

Computing Properties of Hadrons, Nuclei and Nuclear Matter from Quantum Chromodynamics

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(Frithjof Karsch, BNL 12/20/2011)

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1 Abstract

Project Title: Computing Properties of Hadrons, Nuclei and Nuclear Matter from Quantum Chromodynamics

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The proposal describes the software development effort which the nuclear physics lattice QCD community intends to pursue during the next 5 years. This will ensure that lattice calculations can make optimal use of forthcoming leadership-class and dedicated hardware, including those of the national laboratories, and prepares for the exploitation of future computational resources in the exascale era. This work will greatly advance our ability to perform competitive, high precision calculations of properties of hadrons, nuclei and nuclear matter. It has impact on current heavy ion experiments at RHIC and LHC, the nuclear structure programs at RHICspin and JLab, and the study of excited states by CLAS at JLab, and future experimental research programs including GlueX at JLab@12GeV and FRIB. If funded, this project will allow us to greatly improve our understanding of interactions in strongly coupled matter under a broad range of conditions.

We intend to further develop and optimize our simulation software for lattice QCD calculations on leadership class computers and on GPU-accelerated heterogeneous architectures. We will improve and extend our software libraries by providing interfaces for heterogeneous computing environments and through the optimization of gauge field evolution algorithms and sparse matrix inverters. The former includes the development of new multi-time scale integrators and the latter will focus on the development of new multi-grid and domain decomposition inverters for several QCD fermion discretization schemes. We furthermore will develop a domain specific language for lattice QCD computations which will enable the generation of highly optimized code within the ROSE compiler framework. This work will be carried out in cooperation with SUPER.

The proposed work is a project of the USQCD Collaboration, which consists of nearly all of the high energy and nuclear physicists in the United States working on the numerical study of lattice gauge theories. It will be carried out by nuclear physicists in USQCD in collaboration with members of the SciDAC SUPER institute and colleagues in the NVIDIA Emerging Applications group.

All our software developments are coordinated with efforts of the US lattice QCD community which is organized through the USQCD collaboration and will be made publicly available through the collaboration WEB page (<http://www.usqcd.org>).

2 Narrative: Scientific Goals and Software Tasks

2.1 Introduction

A fundamental quest of modern science is the exploration of matter in all its possible forms. The overarching mission of the field of Nuclear Physics is to establish a framework with which to perform high-precision calculations, with quantifiable uncertainties, of the properties and interactions of nuclear matter under a broad range of conditions, including those beyond the reach of laboratory experiment. For the last century, impressive experimental facilities have provided numerous discoveries which have led to the theoretical developments that currently underpin the field. Since the 1970's, quantum chromodynamics (QCD), a non-Abelian quantum gauge field theory constructed in terms of quarks and gluons, has been established as the theory of the strong interactions—which, along with the electroweak interactions, is responsible for all nuclear phenomena. However, many aspects of nuclear physics are dictated by the regime of QCD in which its defining feature—asymptotic freedom—is concealed by confinement and by the structure of its vacuum. The numerical technique of *Lattice QCD* is the only known way to perform *ab initio* QCD calculations of strong interaction quantities in this regime.

The ability to calculate strong interaction observables with quantifiable uncertainties is required in order to better define more complex nuclear systems, and developing such a capability will have profound and transformative impact upon the field. Remarkable progress has been made in the last decade in understanding the structure of hadrons and in establishing bridges between QCD, nuclear interactions and matter under extreme conditions. The 12 GeV upgrade at the Thomas Jefferson National Accelerator Facility (JLab) is designed in part to enable the discovery and exploration of exotic hadrons for which the gluons of QCD may play a visible role in their structure. QCD-consistent forces have emerged from the effective field theory (EFT) framework and are currently being used to calculate the properties and interactions of light nuclei, and are foreseen to be a central component of future calculations of processes involving nucleons. Through collaborative efforts within the nuclear structure community, the field of nuclear physics is presently entering an era in which precise QCD-based calculations of the properties and interactions of nuclei will become possible. Results that emerged from the experimental program at the Relativistic Heavy Ion Collider (RHIC) at Brookhaven National Laboratory and other heavy ion facilities indicate that a new state of matter with a low ratio of viscosity-to-entropy has been produced during the earliest moments of the collision. A complete understanding of these heavy ion collisions, and the development of predictive capabilities for such processes under different conditions requires, at its heart, a detailed map of the QCD phase-diagram and the ability to calculate the properties of matter in each of the phases. QCD-based calculations of nuclear matter at finite temperatures and densities, and of nuclear structure and reactions, will improve the reliability of the input into astrophysical simulations, such as of core-collapse supernovae, enabling the quantification of uncertainties in such simulations.

Lattice QCD is a technique in which strong interaction quantities are calculated by large-scale numerical Monte-Carlo evaluation of the Euclidean space path-integral in a finite-volume discretized space-time, where the effects of the finite volume and the discretization can be systematically removed. With the leadership-class computational platforms that continue to be deployed within the United States, we stand at a new frontier: understanding precisely how the quarks and gluons are assembled to form nucleons and exotic hadrons, and understanding how they interact collectively to generate nuclei and new phases of matter [1].

In order to achieve a precise understanding of the properties of hadrons and of hadronic matter that can confront current and future high precision experiments, and can be used to reliably predict the behavior of matter in environments where experiment is difficult or impossible. Lattice QCD software and algorithms must be upgraded in order to optimally use near-future computational resources on the path to the exascale.

2.2 The Science Case

2.2.1 Matter under extreme conditions (Heavy Ion Collision Physics)

Overview: At low temperatures and densities ordinary hadrons are the prevailing degrees of freedom that determine the properties of nuclear matter. However, under extreme conditions of high temperature or of high density (or both) this is expected to change. The theory of strong interactions (Quantum Chromodynamics (QCD)) predicts that a phase transition occurs that separates the low temperature/density regime from a high temperature/density region where quarks and gluons, the basic constituents of QCD, become the most relevant degrees of freedom. As the temperature and baryon chemical potential are varied, the quark and gluon interactions are modified according to QCD, thereby dictating the properties of matter under extreme conditions.

Deriving detailed predictions for the properties of matter at high temperature and density directly from QCD is paramount in shaping our understanding of nuclear matter in general, as well as for understanding the evolution of the early universe. Large experimental and theoretical programs in the United States and internationally thus exist which explore the properties of matter at high temperature and/or density, with the aim of mapping the boundaries between different phases of strongly interacting matter, and determining quantitatively the properties of matter in this domain.

The progress and future goals of these programs are described in detail in the 2007 Nuclear Science Long Range Plan: The Frontiers of Nuclear Science, a report issued by the DOE/NSF Nuclear Science Advisory Committee

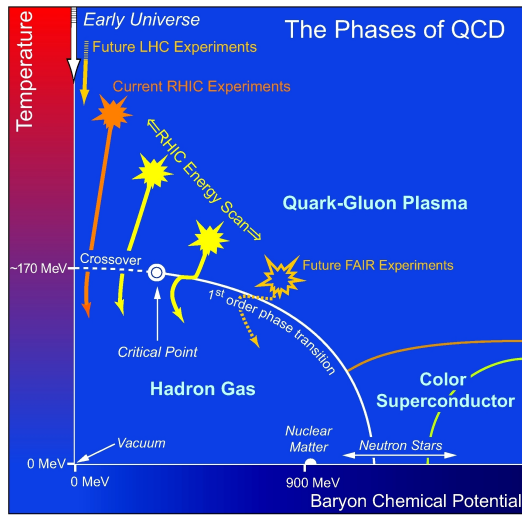


FIGURE 1: Phase diagram of QCD in the temperature and baryon chemical plane.

Past Achievements: During recent years a fairly good quantitative understanding of basic parameters of the transition from ordinary hadronic matter to the quark gluon plasma has been reached in the limiting case of vanishing net baryon number density [2]. The lattice QCD groups in the US contributed significantly to almost all of these new developments. State-of-the art calculations for the thermal transition in QCD [3, 4] led to a first parametrization of the equation of state with almost physical light and strange quark masses. It has been used in the modeling of heavy ion collisions (HIC) [5, 6]. These calculations confirm that the hadron resonance gas, frequently used in phenomenological interpretations of HIC data, provides a fairly good description of the low temperature phase of QCD. A systematic analysis of cut-off effects in calculations with staggered fermions led to a good understanding of the continuum extrapolation of the transition temperature to the quark gluon plasma phase, $T_c = 154(9)$ MeV [7, 8]. Furthermore, it was established that thermodynamics in the transition region is controlled by universal scaling laws that are consistent with those of the three

(NSAC 2007) [1]. As one of the recommendations it states: “...Achieving a quantitative understanding of the quark-gluon plasma also requires new investments in modeling of heavy- ion collisions, in analytic approaches, and in large-scale computing...”

Large scale computation plays a pivotal role in providing answers for the overarching questions in the study of matter under extreme conditions as they have been laid out in the Nuclear Physics Long Range Plan [1],

- What are the phases of strongly interacting matter, and what role do they play in the cosmos?
- What does QCD predict for the properties of strongly interacting matter?
- What governs the transition of quarks and gluons into pions and nucleons?

dimensional $O(4)$ universality class [9]. This observation provided a unique way to predict the curvature of the transition line at non-zero chemical potential [10] and characteristic features of cumulants of conserved charge fluctuations [11, 12]. Although these results still need to be improved so that a controlled continuum extrapolation can be performed, they provide important information about the relative location of the QCD transition line and the freeze-out temperature determined in heavy ion experiments – a prerequisite for the interpretation of the beam energy scan (BES) now underway at RHIC.

A fundamental set of experimental observables that are being analyzed in the BES are fluctuations of conserved charges and their higher order cumulants [13]. They are considered to provide unique signatures for a possible critical point in the QCD phase diagram [11, 14]. Calculations of these observables are computationally demanding. State-of-the-art results for them have been obtained on the USQCD and DOE operated (recently decommissioned) QCDOC computers at BNL [11]. These calculations will be vastly improved through calculations on GPU-accelerated clusters which USQCD operates at JLab [15]. They are crucial for the interpretation of experimental results coming from the BES at RHIC [16].

Any quantitative understanding of electromagnetic signals in heavy ion experiments that emerge from the hot phase has to rely on a hydrodynamic modeling of the expansion of this phase. Such modeling has, for instance, led to an experimental determination of the average emission temperature of dileptons from the quark gluon plasma [17]. Aside from the equation of state, hydrodynamical modeling requires knowledge of transport properties in the quark-gluon plasma. Lattice QCD calculations of bulk and shear viscosities [18] and electrical conductivity [19, 20] have advanced considerably recently. Like the calculation of dilepton rates [19] and thermal masses of hadrons [21], these calculations rely on statistical tools, such as the maximum entropy method, that require input from precise data obtained in lattice calculations on large lattices. The techniques as well as the available data for such an analysis clearly need to be improved in the future.

The state-of-the-art calculations described above would not have been possible without highly optimized software for special purpose (QCDOC) and leadership class (BlueGene L and P) computers that has been developed under the SciDAC-2 program by members of USQCD and the joint effort in the development of software for the rapidly advancing set of applications suitable for calculations on GPU accelerated clusters.

Future Opportunities: Despite the many successes of recent years many questions in the thermodynamics of strongly interacting matter remain open and new ones arise from extensions of the relativistic heavy ion programs in the US and Europe through experiments at the Large Hadron Collider (LHC) at CERN, and the BES at RHIC. These experiments bring new questions into the focus of theoretical studies that are related to (i) the chiral properties of the QCD transition, (ii) transport properties of the Quark-Gluon plasma, (iii) the fate of heavy quark bound states, as well as (iv) the connection between thermal fluctuations of conserved charges, universal critical behavior close to the QCD chiral phase transition and its manifestation in experimentally accessible chemical freeze-out conditions at non-zero net baryon number density.

Properties of the low and high temperature phases and chiral properties of the QCD transition: Many questions in finite temperature QCD are currently being addressed on moderate-sized lattices using improved staggered fermion discretization schemes. All these calculations have been performed in a temperature range up to a few times the QCD transition temperature where it was sufficient to include contributions from the light and strange quark sectors. At the higher temperatures now probed at the LHC, as well as for a proper description of the expansion of the early universe, one needs to also control the contribution of charm quarks to the equation of state. The vastly different energy scale introduced by the charm quarks provides a challenge for such calculations as one needs to control discretization errors on quite different length scales. The highly improved staggered quark (HISQ) action is designed to cope with this problem. Nonetheless systematic thermodynamics studies are missing so far and certainly calculations on larger lattices will be needed.

One of the outstanding problems for future calculations is to confirm the results obtained with staggered fermions by using other fermion formulations. Moreover, subtle features of the QCD transition related to the anomalous axial current, the non-trivial topological structure of the QCD vacuum and its relation to the spectrum of low lying eigenvalues of the Dirac operator at finite temperature may require a chiral discretization

scheme to be addressed appropriately. First steps in this direction have been undertaken using the chiral five-dimensional domain wall fermion (DWF) formulation in studies of QCD thermodynamics [22, 23].

