically free gauge field theory constructed in terms of quarks and gluons. When combined with the standard model of electroweak interactions, it is responsible for the nature and dynamics of nucleons and nuclei. Quarks transform as a triplet under the SU(3) of ``color'', while the gluons are in the adjoint representation.
- Quantum computer: a computation system that makes direct use of quantum-mechanical phenomena, such as superposition and entanglement, to perform operations on data.
- Quantum decoherence time: measures the rate of loss of information in a quantum system.
- Quantum gate: a basic quantum circuit operating on a small number of qubits.
- Quantum information science: an area of study based on the idea that information science depends on quantum mechanical effects. It includes theoretical issues in computational models as well as more experimental topics in quantum physics, including what can and cannot be done with quantum information. [*Wikipedia*].
- Quantum superposition: quantum states can be added together to produce another valid quantum state and, conversely, a quantum state can be decomposed into a sum of valid quantum states.
- Qubit: a unit of quantum information, the quantum analogue of the classical bit. A qubit is a two-state quantum-mechanical system, such as the polarization states of a single photon or the spin-states of a spin-1/2 fermionic system.
- Universal quantum computer: a quantum computer that is capable of performing, in principle, any conceivable quantum computation.

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