Computational Challenge: To make progress with computationally demanding thermodynamic calculations that use the HISQ action and the DWF formulation requires optimized implementations of simulation software on the next generation of leadership class computers, e.g. BlueGene Q, and on GPU accelerated clusters. We have implemented the HISQ action for conventional clusters within the SciDAC-2 software suite. Specific optimizations for BlueGene Q are needed. GPU support for HISQ needs to be developed.

Transport properties, dilepton rates and heavy quark bound states: Unlike thermodynamics calculations for the QCD equation of state, the calculation of transport coefficients, thermal rates and masses requires lattices that are almost two orders of magnitude larger. Recent calculations of the electrical conductivity, performed within the quenched approximation of QCD with vanishing momenta, exploited lattices as large as $128^3 \times 48$. To make contact with experiment these calculations need to be extended to non-zero momenta and a larger temperature range and should include also dynamical light quark effects. A new set of calculations of thermal masses and related screening lengths also becomes important in the context of thermodynamic studies with chiral fermions. The analysis of mass splittings in scalar and pseudo-scalar channels as well as vector and axial-vector channels is needed to disentangle thermal effects related to $SU(2)_L \times SU(2)_R$ chiral symmetry on the one hand and the $U(1)_A$ axial symmetry on the other hand.

The central observables in all these calculations are correlation functions with hadronic quantum numbers. The techniques and the numerical problems one faces in these calculations on large lattices are thus identical to those used in vacuum QCD. Many of these calculations will be ported to GPUs in the future.

Computational Challenge: To make progress we need highly efficient solvers that compute the inverse of the Dirac matrix and codes that support calculations with large lattices and with high statistics. Particularly needed are multicore optimizations specific to the BlueGene Q and to large GPU-enhanced clusters.

The phase diagram at non-zero baryon chemical potential and the QCD critical point: Getting control over the QCD phase diagram at non-vanishing chemical potential is essential for research programs at RHIC and LHC as well as at the future accelerator facilities FAIR in Darmstadt, Germany, and NICA in Dubna, Russia. At present all information on the QCD phase diagram coming from lattice QCD calculations is based on calculations that do not correspond to current state of the art. Likewise, the unsettled question of whether or not a phase transition occurs at non-vanishing net baryon number density is based on calculations that have been performed on rather coarse lattices and thus suffer from large discretization errors.

Direct numerical calculations at non-zero chemical potential or non-zero baryon number are at present not possible; straightforward adoptions of techniques used at vanishing chemical potential are impossible as the high dimensional integrals one needs to analyze do not have positive definite integrands. At present, the Taylor expansion method is most likely to benefit from advances in computing software and hardware, so it looks most promising. The calculation of Taylor expansion coefficients can be performed with HISQ actions at physical quark mass values and vanishing chemical potential. Higher order expansion coefficients need to be calculated at different values of the cut-off. This will allow a direct comparison of higher order cumulants for conserved charge fluctuations with experiment and will provide more reliable estimates for the location of a possible critical point in the QCD phase diagram.

Computational Challenge: The Taylor expansion approach requires the frequent inversion of large sparse matrices with varying random source vectors. These calculations have recently been implemented quite successfully on GPU-clusters. In order to further exploit the potential of GPU-clusters it will be necessary to improve the parallelization and inter-node communication of the QCD code among large GPU arrays as well as to improve algorithms for sparse matrix inversions that take into account the specific structure of the QCD Dirac matrix. Recent successful USQCD work on multi-GPU operation is described in [24, 25]. The outstandingly successful implementation of a multigrid inverter for Wilson fermions is an example of algorithmic improvement [26]. Such a multigrid scheme has yet to be developed for the HISQ action.

2.2.2 Hadron Spectrum (Medium Energy Nuclear Physics)

Overview 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 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 extant experimental data, and to *predict* the outcomes of future experiments.

Past Achievements 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 the presence of exotics in a regime accessible to GlueX [27, 28], illustrated in Figure 2, 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 [29, 30], and the presence of isoscalar exotics at a mass comparable to their isovector cousins [30].

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 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 [32] exhibited a counting of levels consistent with the non-relativistic qqq constituent quark model and inconsistent with a quark-diquark picture of baryon structure.

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 [33, 34]. The method has been successfully applied to extract the momentum-dependent phase shifts in non-resonant

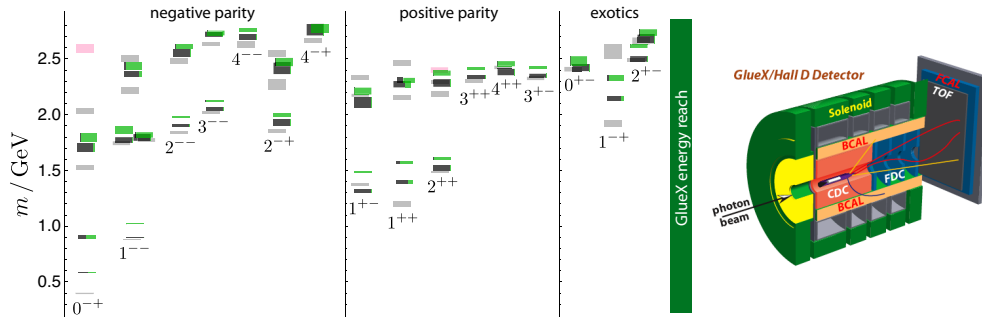


Figure 2: The figure shows the spectrum of states for exotic quantum numbers for both isovectors (grey) and isoscalars (black/green) for light quark masses corresponding to those of a pion of mass 396 MeV [30]. The light/strange quark content is indicated by the fraction of black/green in the rectangle. The pink is the calculation of the pure Yang-Mills glueball [31]. *These results suggest the presence of many exotics in a region accessible to the future GlueX experiment.*

$I = 2\pi\pi$ scattering [35, 36], including those of higher partial waves [35]. The phase shift for the resonant ρ meson has been determined [37, 38], and fitted to obtain a mass and width.

Finally, there have been significant advances in understanding properties of the excited states in QCD, in an approximation in which they are treated as quasi-stable particles. The electromagnetic and axial-vector form factors [39] of the Δ , challenging to determine experimentally, and of the $N \rightarrow \Delta$ transition form factors [40, 41], have been computed adding to our understanding of deformations in the baryon spectrum.

Future Opportunities: The work proposed herein will facilitate significant advances towards the precise studies of the spectrum that can reliably confront experiment. Calculations of the excited meson spectrum, with the effect of decay channels included and the momentum-dependent phase shifts determined, at quark masses approaching the physical light-quark masses, will provide *predictions* for the meson spectrum in advance of experiments such as GlueX. Calculations of the radiative transitions between conventional and exotic mesons, advancing methods developed for charmonium [42, 43], will inform expected production rates at GlueX. The calculation of the flavor-singlet spectrum, including in particular the contribution of the predominantly gluonic “glueballs”, will be performed in advance of searches such as those at PANDA at GSI. The calculation of the spectrum of the narrow, double-strangeness Cascade baryons, Ξ_c , where few states have been discovered and with little knowledge of their quantum numbers, provide an early opportunity for predictions of QCD in the baryon sector in advance of proposed programs at Jefferson Laboratory at 12 GeV, at PANDA, and underpin experimental studies of hypernuclear physics such as those at JPARC.

The spectrum of nucleon and Δ resonances, with the light-quark masses approaching and eventually attaining their physical values, will capitalize on the achievement of the *NSAC performance measures HP3 and HP7* [44]. These calculations will facilitate the interpretation of N^* resonance data extracted from experiment, and help address the key questions in our understanding of the hadron spectrum, such as the status and structure of the low-lying *Roper* resonance, and the anomalously light $\Lambda(1405)^-$.

Measuring the electromagnetic transitions to nucleon resonances is a key effort of CLAS at JLab@12 GeV [47], and their calculation correctly accounting for their decays [48], will provide an important glimpse into their structure. The calculation of the form factors at increasing momentum transfers will elucidate the transition to a perturbative description of QCD in terms of the quark and gluon degrees of freedom [49].

Computational Challenges: The exploitation of leadership-class computers to pursue this program requires that we overcome numerous computational challenges. *Unstable Resonances:* the formalism developed for elastic channels must be extended to inelastic decay channels. *Calculation of hadron correlation functions:* the effective application of the variational method requires a broad variational basis that encompasses the physics, and the resultant efficient computation of many correlation functions including those for multi-hadron states, and for predominantly gluonic states. *High statistical precision:* Calculations of the spectrum are characterized by decreasing signal-to-noise ratios at decreasing quark masses, and with increasing excitation energy. Efficient methods are needed both to generate large lattice ensembles and to make many measurements on those ensembles. *Ensembles at physical quark masses:* Precise comparison with experiment requires large lattice ensembles with the u -, d -, s - quarks close to their physical values, and of sufficient volume for the reliable determination of the momentum-dependent phase shifts.

2.2.3 Hadron Structure (Medium Energy Nuclear Physics)

Overview: One of the great challenges posed by QCD is understanding how protons and neutrons are made from quarks and glue. Just as calculating the structure of atoms was a cornerstone of quantum mechanics, a cornerstone of our effort is to achieve a quantitative, predictive understanding of the structure of nucleons and other hadrons using lattice QCD. Our lattice calculations are directly relevant to experiments at JLab, RHIC-spin, SLAC, and FNAL, and will have significant impact on future experiments at the JLab 12 GeV upgrade and a planned electron-ion collider. They are explicitly required to meet the *2014 NSAC Performance Measure HP9* [44], and address experimental measurements mandated by 6 of the other 9 Performance Measures.

Past Achievements: Electromagnetic form factors reveal the distribution of charge and current, and recent calculations[50, 51, 52, 53] have shown the emergence of the pion cloud at the periphery of the nucleon. The axial charge, g_A , governing neutron Beta-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[50, 54, 55] with errors as low as 7%. Precision calculation 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 , [56] will be valuable in searching for physics beyond the standard model in ultra-cold neutron Beta-decay experiments.

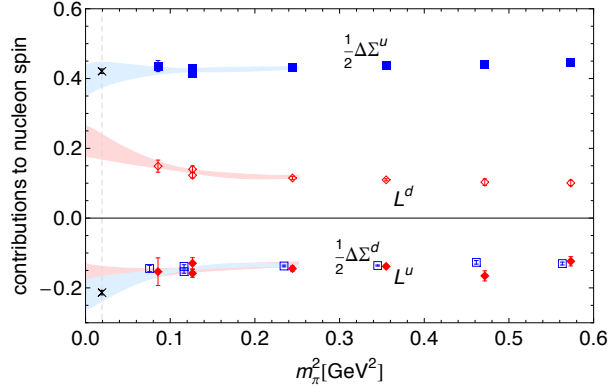


Figure 3: Contributions of quark spin $\Delta\Sigma^{u,d}/2$ (blue error bars) and orbital angular momentum $L^{u,d}$ (red error bars) to the spin 1/2 of the proton for up and down quarks. Chiral extrapolations (shaded error bands) agree with HERMES data (crosses).

Quark parton distributions, measured in deep-inelastic scattering, specify quark density, spin, and transversity distributions as functions of the momentum fraction, x , of the struck quark. Their lowest three moments have been calculated[50, 57, 58, 59] showing, for example, that chiral extrapolations of the fractions of the nucleon spin and momentum arising from quark spin and momentum agree with experiment.

Generalized Parton Distributions (GPD's) specify quark density, spin, and transversely 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[50, 61], and the combination of these moments with convolutions of GPDs measured at JLab and elsewhere will provide a more complete under-

standing than either effort could obtain separately. Moments of GPD's specify the total angular momentum of quarks in the nucleon, 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 [50, 61, 57, 60] shown in Fig 3, are striking. Only about 30% comes from quark spin and the substantial orbital contributions of up and down quarks cancel so that the remaining 70% must come from 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, and an important initial step has been taken by calculating the contribution of gluons to the momentum fraction $\langle x \rangle$ of the pion[62].

Transverse momentum distributions show the quark momentum distribution, and initial calculations in a nucleon [63] 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 by calculating its quark transverse charge densities[64] and the transition form factors to it from the nucleon[41].

Future Challenges: These recent accomplishments and emerging computer resources, combined with the requisite algorithms and software provide the opportunity to meet a range of exciting challenges.

Precision calculations at the physical pion mass Although calculations at the physical pion mass are finally becoming possible, an unexpected challenge has arisen. Instead of following chiral extrapolations of existing calculations that lead to the correct experimental values, calculations[65, 66] in the nucleon for g_A , the momentum fraction, and RMS radius by several groups using standard methodology have shown deviations arising from contamination by excited states. Hence, it will be necessary to dramatically increase statistics to explicitly remove excited states or use distillation[67] to expand in a basis including the relevant multi-particle states.

Disconnected diagrams Disconnected diagrams involve quark propagators that can start at any point on the

lattice and are computationally far more expensive than isovector matrix elements that have been the primary focus of past calculations. They are required to calculate flavor singlet quantities such as the properties of a neutron or proton separately, and testing algorithms on large lattices at the physical pion mass and developing efficient software for them will be crucial.

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} . To determine this scale for asymptotic scaling, form factor calculations must be extended to high momentum transfer where new techniques[68] need to be explored and applied in large volumes at the physical pion mass.

Higher moments of quark structure functions Due to operator mixing on a discrete lattice, only the lowest three moments of quark distributions can be calculated with present techniques. To reconstruct the full quark distributions, it is necessary to explore new algorithms for calculating higher moments, such as introducing a heavy quark field [69], and to exploit them at the physical pion mass.

Gluon contributions Calculation of gluon contributions to the nucleon mass, momentum, and angular momentum, and gluon mixing with quark disconnected diagrams is complicated by the fact that fluctuations grow strongly as the lattice spacing is decreased. Hence, extracting the continuum limit will require a combination of techniques for obtaining extremely high statistics and new algorithms.

Transverse momentum distributions To relate lattice calculations of transverse momentum distributions to semi-inclusive deep inelastic scattering and Drell-Yan experiments, these calculations must be extended to much higher nucleon momenta and lattice volumes. Because of the rapid decrease of the signal-to-noise ratio with momentum, extremely high statistics will be required.

Computational Challenges: One theme pervading these physics challenges is the need for unprecedentedly large numbers measurements on very large lattices at the physical pion mass. Although deflation is useful for present lattice sizes, evolution to larger lattices will require multigrid algorithms. Optimized inverters implementing these and other algorithmic advances are needed for all the relevant fermion actions on BG/Q, GPU's, and subsequent emerging architectures.

A second theme is the need for nimble exploration of algorithms at scale. Exploration of multigrid methods, distillation, step scaling, schemes for higher moments, noise reduction methods, improved gluon operators as well as performance optimization on each architecture will only be feasible if tools are developed to do this quickly.

2.2.4 Hadron Interactions (Medium and Low Energy Nuclear Physics)

Overview: 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, conspire to produce the spectrum of nuclei and the complicated chains of nuclear reactions that allow 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 provided a precise set of measurements 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 potentials such as AV_{18} [70] and the chiral potentials [71], when supplemented with three-body interactions, and implemented using the renormalization group [72], 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 (under the SciDAC2 UNEDF collaboration [73]) show that three-nucleon forces are required to determine the structure of light nuclei [74, 75]. 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 [76] that can be found, for instance, in the interior of core-collapse supernova. One of the motivations for building FRIB (Facility for

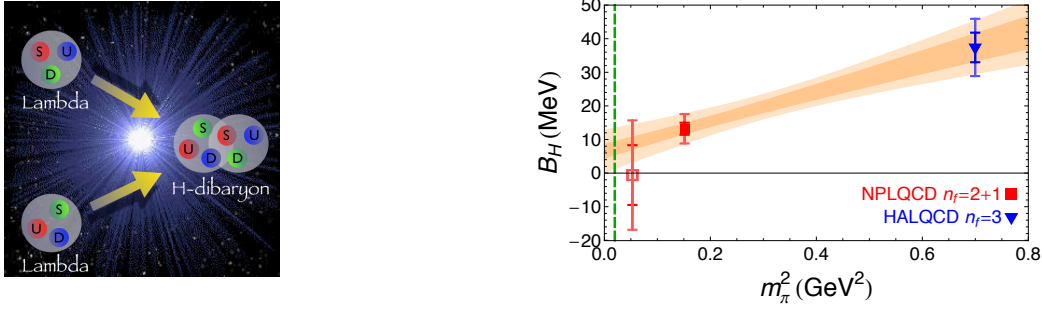


Figure 4: The H-dibaryon has the quantum numbers of $\Lambda\Lambda$ (left panel). The right panel shows the results of Lattice QCD calculations [46, 45, 88, 87]. The green dashed line corresponds to the physical pion mass.

Rare Isotope Beams) is to better constrain the multi-neutron interactions from very neutron-rich nuclei.

The connection between nuclear physics and the underlying theory of fundamental forces, the standard model of the strong and electroweak interactions, 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* [44]. 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 [77], FAIR [78], JLab, and the relativistic heavy ion experiments at BNL and CERN, may be able to observe or constrain the simplest exotic systems.

Past Achievements: A pioneering study of baryon-baryon scattering with Lattice QCD was performed more than a decade ago by Fukugita *et al* [79, 80], but it involved large light-quark masses and did not have dynamical sea quarks (quenched). More recently, Lattice QCD calculations of nucleon-nucleon [81, 82, 83, 84, 85] and hyperon-nucleon [86] interactions were performed but with unphysical pion masses, and the nucleon-nucleon scattering lengths were found to be of natural size. The fine-tunings in nature indicate that LQCD calculations with quark masses much closer to the physical values are needed to extrapolate to the experimental values. During 2010, lattice QCD calculations [46, 45, 87], have provided evidence that the H-dibaryon (with the quantum numbers of $\Lambda\Lambda$) is bound at heavier light-quark masses. While the form of the light-quark dependence of such a system has not been rigorously constructed, possible extrapolations suggest a weakly bound H-dibaryon or a near threshold resonance exists [88, 89, 90] (right panel of Figure 4). It has also been found that the $\Xi^-\Xi^-$ forms a bound state at heavier light-quark masses [45], which is consistent with previous estimates constrained by experimental data and the approximate SU(3) flavor symmetry of QCD. Following work on three-baryon systems [91], in late 2009 the PACS-CS collaboration performed the first, but quenched, calculation of ^4He [92]. The pion mass was $m_\pi \sim 800$ MeV and surprisingly the calculated binding energy of ^4He was found to be close to its actual value.

Calculations of finite-density, Bose-Einstein condensed multi-meson systems containing up to 12 π^+ 's or K^+ 's have been performed [93, 94, 95] (and extended up to 72 mesons [96]). Precise determinations of the $\pi^+\pi^+$ scattering length [97] and extractions of the effective range and shape parameter, along with the scattering phase-shift [35, 36], have been performed by combining Lattice QCD calculations with chiral perturbation theory (χ PT). Further, analysis of multi-pion systems has led to a determination of the three-pion interaction [93]. A surprising result is that tree-level χ PT describes these systems even at the heavy light-quark masses, and hence tree-level χ PT should provide reasonable estimates of the properties of a possible kaon-condensed phase in dense matter. However, condensed systems containing baryons have not yet been explored, leaving a significant systematic uncertainty in such calculations. 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 [98].

Future Challenges: 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 (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 hyper-nuclei, that may be tested in the upcoming experimental programs.

2.2.5 Fundamental Symmetries (Low Energy Nuclear Physics)

Overview: Research efforts to uncover particles and symmetries beyond those of the standard model of the strong and electroweak interactions are multi-pronged. One of the approaches in this effort is to perform precision measurements of the properties of known particles, such as 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.

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 [99], 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.

Past Achievements: There have been a number of efforts, part of the broader effort to support the 2020 NSAC Performance Measure FII5 [44], to calculate the neutron edm arising from the QCD θ -term using Lattice QCD [100, 101], 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 [102], in which the “connected diagrams” contributing to the weak one-pion-nucleon vertex, $h_{\pi NN}^1$, were determined. 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 [103] at the SNS promises to greatly reduce the experimental uncertainties in the value of $h_{\pi NN}^1$, likely in a similar time-frame to the Lattice QCD calculations.

Exploratory Lattice QCD calculations of the muon $g - 2$ are underway to understand how to calculate the strong interaction contributions, and this years *Kenneth Wilson Prize* [104] was awarded to Dru Renner and collaborators of the *European Twisted Mass Collaboration* [105] (now at JLab) for calculations of the leading contributions to the magnetic moments of the leptons.

Future Challenges: The currently exploratory calculations of nuclear parity violation must be greatly refined with the inclusion of the currently omitted quark-loop contributions. The neutron edm calculations have to

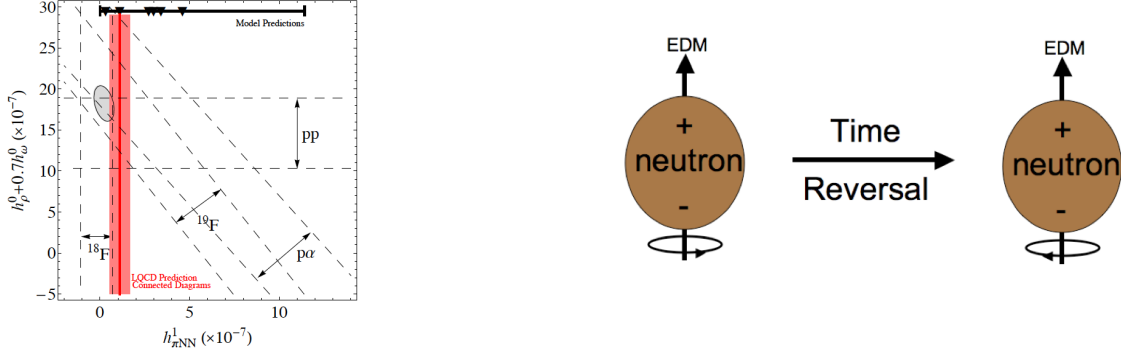


Figure 5: The left panel shows constraints on nuclear parity-violating interactions including the recent Lattice QCD result [102] (shaded (red) region), and the experimental 1σ uncertainty ellipse (gray). The upper panel is a cartoon showing the behavior of the neutron electric dipole moment under time-reversal.

be performed at the physical quark masses, and the impact of higher dimension operators evaluated. Efforts must be made to determine the strong interaction contributions to the light-by-light contributions to the muon $g - 2$.

2.3 The Computational Approach: Lattice QCD

QCD is a quantum field theory defined in four-dimensional space-time, with a gauge symmetry analogous to that of quantum electrodynamics (QED) with the distinction that the gauge group, $SU(3)$, is non-Abelian. In order to study the theory numerically, one must reformulate it on a four-dimensional lattice. Physical results are obtained by performing calculations for several small values of the lattice spacing, and then extrapolating to the continuum, or zero-lattice-spacing, limit. The gauge fields which carry the forces, known as *gluons*, are represented by elements of the gauge group, with one element assigned to each link of the lattice. The quarks, which are the matter fields, are associated with the lattice points. Physical observables can be expressed in terms of Feynman path integrals:

$$\langle O \rangle = \frac{\int \mathcal{D}U O(U) \exp[-S(U)]}{\int \mathcal{D}U \exp[-S(U)]}. \quad (1)$$

Here U represents the gauge field, and $\int \mathcal{D}U$ an integral over all of the components of U using the Haar measure. Because the quarks are fermionic, they are represented in the path integrals by anti-commuting elements of a Grassmann algebra, that are integrated out in the above expression. As a result, the effective action $S(U)$ is non-local. Indeed, it contains a term proportional to the logarithm of the determinant of the Dirac operator, which describes the propagation of a quark in the gauge field U . On the lattice, the Dirac operator is a large, sparse matrix with dimension proportional to the number of lattice sites. Finally, O is the physical observable being computed, and $O(U)$ is the value of O in the gauge configuration U .

The first step in the calculation is to use importance sampling techniques to generate an ensemble of gauge configurations, U_i , $i = 1, \dots, N$, with the probability distribution

$$P(U_i) = \frac{\exp[-S(U_i)]}{\int \mathcal{D}U \exp[-S(U)]}. \quad (2)$$

Once an ensemble of representative gauge configurations is available, an unbiased estimator for any physical observable O is given by

$$\langle O \rangle = \frac{1}{N} \sum_i^N O(U_i). \quad (3)$$

In generating an ensemble of gauge configurations, each configuration evolves from the one before it. Because of the non-locality of $S(U)$ it would be prohibitively expensive to use a local updating scheme in which one

or a few links of the lattice are updated at a time. Instead, one uses an algorithm, such as hybrid Monte Carlo (HMC) [106], or one of its variants [107, 108], in which all components of U are updated simultaneously. The most time consuming step in this class of algorithms is the numerical integration of a set of molecular dynamics equations, which are non-linear, coupled first-order differential equations of dimension proportional to the number of lattice sites. We are currently using a multiple time-step symplectic Omelyan integrator [109] for this calculation. However, as described below, we propose to explore and develop improved integrators for these equations since even a modest improvement would lead to major advances in our program.

At each step of the integration of the molecular dynamics equations one must solve a set of linear equations of the form $(D^\dagger D + \sigma_j I)x_j = y_j$, where D is the Dirac matrix, I is the unit matrix, and the σ_j are real positive numbers. These equations are solved using Krylov space methods. Their solution consumes the largest fraction of floating point operations in the generation of gauge configurations. The vast majority of the floating point operations in the observable calculations, that is the determination of $\langle O \rangle$ from Eq. 3, go into solving linear equations of the form $D^\dagger D x = y$, for which we again use Krylov space techniques. The systems of linear equations encountered in both configuration generation and observable calculation become increasingly ill-conditioned as the masses of the quarks decrease. For this reason, almost all QCD simulations to date have used heavier-than-physical values of the masses of the two lightest quarks, the up and the down, and then relied on extrapolations in the light quark masses to obtain physical results. A major goal of this project is to perform simulations directly at the physical light quark masses. The proposed work to develop and implement improved techniques for solving the linear equations will play an important role in reaching this goal. This work will include the development of multigrid and deflation methods, the latter requiring efficient evaluation of the lowest eigenvalues of the Dirac matrix and their eigenvectors.

As one approaches the continuum limit by decreasing the lattice spacing, the number of lattice points in each direction must be increased if the linear spatial size L of the box is to remain fixed. For a stable single-particle state, the leading finite-size artifacts are of order $\exp(-m_\pi L)$, where m_π is the pion mass. Since m_π decreases with the masses of the up and down quarks, movement towards physical values of the quark masses and small lattice spacings both require that we work on increasingly large lattices. Performing computations at several volumes provides an important systematic test of our calculations, and is key to the study of unstable resonances and of hadronic interactions.

Because each configuration follows from its predecessor, this part of the calculation must be run in a single stream, or a small number of them, and is performed on the most-capable leadership-class computers. By contrast, observable calculations can be performed on many configurations in parallel. This creates a capacity challenge, but is an increasingly demanding element of lattice calculations in nuclear physics. It can be run both on leadership-class computers, and on dedicated clusters including those funded by the DOE for our research. We have developed code for Krylov space solvers that runs on clusters with graphics processing unit (GPU) accelerators, and it is having a major impact on calculations of observables.

There are three different formulations of lattice fermions that we will use in this work; each has advantages for different components of the program, but all should give the same results in the continuum limit. Highly-improved staggered quarks (HISQ) will be used extensively in the study of QCD at finite temperature and finite density. Domain-wall fermions (DWF) will also be used for QCD at finite temperature and density, and for the study of hadron structure. Wilson-clover fermions, and their anisotropic variant, will be the principle discretisation for the investigation of the excited-state spectrum of QCD and of hadronic interactions, but also employed for hadron structure, fundamental symmetries and to examine thermal correlation functions in QCD at finite temperature.

2.4 Past Accomplishments: SciDAC-1 and SciDAC-2 Software

The USQCD Collaboration has developed the software and algorithmic infrastructure needed for the numerical study of lattice gauge theories. The software and its documentation are publicly available at the USQCD

software web site <http://www.usqcd.org/usqcd-software>. The software libraries have been widely adopted within the United States, and are used extensively abroad. They have been instrumental in our effective use of leadership class computers, and of dedicated computers including those funded for USQCD by the DOE's Offices of High Energy and Nuclear Physics; the committees which review the USQCD hardware effort on a yearly basis have consistently emphasized the importance of the work done under the SciDAC grants and the need for its continuation. The work proposed builds upon our accomplishments under the two SciDAC grants, so we briefly summarize them here.

2.4.1 The QCD Applications Programming Interface

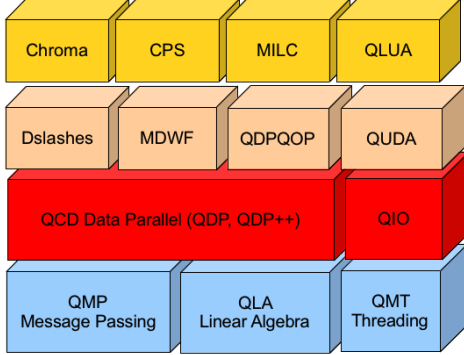


Figure 6: Levels 1, 2 and 3 of the QCD API, and the application code bases that exploit them (bottom to top).

The USQCD Collaboration has created a unified programming environment that enables its members to achieve high efficiency on leadership class computers and commodity clusters. Among the design goals were to enable users to quickly adapt existing codes to new architectures, easily develop new applications and incorporate new algorithms, and preserve their large investment in existing codes. To achieve these goals the QCD Applications Programming Interface (QCD API) was developed as a layered structure which is implemented in a set of independent libraries. It is illustrated in Fig. 6, which shows the three levels of the API and the application codes that sit on top of them.

Level 1 provides the code that controls communications and the main single-processor computations. Versions exist in C and C++ using MPI for transparent portability of all application codes.

Message Passing: QMP defines a uniform subset of MPI-like functions with extensions that (1) partition the QCD spacetime lattice and map it onto the geometry of the hardware network and (2) contain specialized communication routines designed to access the full hardware capabilities of computers, such as the BlueGene line, and to aid optimization of low level protocols on cluster networks. New versions are developed as needed to accommodate changing architectures and algorithms, as we illustrate below. For example hooks to combine message passing and threaded code are being added, as is the ability to work with multiple lattice geometries, which is needed for multigrid and domain decomposition algorithms.

Linear Algebra: QLA contains the linear algebra operations common to all lattice QCD calculations in which the basic elements are three-dimensional complex matrices. These operations are local to lattice sites or links, and do not involve interprocessor communications. The C implementation has about 19,000 functions generated in Perl, with a full suite of test scripts. The C++ implementation makes considerable use of templates, and so contains only a few dozen templated classes; the required specific classes are generated on demand by the compiler. For both C and C++ it is important to optimize the code for the most heavily used linear algebra modules.

Level 2: QDP is the *data-parallel interface* containing data parallel operations that are built on QMP and QLA, thereby hiding the details of communication barriers, vectorization over multiple sites on each node, etc., from the user enabling him or her to focus on the physics. As in the case of QLA, there are both C and C++ versions. QDP and QDP++ significantly accelerate the process of developing new codes and optimizing existing ones, and codes based on these layers become significantly easier to comprehend thereby lowering the barriers for entry into the field by graduate students, post-docs and senior researchers from other fields.

Data Management (QIO): A large fraction of the computing resources used in lattice QCD calculations go into the generation of ensembles of gauge field configurations which are then used to calculate many physical quantities. To facilitate sharing of gauge configurations, we have created standards for file formats, and written

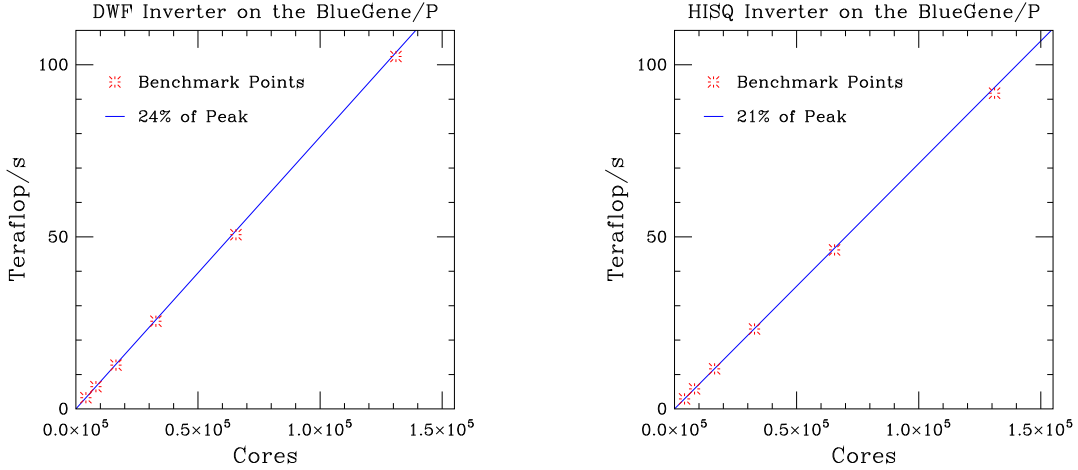


Figure 7: Performance of the Dirac solver on the Blue Gene/P in Tflops as a function of the number of cores for domain wall fermions (left panel) and HISQ quarks (right panel). The red bursts are the benchmark points, and the solid blue lines indicate 24% and 21% of peak, respectively. These are weak scaling tests with the number of lattice points per core being held fixed at 6^4 for the DWF solver, and 8^4 for the HISQ solver.

an I/O library (QIO) that adheres to them. It supports a logical partitioning of the computer into I/O partitions, with one core per partition handling I/O for the data in just that partition. Thus, our codes can read and write data in multiple files, and these files can be flattened into one large file offline on a single-processor machine; this file can then be fragmented on a single-processor machine, and copied to the local disks for subsequent reading by individual partitions. By tuning the size of the I/O partitions, we can maximize the bandwidth and avoid contention. Finally, we are members of the International Lattice Data Grid, which established a basic set of meta-data and middleware standards to enable international sharing of data.

Level 3 consists of highly optimized code for a limited number of subroutines that consume a large fraction of the resources in any lattice gauge theory calculation. Most notable among these is the subroutine for the solution of the linear, sparse matrix equations involving the Dirac operator. To obtain the highest level of performance, it is necessary to optimize these subroutines for each architecture. These routines are generally written with extensive assembly language coding, either employing hand coding or specialized tools, such as Bagel [110] and QA(0) [111], which were developed to generate optimized codes. Data layout to improve cache behavior and hand coded assembly kernels are common place. For example the Möbius Domain Wall Fermion (MDWF) and clover solvers both use Morton ordering (a cache-oblivious ordering) in their internal data representation. In Fig. 7 we show the performance of the Dirac solver for DWF and HISQ quarks on the Blue Gene/P; the Wilson-clover solver also scales linearly, achieving 17-20% on the BlueGene/P at ANL.

Extensions to these libraries and the maintenance of the API code are ongoing activities as computer architectures and algorithms change. The API is a critical software underpinning for all the application codes, which requires maintenance, testing, version control, documentation and distribution.

Application Codes: There are four publicly available application code suites developed by members of USQCD that take advantage of the QCD API; each is publicly available at the USQCD website.

Chroma [112] was built directly on top of QDP++, and is now the principle framework for our studies of the spectroscopy of hadrons and of their interactions, including the generation of Wilson-clover gauge field configurations on leadership facilities. It is widely adopted worldwide with over 200 citations. The package is highly object oriented, and makes extensive use of modern software engineering design techniques, such as object-orientated design patterns [113]. Significant effort has gone into designing a gauge field generation framework that supports the plug and play of different solvers, including level 3 packages for GPUs as well as optimized solvers, including EigCG, for leadership facilities.

Qlua is a framework for integration and optimization that uses the scripting language Lua [115] and was built

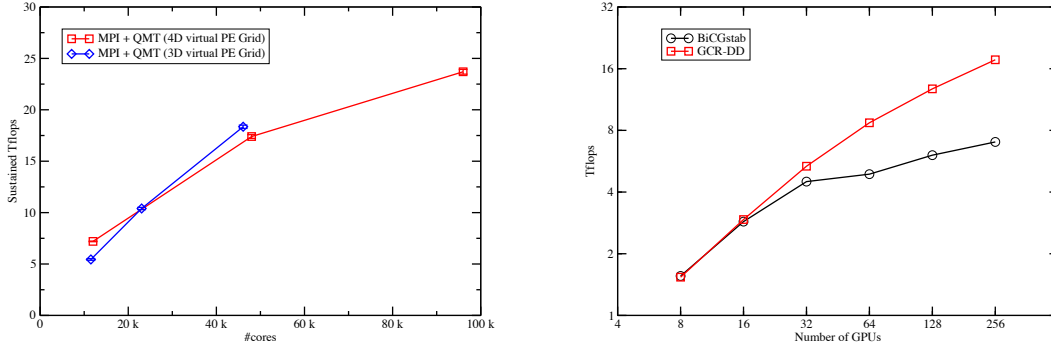


Figure 8: Strong scaling tests of the Wilson-clover inverter with threaded codes. On the left, results on a $40^3 \times 384$ lattice on the NERSC Cray XE6, Hopper, using hybrid code with MPI and the QMT library; and on the right, results on a $32^3 \times 256$ lattice on the LLNL Edge cluster for up to 256 GPUs with MPI and CUDA threads [114].

on top of QDP/C. It has been used for developing optimized Möbius domain wall and Wilson-clover solvers and incorporates EigCG, Morton order, and improved IO performance. It has been used as a platform for rapid algorithm research and software prototyping, and is the workhorse for a broad range of hadron structure calculations. Particular attention was paid in its design to straightforward portability for the user: the same scripts can be run on machines ranging from a laptop to leadership-class computers.

The Columbia Physics System (CPS) and the MILC code predate the API, but incorporate key features of it. Thus rewriting computationally intensive subroutines of the MILC code base in QDP yielded a significant increase in performance, despite the careful optimizations performed over the previous fifteen years. These code suites provide extensive support for QCD calculations based on domain wall fermion (DWF) and staggered fermion discretization schemes, respectively. Both are heavily used in calculations of QCD at non-zero temperature and density. Each of these application suites is used extensively in nuclear physics, and benefits immediately from any extensions to or optimizations of the QCD API.

2.4.2 Recent Software and Algorithmic Advances

Although the QCD API and the application codes are highly portable, as we move to new computers, we typically have to upgrade and augment the Level 1 and Level 3 routines. The advent of computer nodes with large numbers of cores and the use of GPU accelerators on the nodes have required that we develop threaded versions of our codes. In addition, algorithmic improvements must be exploited and new theoretical ideas implemented. Here we give some recent highlights of these phases of the work.

Hybrid MPI/Threaded Code: It is clear that in the near future computer nodes will contain large numbers of cores, and that for such machines we will need to employ a hybrid programming model in which communication between nodes is programmed in MPI or QMP, and work on nodes is performed with threaded code. We have addressed these challenges in a variety of ways. We have developed a new threading library, QMT, whose light-weight barriers outperform those of OpenMP on a variety of AMD Barcelona and Xeon systems, and exploited it for performance on the Cray XT series. We have collaborated with Intel Corporation to craft a highly-tuned multi-threaded Dirac operator for multicore Xeon CPUs, and the lessons learned will be applicable to all architectures with large shared caches and short vector units. We are developing an optimized DWF solver in a hybrid MPI/OpenMP approach for the forthcoming BlueGene/Q, and similar code for other discretizations is planned. The success of these approaches is apparent in the left-hand panel of Fig. 8, where we show strong scaling results for threaded code on NERSC’s Hopper, the Cray XE6.

GPU Library QUDA: Starting in 2008, we have implemented high performance Dirac solvers in CUDA on NVIDIA GPUs [116]. This effort was initially supported by NSF funding, but has rapidly expanded into a major SciDAC project with the development of the QUDA (QCD in CUDA) library [117, 118, 119], and the rapid deployment of GPU accelerated clusters at Jefferson Laboratory and Fermilab. The QUDA library now includes solvers for most of the fermion actions we use: Wilson-clover, Staggered, and Domain Wall. The most recent advance has been the extension of code from single to multiple GPUs, using CUDA threads on the GPUs combined with POSIX threads on the CPU and MPI between the nodes. The solvers implement a novel multi-precision strategy incorporating “reliable updates” [117, 120], thus achieving double precision accuracy while doing most of the work in single or even half (16-bit) precision. This greatly improves performance by reducing memory traffic and inter-GPU communication. We have achieved good strong scaling up to 256 GPU for the staggered and Wilson-clover solvers running on the Edge cluster at LLNL, based on NVIDIA Tesla M2050 GPUs; the latter is illustrated in the right-hand panel of Fig. 8 [114]. The result has been a dramatic improvement in the price/performance for a range of observable-computation work that is dominated by Dirac solvers.

Improved solvers for the Dirac Operator: The solver for the lattice Dirac operator has traditionally been a dominant focus of algorithm and specialized software development because of its central role in all QCD codes. A large variety of Krylov solvers have been explored with the Conjugate Gradients (CG) and Stabilized Bi-Conjugate Gradients (BiCGstab) being the current work horses in many production codes.

A new area of activity that shows great promise is the use of multigrid methods that have eluded lattice gauge theorists for over twenty years. In collaboration with applied mathematicians from TOPS (Towards Optimal Petascale Solvers), we have finally succeeded in formulating a multigrid solver for Wilson-clover quarks [121] that gives a 10 to 15 times speed up on current production lattices. This opens a new opportunity to apply multi-level algorithms for other parts of our code and for other fermion discretizations, and will become increasingly important as the quark masses are reduced and lattice sizes increased. In this same spirit, we are exploring and implementing a variety of “deflation” and Schwarz domain decomposition methods. To successfully explore these algorithms, we implemented support for multiple lattice geometries within QDP/C and Qlua, enabling them to be used as a platform for multigrid algorithm development and prototyping.

Improved Hybrid Monte Carlo (HMC) Evolution: The other major ingredient in lattice field theory codes is the configuration generation algorithm and its components such as the symplectic integrator for molecular dynamics in HMC methods. Over the period of previous SciDAC grants, improved evolution has been achieved by a combination of effectively splitting the HMC Hamiltonian, for example by using rational approximations, and improved molecular-dynamics integration schemes. This development has led to a highly efficient class of algorithms called Rational HMC (RHMC), which are implemented in all of our major application codes. It typically results in a two to four times speedup in the generation of gauge field configurations. A higher order symplectic Force Gradient integrator has been designed, which promises further improvements in the next generation of gauge field configuration generation algorithms on very large lattices.

Highly Improved Staggered Quarks (HISQ): Many of our studies of QCD at finite temperature and at finite density have been performed using the improved staggered (asqtad) formulation of lattice quarks. However, controlling the contribution of the charm quarks, needed at the higher temperatures being probed at the LHC, is challenging. Members of our collaboration have developed highly improved staggered quarks (HISQ) [122]. This formulation incorporates improvements in the quark dispersion relation that enable charm quarks to be treated on the same basis as up, down and strange quarks at lattice spacings accessible with today’s supercomputers [122, 123]. In order to generate gauge field configurations with HISQ sea quarks, we had to develop a new algorithm for the molecular dynamics evolution of the system [123]. Both the formulation of the HISQ quarks, and the rapid development of high performance production code for simulations with it were made possible by USQCD software.

Anisotropic Wilson-clover Lattices: Studies of the excited-state spectrum of QCD, and of the interactions between hadrons, are characterized by the need to precisely resolve many low-lying energy levels contributing

to the temporal decay of hadron correlation functions. The signal-to-noise ratio for these correlators degrades rapidly with increasing temporal separations, and this degradation becomes more severe with decreasing quark mass, and with increasing numbers of quarks. To ameliorate this, we introduced so-called anisotropic Wilson-clover lattices [124, 125], with finer temporal than spatial discretization, to enable the time behavior of correlation functions to be resolved at short separations; this effort is core to our study of spectroscopy and hadron interactions.

Distillation – efficient calculations of hadron correlation functions: The need for hadron correlation functions between increasingly complex operators is a feature of nuclear-physics calculations. “Distillation” [126] enables such correlation functions to be computed efficiently, and in such a way that additional operators can be added *a posteriori*, without the need for additional Dirac inversions. This method has been efficiently implemented and exploited extensively on GPUs, and used for the calculation of the excited-state spectrum.

2.4.3 Computational Science: Improved Performance Tools

Collaborative interactions with PERI (Performance Engineering and Research Institute) have benefitted the research efforts both of USQCD and of PERI. The improvements to PERI tools and methods motivated by LQCD problems have been applied in multiple other domains, and thus had a widespread impact on the DOE computational science community.

The data-parallel interface QDP++ is implemented using C++ template meta-programming, especially expression templates, in which syntactically simple programming constructs such as arithmetic and assignment operators expand into deep and complex binary code. The “tower” of inlined fragments and loops in the binary file has no single corresponding fragment in the original source, so analyzing performance and attributing problems to source is very difficult. To meet this challenge RENCi and Rice personnel in PERI collaborated to extend HPCToolkit to handle such codes [127, 128]. In collaboration with USQCD, these improvements were used to identify several performance issues previously buried under the template framework. The tools were also used in developing parallelization strategies for the current generation of multi-core chips [129, 130]. RENCi and Rice researchers worked with Robert Harrison of ORNL to apply the tools and methods developed for QDP++ to successively identify and fix performance issues in the MADNESS chemistry code. Experience gained working with multi-core Chroma was applied to identify inter-thread synchronization dependence issues in MADNESS that have further driven PERI tool development [131]. Other DOE codes that have benefited from the HPCToolkit extensions for templates include the Omen 2011 Joule code from Purdue, the sparse matrix-vector multiply component of Trilino from Sandia, the DENOVO radiation transport code from ORNL, and the GEANT4 particle code.

2.4.4 Collaboration with Industry

Members of USQCD from Columbia and BNL, together with the University of Edinburgh, are working with IBM to develop some hardware features of the BlueGene/Q, enabling us to have highly optimized code elements running on prototype hardware. The collaboration with NVIDIA Corporation is key to the exploitation of GPUs and other accelerators, and will advance our nuclear physics scientific goals and contribute to the design of next-generation GPU architectures. Members of USQCD from Jefferson Laboratory have collaborated with Intel Corporation to develop a highly optimized Dirac operator for multi-core Xeon CPUs, and have an ongoing collaboration exploiting features of the new AVX and MIC architectures.

2.5 Software Development Proposal

The proposed software development will be focused on two campaigns. Firstly, we will optimize our software infrastructure to ensure that we achieve the highest possible performance on anticipated architectures, including the BlueGene/Q, Cray XE, and heterogeneous systems such as the Cray XK series or the recently announced Stampede System, featuring acceleration via GPUs or other accelerators like the Intel MIC. To ensure future readiness in the approach to the exascale, we will develop a domain-specific language and com-

piler in cooperation with the SUPER institute that will provide high performance while maintaining portability. Secondly, we will aggressively pursue algorithmic advances. This includes the development of efficient solvers for physics measurements, of integrators for gauge field generation and improved methods of importance sampling. This will satisfy the requirements of high statistics and large volumes that characterize many calculations in nuclear physics. Further, we will develop new methods for the efficient enumeration and construction of hadron correlation functions, the computation of which increasingly dominate studies of spectroscopy, hadron structure, and nuclear interactions. In each case, our algorithmic development will be cognisant of emerging architectures.

Our program will capitalize on the achievements which to some degree anticipated many of the developments proposed below. Furthermore, we expect the proposed work will strongly benefit the high-energy-physics (HEP) program of USQCD, in addition to enabling us to perform the nuclear-physics topics in this proposal.

2.5.1 Optimization of Software Infrastructure on Leadership Class Machines

QCD on the BlueGene/Q and its Successors

The new IBM Blue Gene/Q architecture is a promising architecture that is key to our computational program. ANL and LLNL are expecting large installations of BG/Q within the next year, and BNL is expecting early hardware soon. We already have some highly optimized code elements running on prototype BG/Q hardware: Peter Boyle, of the University of Edinburgh, has a multi-threaded assembly version of a conjugate gradient solver that efficiently uses all 64 threads on a compute node, and achieves a performance of 50% of peak. We have started to use this for the development of a DWF code for QCD thermodynamics.

The HISQ fermion discretization is extensively used in QCD at finite temperature and density. Therefore we will strive to produce optimized code on BG/Q that can be used effectively by the CPS and MILC codes. This will involve optimizing the key QLA routines needed for the HISQ implementation, in addition to the threading and QMP work mentioned below. We will also investigate the benefit of writing a highly optimized HISQ solver from scratch to maximize the performance of the code.

The Domain Wall Fermion discretization is employed both in studies of QCD at finite temperature and of hadron structure. Thus the aggressive optimization of the CPS code base is a high priority, and we will port the extant Level 3 libraries for the Möbius DWF solver to the BG/Q.

The Wilson-clover discretization is used for the study of the excited-state spectrum, for the study of the origin of the nuclear force, and provides an important additional discretization to refine our calculations of hadron structure. Furthermore, an optimized clover inverter is needed for the calculations of transport coefficients and spectral functions from thermal meson correlation functions at finite temperature on gauge configurations generated using the HISQ and DWF discretizations. We will therefore develop an optimized inverter for Wilson-clover fermions, and integrate it into the application codes.

Year	Task	Team
1	Optimize QDP++ and Chroma to efficiently use the new floating-point features of the BG/Q	JLab
	Port and optimize existing Level 3 Clover and Möbius domain-wall fermion libraries	JLab, MIT
	Optimize the HISQ and DWF evolution code for thermodynamics within the CPS software package	BNL
2	Completion of optimizations started in year 1	BNL, JLab, MIT
	Integrate the thermodynamics measurement codes in CPS with the optimized DWF and HISQ inverter codes	BNL
3-5	Optimization within <i>Domain-Specific Framework</i>	BNL, JLab, MIT

QCD on Cray XK6 and other Hybrid Accelerated and Multi-core Architectures

The exploitation of GPUs by USQCD has already enabled us to address questions in nuclear physics that would otherwise be computationally prohibitive; the calculation of fluctuations of conserved charges in finite temperature QCD and the excited meson and nucleon spectrum are outstanding examples. The latter was made possible through the novel algorithmic technique of “distillation”, together with the highly cost-optimized implementation of the key solver needed for the method on GPUs within QUDA. Thus the continued exploitation of GPUs, and the exploration of other promising many-core, accelerated architectures such as the Intel Many Integrated Core (MIC) architecture is paramount. We will extend the scaling of the solvers needed for the observable computation phase of our calculations from the tens or hundreds of GPUs currently demonstrated within QUDA, to the many thousands that characterize these emerging architectures, and to perform this task for each of the fermion discretizations that we require. The long-term objective is to combine the development of new multigrid solvers described below, with the raw computational power provided by GPUs and other accelerators.

The emergence of leadership class, hybrid multicore-accelerated systems such as Titan at ORNL and Blue-Waters at NCSA based on the Cray XK6, GPU-accelerated architecture, as well as the Stampede System at the Texas Advanced Computing Center (TACC) based on the Intel MIC architecture makes it imperative for us to continue to go beyond solver libraries, and to port our full gauge field generation infrastructure to these new machines. Such work has already begun for the HISQ discretization of the fermion action that is central to our studies of QCD at finite temperature and densities. Integrating this within the CPS code so as to exploit the thermodynamic measurement routines is therefore an early priority of our efforts.

We have also made initial advances on moving the Wilson-Clover gauge field generation framework to GPUs, through initial conversion of the QDP++ framework (Just-in-Time) to utilize single GPU systems. We will extend this to support multiple GPUs. Further, we are working in partnership with Intel Corporation on early evaluation of, and the development of optimized code for, the Intel MIC architecture. The continuation of this work will allow the deployment of the Chroma gauge field generation frameworks on large-scale multi-node accelerated systems and forms a key part of our software deliverables and our partnership with the SUPER institute.

This development, combined with the use of current and to-be-developed highly optimized solvers, will enable a Wilson-clover hybrid-Monte-Carlo (HMC) gauge field generation on large heterogeneous systems, which will be key in enabling the generation of large lattices with light quarks on leadership class systems for hadronic and multi-hadron studies.

Year	Task	Team
1	Extend the Just-in-Time (JIT)-based version of QDP++ to use multiple GPUs for deployment on large-scale GPU-based systems	JLab
	Optimize QDP++ and Chroma for large-scale multi-GPU resources	JLab
	Continue collaboration with Intel corporation for MIC	JLab
	Optimize the HISQ evolution and measurement code for QCD thermodynamics on GPUs within CPS	BNL
	Implement Qlua interface to GPU libraries	MIT
2	Continue optimizations for Cray XK6	JLab
	Continue work with Intel on MIC architecture, deployment of Chroma and analysis of Chroma performance on Stampede	JLab
	Optimize analysis code for finite-density QCD calculations within CPS by including calls to GPU-based HISQ solver	BNL
	Develop an interface between CPS and DWF and overlap fermion GPU inverters	BNL
	Incorporate a Wilson-clover HMC implementation within the QUDA library	UW
3-5	Develop optimized codes for emerging generation of GPU and many-code architectures using <i>Domain-Specific Languages</i>	BNL, JLab

2.5.2 Domain-specific Frameworks for Lattice QCD

The development of domain-specific frameworks to facilitate the rapid development of highly optimized code that takes account of the emerging hardware features, such as many-core nodes, heterogeneous architectures, and an abundance of floating-point performance compared with limited memory bandwidth, is key to our longer-term optimization strategy. This we will accomplish through the development of a domain-specific language and compiler in cooperation with the SUPER Institute, together with the further development of the Qlua integration and optimization framework.

A domain specific language and compiler in partnership with SUPER: We propose to build a successor to the current implementation of the data parallel level of our QCD API by creating a *domain specific language* (DSL) for lattice computations using the ROSE compiler framework [132]. We will undertake this as a partnership between USQCD and the Institute for SUstained Performance, Energy and Resiliency (SUPER), in particular members at RENCi. SUPER has expertise in compiler technologies in general and the ROSE compiler framework in particular, required to bring this project to fruition.

The objective of this effort is to improve scientific productivity while simultaneously achieving an uncompromised level of execution performance that will be portable across the widest variety of platforms, including conventional cluster architectures, heterogeneous systems with many-core accelerators, and the power efficient systems that will emerge on the way to extreme scale. The compiler will recognize common computational, mathematical, and physical idioms and use specific knowledge of these idioms to either enable aggressive optimization methods, or in some cases, select the best hand-coded solutions for the target architecture by either calling a library or by inlining the code directly. DSL approaches have been successful in several areas including tensor calculations in chemistry (Tensor Contraction Engine) [133], digital signal processing (SPIRAL) [134], PDE's on irregular meshes (Liszt) [135], and stencil calculations on large-scale GPU-accelerated systems [136].

As developing such a system is a long term effort, we will concurrently carry out the crucial activities of extending the QCD implementations for specific architectures listed in the previous sections. This dual approach will allow for the exploitation of near-term expected resources at leadership computing facilities with high performance, while developing techniques and idioms to include in the domain specific compiler in the longer term, and serve as a basis for moving lattice QCD towards the exascale.

The domain specific compiler will use the abstraction specified by the QDP++ layer. It will eliminate the need for expression templates or third-party library code generation, and will allow high level transformations to be applied at the abstraction level, where programmer intent is available and where properties such as independence (absence of aliasing) are known. On the back end, the domain specific language can apply code transformations to allow efficient vectorization, to subdivide work into tasks for efficient threading, and to order loops to make efficient uses of caches. Since the ROSE compiler can generate both CUDA and OpenCL code, the domain specific compiler will be able to deal with the challenge posed by heterogeneity without the need for Just-In-Time compilation of expressions.

The production of a system which is sufficiently capable to completely replace the current QDP++ system will take at least the first 3 years of the SciDAC project. Useful prototypes that address core issues will be available earlier and we expect to use these prototypes to generate production-quality code on restricted, high-impact examples.

Chroma: The extension of QDP++ to use a domain-specific implementation is a key part of the development of Chroma to fully exploit heterogeneous architectures, and the expected near- and longer-term leadership facilities.

Year	Task	Team
1	Implement a domain-specific compiler through source-to-source translation, using ROSE to generate loops that are currently handled through expression templates	BNL, JLab, RENCi
2	Perform optimizations based on local rewriting of operators, and investigate autotuning of the code	JLab, RENCi
3	Design mechanism to describe target architectures, and use descriptions to produce machine-specific code	JLab, RENCi
	Perform machine-specific optimizations for the BG/Q, many-core architectures, and for heterogeneous architectures such as the Cray XK6	BNL, JLab RENCi
4-5	Investigate whole-program optimization and deliver auto-tunable code	JLab, RENCi
	Perform optimizations for emerging architectures, emphasizing code generation for heterogeneous systems, and dynamic scheduling to improve code reuse at all levels of memory hierarchy	JLab, RENCi

Qlua – integration and optimization framework for lattice QCD: We will refine Qlua to support machine-level optimization based on experience with the development and prototyping of multigrid algorithms, as described below. The resulting implementations will share a common front end and scripting language interpreter, but have machine-specific back ends targeting the emerging architectures. We will also include support for theories with differing numbers of “colors”, enabling us to investigate Beyond-the-Standard-Model theories sought in precision nuclear-physics experiments.

Year	Task	Team
1	Begin exploration of algorithms at scale for disconnected diagrams, form factors at high momentum transfer, higher moments of structure functions and improved gluon operators	MIT
	Include support for multiple colors	MIT
2	Develop prototype implementation of optimized Qlua	MIT
3	Implement a Qlua interface to 3rd party libraries	MIT
4-5	Provide support for Level 3 libraries using back-end optimization optimization for emerging architectures: BlueGene/X, Intel MIC, etc.	MIT

2.5.3 New Algorithms for Nuclear Physics

High fidelity studies of hadron structure, of excited hadronic states, and of nuclei as well as thermal hadron correlation functions or transport coefficients demand lattices of large physical volume, quark masses that approach the physical light-quark masses, and large statistical samples to overcome the poor signal-to-noise ratio inherent to lattice studies in nuclear physics. Thus the development of efficient solvers, their exploitation both in gauge field generation and physics observable computation, and new gauge field generation algorithms are essential prerequisites for our science goals. A further characteristic of studies in nuclear physics is the increasing complexity of the correlation functions with a resulting need to automate their tabulation, and the computational cost of computing them. Thus a program addressing these challenges is essential if the physics goals are to be satisfied.

Improved Solvers

A high priority is to capitalize on the first successful applications of advanced multigrid and, more generally, domain decomposition methods to lattice QCD. The full exploitation of multiscale algorithms is a major project starting with solvers for the Wilson-clover, Domain Wall and HISQ discretizations, then integrating

them into analysis code and finally into HMC evolution code, all the time tuning parameters and mapping data layouts for increasingly complex heterogeneous architectures. This strategy will continue throughout this five-year project, capitalizing on applied-mathematics expertise within FASTMath and in collaboration with Boston University, the Argonne Leadership Computational Facility and the USQCD community. We will begin by integrating the Wilson-clover multigrid solver into our application codes and starting the development of new multigrid solvers for Möbius domain-wall fermions and for HISQ. Each solver will be distributed as a Level 3 library for inclusion in our application codes. These multiscale methods have the potential to greatly advance our campaigns on the hadron spectrum, hadron structure and the hadronic interactions through accelerating the computation of observables, as well as to improve QCD thermodynamics calculations.

Year	Task	Team
1	Integrate a multigrid algorithm for the Wilson-clover discretization into Chroma	JLab, UW
	Develop multigrid solver for the HISQ action, leveraging HYPRE and the FASTMath	BNL
	Develop a multigrid algorithm for Möbius Domain Wall fermions, leveraging Qlua and FASTMath.	MIT
2	Investigate the performance of HISQ multigrid for QCD thermodynamics	BNL
	Implement a Qlua interface to HYPRE, in cooperation with FASTMath	MIT
	Integrate multigrid algorithm for Wilson-clover discretization on GPUs and the BlueGene/Q within QDP++ and Chroma	JLab, UW
3-5	Implement a MDWF multigrid algorithm within Level 3 and investigate use in HMC evolution code	MIT
	Investigate, in collaboration with BU, the combined role of multigrid and domain decomposition on evolution code on capability computers	BNL, JLab MIT, WM
	Use the Qlua framework, in collaboration with BU, for rapid prototyping and code generation for use of multigrid in hadron structure calculations on emerging architectures	MIT

Low Eigenvector Methods:

The estimation of the trace of the inverse of a Dirac matrix is important for nuclear physics in a variety of ways, most notably the calculation of flavor-singlet contributions to hadron structure and in reweighting methods to account for isospin-breaking effects. In finite density QCD products of traces over powers of the inverse of the Dirac matrix are needed, which requires frequent inversions of the same matrix using thousands of different source vectors. Though there have been studies of the improvement of solvers by handling the low eigenvalue spectrum of the Dirac matrix separately [137, 138, 139], their use has been limited due to the lack of better trace-estimation methods. Improved methods are also of interest in other fields, for example in data mining where the estimation of the traces of very large covariance matrices is required.

The trace of the inverse of a matrix is typically estimated through Monte Carlo (MC) averaging over a sample of Gaussian quadratures, each computed with a Krylov method. Therefore, any computational improvements should come by speeding up convergence of the Krylov method and/or by reducing the variance of the MC. We will focus on techniques that perform both tasks at the same time: deflation, preconditioning, and use of low variance samples (vectors).

It has been shown that deflation can reduce the number of linear system iterations by a factor of 5–10 [140]. In preliminary results, deflation reduces also the MC variance by factors of 10^2 – 10^4 [141], yielding overall speedups of 1000 over undeflated methods. Methods for non-hermitian systems will be developed, including the eigBiCG method. These methods will also be extended to other functions of a matrix such as the log. In LQCD the concept of dilution has been used extensively to reduce the MC variance using graph coloring.

Dilution can be combined with other variance reducing vectors such as Fourier or Hadamard. An efficient generation and application of these vectors will also be performed.

Year	Task	Team
1	Implement eigBiCG inverter at Level 3, callable from high level QCD software packages; provide an interface to PRIMME eigenvalue package	JLab, WM
2	Implement deflated MC trace estimators	JLab, WM
3	Explore preconditioners to improve convergence, and reduce MC variance	BNL, JLab, WM
4	Explore variance reducing vector samples	BNL, JLab, WM
5	Provide methods and implementations that combine deflation, preconditioning and variance reducing vectors	BNL, JLab, WM

Improved algorithms for gauge generation

The large performance improvements in gauge field generation that have been made in the last few years rely on multi-timescale integration methods coupled with various kinds of preconditioning strategies. These techniques have relied on heuristic methods to balance the work among the various timescales. A more rigorous approach to tuning integration parameters relying on the properties of symplectic integrators has recently been proposed in [142] using the technology of Poisson Brackets (PBs) and the Shadow Hamiltonian – the version of the original Hamiltonian that is integrated exactly by the finite time-step integrator.

The *Shadow Hamiltonian HMC (SHMC)* [143] and its variants (e.g. [144]) are techniques pioneered in numerical chemistry simulations of biological molecules to improve over the performance of HMC. The main benefit is that integration of the shadow Hamiltonian can be reformulated as a higher order integration of the original Hamiltonian. The new technology of Poisson Brackets can be used to predict the optimal form of the integration parameters. Coupled with the new kind of higher order symplectic integrator known as the *Force-Gradient integrator* [142, 145] made possible by the Poisson Bracket technology, there are opportunities for performance improvements in our gauge field generation programs.

With the approach to precision calculations at the physical light-quark masses, additional issues become crucial. Firstly, the gauge field generation algorithms must rapidly sample the different topological sectors of QCD. We will therefore explore new Monte-Carlo sampling methods, such as cluster algorithms [146]. Secondly, the inclusion of isospin breaking effects, through the different masses of the light u and d quarks, becomes a priority. Thus we will exploit the low-eigenmode developments described above to directly include isospin-breaking effects in gauge field generation.

Year	Task	Team
1	Extend the Poisson bracket technology for use with the clover action; use these methods to optimize and carry out efficacy tests of the force gradient integrator technique on large lattice sizes made possible on new leadership class facilities	BNL, JLab
2	Carry out the initial feasibility study of Shadow Hamiltonian techniques for use in gauge field generation	JLab
	Carry out an initial feasibility study on updating deflation spaces within the gauge field integration.	JLab
3-5	Investigate improved Monte Carlo sampling techniques, to increase topological tunnelling rates, which are expected to slow down at light quark masses	JLab, WM
	Exploit developments in low-eigenmode methods for use in Hybrid Monte Carlo algorithm so as to include isospin-breaking effects in gauge generation framework	JLab, WM

Multi-quark contractions and contraction combinatorics

The construction of correlation functions represents an increasingly significant fraction of the cost of lattice calculations for nuclear physics, driven both by the explosion in the size of the operator basis and the increasing numbers of elemental quark fields in multi-hadron systems. Thus the development of a powerful computational framework for analysis is an important emphasis of this proposal.

Performing the required contractions is more suited to a 3-dimensional data-parallel code than a 4-dimensional one. Currently a 3-dimensional version of QDP++ provides suitable data types and operations to express contractions, however, for greater efficiency a style of data parallelism where elemental functions (much like CUDA kernels) are mapped onto the lattice sites may be more suitable, especially for re-expressing data-reuse. We propose to extend QDP++ to support such a style of programming.

The use of accelerator technologies such as GPUs affords a means to speed up the analysis computations. Initial steps in this direction have already been taken, for example where QDP++ statements are Just-In-Time (JIT) compiled into CUDA kernels for execution on NVIDIA GPUs. The previously mentioned extension of QDP++ should map straightforwardly to heterogeneous systems. New analysis techniques such as distillation [126] can be reduced to a number of linear algebra operations on dense matrices. We will evaluate the operations required, and design a library of primitives that can be efficiently implemented on GPUs and forthcoming accelerator technologies.

The combinatorial explosion of basis operators represents a complexity frontier for lattice calculations which rely on the variational method. The mechanics of LQCD require that all pairs of quark and antiquark fields within a correlation function be combined in all possible ways resulting in a large number of contractions. For complex systems, it is impractical to construct code by hand that implements the contractions for an n-point correlator of given quantum numbers. We propose to construct automatic code generation tools that either explicitly realize the full set of contractions or make use of more advanced methods such as applying recursions [98]. Moreover, the short range confining nature of QCD suggests that contraction of these correlation functions can be reorganized following clustering techniques familiar in many-body studies in nuclear and atomic physics. Investigations of these new techniques will foster new fruitful collaborations with other well established fields of computational and computer science domains.

Year	Task	Team
1	Port the current contraction code for multi-nucleon systems to GPUs	UW
	Develop a generalized contraction code that is suitable for a small number of initial and final-state particles using a three-dimensional implementation over QDP++	JLab
	Implement “distillation” for the study of hadronic structure and matrix elements	JLab, MIT
2	Extend general graph contraction to use GPUs through the use of the JIT-based implementation of QDP++	JLab, UW
	Begin development of third-generation nuclear contraction code that incorporates realistic nuclear wavefunctions in both the source and sink construction, and port to GPU-based systems	UW
	Develop an interface to HDF5 I/O framework	MIT, UW
3	Complete port of third-generation contraction code to heterogeneous architectures	JLab, UW
	Coordinate with emerging SciDAC Data storage institutes to incorporate new lattice file storage techniques within analysis codes	JLab
4-5	Continue optimization of the contraction code(s) on the existing and new architectures	JLab, UW
	Extend the scope of the nuclear contraction code to larger nuclear systems	UW
	Port the nuclear contraction code to new architectures aligned with the exascale architecture(s)	JLab, UW

2.6 Management Structure and Performance Control

The Project Director and lead principal investigator for this effort will be Frithjof Karsch. He will have overall responsibility for the project, and will be the point of contact for the Department of Energy. The co-director for Computation, Richard Brower, will have overall responsibility for the software and algorithm work, providing direction and coherence to the work, and monitoring progress on all tasks. He will also coordinate work with other collaborators in the U.S. lattice gauge theory community (USQCD), and our partners in the SciDAC SUPER Institute¹ and in the Emerging Applications Group at NVIDIA. He will provide quarterly reports to the Director on the progress of the software effort. The co-director for Science, David Richards, will track progress towards meeting the scientific goals of the project, and will advise the Director on new scientific opportunities that arise during the course of the project. He will also advise the Director and co-director for Computation on priorities for software and algorithm development needed to advance the scientific program².

Each institution receiving funds under this grant has a local principal investigator, who has first level responsibility for the work carried out at his or her institution. The principal investigators will report to the Director and co-directors during monthly phone conferences.

The Director and the two co-directors are also members of the USQCD Executive Committee, whose other members are N. Christ, J. Kuti, P. Mackenzie (chair), J. Negele, S. Sharpe, and R. Sugar. The USQCD Executive Committee serves as the Advisory Board to the Director and co-directors. It gives advice on the scientific goals of the project, the software development plan designed to meet these goals and the distribution of funds available. At the end of each project year, the Executive Committee will review progress towards meeting the scientific and computational goals of the project and will advise the Director. Schedule slips of more than two months must be reported to the Executive Committee. In consultation with the Executive Committee the Director and co-directors will then decide if a reallocation of resources or a scope change is needed.

As the USQCD Executive Committee monitors the physics program of the lattice QCD community in the US, this process will insure that the software development performed within this project gets coordinated with other efforts of the USQCD.

USQCD Executive Committee:

The Executive Committee has been leading the effort to construct computational infrastructure for the U.S. lattice gauge theory community for over twelve years. It holds approximately two conference calls per month, and communicates via email between calls. The Executive Committee has been actively involved in the preparation of this proposal.

USQCD Software Committee:

The USQCD Software Coordinating Committee consists of software leaders in the U.S. lattice gauge theory community. It works with the Software Coordinator to provide leadership of the USQCD software effort. The co-director for Computation, Prof. Brower, also is USQCD's Software Coordinator. He has responsibility for all USQCD software projects, providing direction and coherence to the work, and monitoring progress on all tasks. The Committee meets weekly in conference calls to track progress of software tasks, to discuss technical approaches for completing them, and to further clarify the tasks. The Software Coordinating Committee works in consultation with the Executive Committee to insure that critical components are available in time to keep the overall software project, and the scientific work which depends on it, on track. It proposes changes in task priority and schedule to the Executive Committee as appropriate.

¹ To ensure the effectiveness of the partnership, a postdoctoral researcher from the field of Lattice QCD with demonstrated ability and interest in the development of optimized software for lattice QCD will be hired by SUPER at RENCi, but will spend the majority of his or her time working with the nuclear physics groups on this proposal.

²In Section 2 we listed software development tasks grouped according to topics. Summary tables for tasks to be performed at the various participating institutes are given in the Appendix.

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- [128] J. Mellor-Crummey, and N. Tallent, “A Methodology for Accurate, Effective and Scalable Performance Analysis of Application Programs”, IEEE International Symposium on Performance Analysis of Systems and Software: Workshop on Tools, Infrastructures and Methodologies for the Evaluation of Research Systems (2008).
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D. Unat, X. Cai and S. Baden, “Mint: Realizing CUDA performance in 3D stencil methods with annotated C”, published in *Proceedings of the 25th International Conference on Supercomputing (ICS’11)*, 214 (ACM Press, 2011).
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- [141] A. Stathopoulos, K. Orginos, and A. Abdel-Rehim, presentation at Copper Mountain Conference on Iterative Methods (2010).
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- [145] A. D. Kennedy, M. A. Clark and P. J. Silva, “Force Gradient Integrators,” *PoS LAT2009*, 021 (2009) [arXiv:0910.2950 [hep-lat]].
- [146] C.H. Mak and Arun.K. Sharma, ”Reverse Monte Carlo Method and Its Implications for Generalized Cluster Algorithms”, *Phys. Rev. Lett.* **98** (2007) 180602.

4 Biographical Sketches

- Richard Brower (Boston University)
- Robert Edwards (Thomas Jefferson National Accelerator Facility)
- Rob Fowler (University of North Carolina)
- Frithjof Karsch (Brookhaven National Laboratory)
- John Negele (Massachusetts Institute of Technology)
- David Richards (Thomas Jefferson National Accelerator Facility)
- Martin Savage (University of Washington)
- Andreas Stathopoulos (College of William and Mary)

Curriculum Vitae

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Professional Preparation

Ph.D. Physics, University of California, Berkeley, 1969
M.S. Applied Math, Harvard University, 1964
B.S. Physics, Harvard University, 1963

Appointments and Visiting Positions

1987-present, Professor of Physics and Engineering, Boston University
1973-86, Professor of Physics, University of California, Santa Cruz, CA
1978-86, Research Professor, Santa Cruz Institute of Particle Physics
1972-73, Senior Research Associate, Cal. Tech, Pasadena, CA
1969-72, Research Associate, MIT, Cambridge, MA
2006-present, Visiting Professor of Physics, Brown University, Providence R.I.
1992-present, Visiting Scientist, MIT Center for Theoretical Physics
1980-81, Visiting Associate Professor of Physics, Harvard Cambridge, MA

Honors and Awards

1974-76, A. P. Sloan Research Fellow, SLAC and MIT
1970-71, NSF Postdoctoral Fellow, C.E.R.N., Geneva, Switzerland

Research Interests and Expertise

Professor Brower has worked in several fields of theoretical and computational physics — string theory, hadron phenomenology, Quantum Chromodynamics, lattice formulations of quantum field theory and statistical mechanics and molecular dynamics. He has experience with parallel algorithms starting with data parallel methods on the the Connection Machine to GPU cost effective clusters architectures. Algorithmic research includes in multi-grid Dirac solvers, the Möbius Domain Wall algorithm, chronological inverter and cluster algorithms for bosonic and fermionic systems. He serves on the USQCD Executive Committee and as the National Software Co-ordinator for the SciDAC software infrastructure project.

Synergistic Activities

Organizer of Aspen QCD Workshop 1997 and Strong Dynamics BSM Workshop 2010.
Member, USQCD Executive Committee, 2001-present.
SciDAC software co-ordinator, chair of Software Committee, 2001-present.
International Lattice Data Grid (ILDG)2003-pres; Chair in 2005, 2010.
International Advisory Committee for Lattice Field Theory, Virginia 2008.
Member, Organizing committee, SciDAC 2007.

Thesis, Postdoctoral Advisors and Advisees

Geoffrey Chew (U.C. Berkeley); Francis Low (MIT), Murray GellMann (CalTech); Ronald Babich (NVIDIA/PSC), Michael Cheng (BU), Mike Clark (NVIDIA/Harvard), Saul Cohen (INT Seattle), James Osborn (ANL), Oliver Witzel (BU)

Collaborators

T. Appelquist (Yale), R. C. Babich (Boston University), James Brannick (Penn. State U), S. Catterall (Syracuse), M. A. Clark (Harvard), S. Cohen (INT Seattle), Marko Djuric (Universidade do Porto), Robert Edwards (Jeff Lab), George T. Fleming (Yale), J. Giedt (Rensselaer), S. Gottlieb (Indiana U.), B. Joo (Jeff Lab), J. Kiskis (U.C. Davis), T. A. Manteuffel (U. of Colorado, Boulder), S. McCormick (U. of Colorado, Boulder), Meifeng Lin (Yale), J. Negele (MIT), E. Neil (FNAL), K. Orginos (William and Mary), J. C. Osborn (ANL), J. Polchinski (Kavali Institute), C. Rebbi (BU), Ina Sarcevic (Arizona U), David Schaich (Boulder Colorado), G. Shi (NCSA), M. Strassler (Rutgers), C-I Tan (Brown), Pavlos Vranas (LLNL)

Publications Most Relevant to Proposal

- R. Babich, M. A. Clark, B. Joo, G. Shi, R. C. Brower and S. Gottlieb Scaling Lattice QCD beyond 100 GPUs SuperComputing 2011 paper, arXiv:1109.2935 [hep-lat].
- T. Appelquist, R. Babich, R.C. Brower, M.Cheng, M.Clark, S. Cohen, G. Fleming, J. Kiskis, E. Neil, J. Osborn, R. Claudio, D. Schaich and P. Vranas, Parity Doubling and the S Parameter Below the Conformal Window, Phys. Rev. Lett. 106, 231601 (2011), arXiv: 1009.5967v1 [hep-ph].
- T. Appelquist, A. Avakian, R. Babich, R.C. Brower, M.Cheng, M.Clark, S. Cohen, G. Fleming, J. Kiskis, E. Neil, J. Osborn, R. Claudio, D. Schaich and P. Vranas, Toward TeV Conformality Phys. Rev. Lett. 104, 071601 (2010), arXiv:0910.2224 [hep-ph].
- M. A. Clark, R. Babich, K. Barros, R. C. Brower and C. Rebbi, Solving Lattice QCD systems of equations using mixed precision solvers on GPUs Comput. Phys. Commun. 181, 1517 (2010), arXiv:0911.3191 [hep-lat].
- R. Babich, J. Brannick, R. C. Brower, M. A. Clark, T. A. Manteuffel, S. F. McCormick, J. C. Osborn and C. Rebbi, Adaptive multigrid algorithm for the lattice Wilson-Dirac operator Phys. Rev. Lett. 105, 201602 (2010); arXiv: 1005.3043 [hep-lat].
- J. Brannick, R. C. Brower, M. A. Clark, J. C. Osborn and C. Rebbi, Adaptive Multigrid Algorithm for Lattice QCD Phys. Rev. Lett. 100, 041601 (2008), arXiv: 0707.4018 [hep-lat].
- R. C. Brower, R. Babich, K. Orginos, C. Rebbi, D. Schaich and P. Vranas Möbius Algorithm for Domain Wall and GapDW Fermions LATTICE2001, arXiv: 0910.2813 [hep-lat].

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Professional Preparation

University of Texas at Austin: B.S. (Physics), 1984
University of Texas at Austin: B.S. (Mathematics), 1984
New York University: PhD. (Physics), 1989
New York University: M.S. (Physics), 1989

Appointments

1999–present, Senior Staff Scientist, Jefferson Lab, USA
1997-1999, S.C.R.I., Florida State University, Associate Research Scientist
1992-1997, S.C.R.I., Florida State University, Assistant Research Scientist
1989-1992, S.C.R.I., Florida State University, Postdoctoral Research Scientist

Synergetic Activities

Member at Large - American Physical Society: Topical Group on Hadronic Physics.
Panel, DOE/ASCR/NP Computational Requirements for NERSC, 2011.
Member, USQCD Scientific Program Committee and Software Committee.
Developer of Chroma/QDP++ software system, <http://usqcd.jlab.org/usqcd-docs/chroma>
Co-designer of the QCDSP supercomputer. Developed in collaboration with Columbia Univ. & Brookhaven Lab. Won the 1998 Gordon Bell prize.

Awards

Fellow of the American Physical Society, 2011
Gordon Bell Prize, 1998
New York University, Deans Dissertation Fellowship 1988
New York University, Andre Meyer Fellowship 1984

Organizing Committee:

Lattice 90, Tallahassee, Lattice 02, MIT; Lattice 08, Williamsburg; Gluonic Excitations, JLab, 2003; Lattice Hadron Physics, Cairns, 2003; Chiral Dynamics, JLab, 2012.

Graduate Advisor: Prof. Alan Sokal, New York University

Postdoctoral Advisor: Prof. Anthony Kennedy, Univ. of Edinburgh

Selected Publications: Robert Edwards

- 1.) R.G. Edwards, J.J. Dudek, D.G. Richards, S.J. Wallace, “Excited state baryon spectroscopy from lattice QCD”, Phys. Rev. D84, 074508 (2011)
- 2.) J.J. Dudek, R.G. Edwards, B. Joo, M.J. Peardon, D.G. Richards, C.E. Thomas, “Isoscalar meson spectroscopy from lattice QCD”, Phys. Rev. D83, 111502 (2011)
- 3.) J.J. Dudek, R.G. Edwards, M.J. Peardon, D.G. Richards, C.E. Thomas, “Highly Excited and Exotic Meson Spectrum from Lattice QCD”, Phys. Rev. Lett. 103, 262001 (2009)
- 4.) M.J. Peardon, J. Bulava, J. Foley, C. Morningstar, J.J. Dudek, R.G. Edwards, B. Joo, H.-W. Lin, D.G. Richards, K.J. Juge, “A Novel Quark Field Creation Operator Construction for Hadronic Physics in Lattice QCD”, Phys. Rev. D80, 054506 (2009)
- 5.) H.-W. Lin, S.D. Cohen, J. Dudek, R.G. Edwards, B. Joo, D.G. Richards, J. Bulava, J. Foley, C. Morningstar, E. Engelson, S. Wallace, K.J. Juge, N. Mathur, M.J. Peardon, S.M. Ryan, “First results from 2+1 dynamical quark flavors on an anisotropic lattice: Light-hadron spectroscopy and setting the strange-quark mass”, Phys. Rev. D79, 034502 (2009)
- 6.) J. Dudek, R.G. Edwards, “Two Photon Decays of Charmonia from Lattice QCD”, Phys. Rev. Lett. 97, 172001 (2006)
- 7.) R.G. Edwards, G.T. Fleming, Ph. Hagler, J.W. Negele, K. Orginos, A.V. Pochinsky, D.B. Renner, D.G. Richards, W. Schroers, “The Nucleon axial charge in full lattice QCD”, Phys. Rev. Lett. 96, 052001 (2006)
- 8.) Ph. Hagler, W. Schroers, J. Bratt, J.W. Negele, A.V. Pochinsky, R.G. Edwards, D.G. Richards, M. Engelhardt, G.T. Fleming, B. Musch, K. Orginos, D.B. Renner, “Nucleon Generalized Parton Distributions from Full Lattice QCD”, Phys. Rev. D77, 094502 (2008)
- 9.) G. Kilcup, S. Hanson, J. Sexton, R. Edwards, T. Kennedy, I. Arsenin, D. Chen, P. Chen, N.H. Christ, G.T. Fleming, C. Jung, A. Kaehler, S. Kasow, R. Luo, C. Malureanu, R.D. Mawhinney, J. Parsons, C. Sui, P. Vranas, A. Gara, “The 0.8Tflop project at Columbia”, IEEE/ACM, SC97: High Performance Networking and Computing (1997)
- 10.) R.G. Edwards, B. Joo, “The Chroma Software System for Lattice QCD”, Nucl. Phys. Proc. Suppl. 140:832 (2005)

Collaborators and Co-Editors: C. Aubin (Fordham), J. Bulava (CERN), S. Cohen (U. Wash.), J. Dudek (Old Dominion), M. Engelhardt (New Mexico State), J. Foley (Utah), Ph. Hägler (Munich), G. Fleming (Yale), B. Joo (JLab), K.J. Juge (U. Pacific), H.W. Lin (U. Wash.), N. Mathur (Mumbai), H. Meyer (Bonn), C. Morningstar (CMU), J. Negele (MIT), K. Orginos (W&M), M. Peardon (Trinity), A. Pochinsky (MIT), D. Renner (JLab), D. Richards (JLab), S. Ryan (Trinity) S. Syritsyn (LBNL) H. Thacker (U. Virginia), C.E. Thomas (Trinity), S. Wallace (U. Maryland)

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Education and Training:

Harvard College, Physics, A.B. (cum laude), 1971.
University of Washington, Computer Science, M.S, 1981.
University of Washington, Computer Science, Ph.D. 1985.

Research and Professional Experience:

Director of High Performance Computing. Renaissance Computing Institute, University of North Carolina, June 2006- present. (Previous titles: Chief Domain Scientist for HPC, Director of High Performance Computing Research)

Adjunct Professor of Computer Science, appointments at Duke University, University of North Carolina, and Rice University, 2006-present.

Senior Research Scientist and Associate Director, Center for High Performance Software Research, Rice University, Sept 1996-May 2006.

Visiting Associate Professor, Rice University, January 1985-August 1996.

Visiting Associate Professor, DIKU, University of Copenhagen, August 1993-December 1994.

Assistant Professor, University of Rochester, September 1986-June 1993.

Acting Assistant Professor, University of Washington, September 1985-June 1986.

Publications Relevant to Proposed Project:

1. Ken Kennedy, Bradley Broom, Arun Chauhan, Robert Fowler, John Garvin, Charles Koelbel, Cheryl McCosh, and John Mellor-Crummey. Telescoping languages: A system for automatic generation of domain languages. *Proceedings of the IEEE*, 93(2):387-408, February 2005.
2. John Mellor-Crummey, Vikram Adve, Bradley Broom, Daniel Chavarra-Miranda, Robert Fowler, Guohua Jin, Ken Kennedy, and Qing Yi. Advanced optimization strategies in the Rice dHPF compiler. *Concurrency: Practice and Experience*, 14(8 & 9):741-768, August 2002.
3. Anirban Mandal, Rob Fowler, and Allan Porterfield. Modeling memory concurrency for multi-socket multi-core systems. In *Proceedings of the 2010 IEEE International Symposium on Performance Analysis of Systems and Software (ISPASS2010)*, pages 56-75, White Plains, NY, March 2010.
4. N. Froyd, J. Mellor-Crummey and R. Fowler. Efficient call-stack profiling of unmodified, optimized code. *Proc. of the 19th ACM Intl. Conference on Supercomputing*. Cambridge, MA, June, 2005.
5. J. Mellor-Crummey, R. Fowler, G. Marin, and N. Tallent. HPCView: A tool for top-down analysis of node performance. *The Journal of Supercomputing*, 23, 81-101, 2002.
6. Bradley Broom, Rob Fowler, Ken Kennedy, Charles Koelbel, and Michael Paleczny. Compiler support for out-of-core arrays on parallel machines. In Daniel Reed, editor, *Scalable Input/Output*, pages 155-174. MIT Press, Cambridge, MA, October 2003.
7. Alain Darte, John Mellor-Crummey, Robert Fowler, and Daniel Chavarra-Miranda. Generalized multi-partitioning of multi-dimensional arrays for parallelizing line-sweep computations. *Journal of Parallel and*

Distributed Computing, 63(9):887-991, September 2003.

8. Bradley Broom, Daniel Chavarra-Miranda, Guohua Jin, Rob Fowler, Ken Kennedy, and John Mellor-Crummey. Overpartitioning with the rice dhp compiler. In Proceedings of the 4th Annual HPF Users Group Meeting, Tokyo, Japan, October 2000.
9. Robert Fowler, John Mellor-Crummey, Guohua Jin, and Apan Qasem. A source-to-source loop transformation tool (extended poster abstract). In Proceedings of the Los Alamos Computer Science Institute 3rd Annual Symposium, Santa Fe, NM, October 2002.
10. Todd Gamblin, Rob Fowler, and Daniel A. Reed. Scalable methods for monitoring and detecting behavioral classes in scientific codes. In Proceedings of the International Parallel and Distributed Processing Symposium 2008, Miami, FL, April 2008.

Synergistic Activities:

Fowler is principal investigator for the UNC component of the SciDAC Sustainable Performance, Energy, and Resilience (SUPER) institute. Prior to that he was PI for UNC in the PERI institute. He was also PI of the UNC part of the SciDAC 2 USQCD project for which he was involved in the performance measurement, analysis, and tuning of LQCD libraries and codes.. In conjunction with state-funded projects within RENCi, he is involved in the analysis and tuning of HPC codes in the geo-sciences (weather, flooding) and in computational biology. Fowler is Co-Investigator on the MAESTRO project, a DoD-funded research project focusing on the problem of building language (user) level multi-threaded runtime environments for multi- and many-core processors. MAESTRO uses real time performance reflection to adapt threading strategies based on real-time measurement of power and of the utilization of shared hardware resources.

Fowler was the Program Chair for the inaugural HPCWeek Symposium held in conjunction with the DOE ASCR PI meeting in March 2008. Previously he served several times as the program chair for the Los Alamos Computer Science Institute Symposium and on the program committees of numerous conferences. He has done recurring service on proposal review panels for NSF and DOE, and has served on programming committees and as a reviewer for numerous journals and conferences..

Collaborators and Other Affiliations since Dec.2005

Alan Cox (Rice), Bronis de Supinski (LLNL), Patrick Dreher (UNC), Nathan Froyd (Code Sourcery), Todd Gamblin (LLNL), Kevin Huck (Oregon), Balint Joo (JLab), Gopi Kandaswamy (UNC), Ken Kennedy (Rice), Howard Lander (UNC), Allan Malony (Oregon), Anirban Mandal (UNC), John Mellor-Crummey (Rice), Cheryl McCosh (Rice), Dan Reed (Microsoft), Mark Neyer (Blue Capital), Rodney Oldehoeft (Krell Inst.), Allan Porterfield (UNC), Lavanya Ramakrishnan (Indiana), Prasun Ratn (NCSU), Martin Schulz (LLNL), Sameer Shende (Oregon), Allen Snavely (SDSC), Nathan Tallent (Rice), Varerie Taylor (TAMU), Steven Thorpe (MCNC), Ying Zhang (UNC) (Note: For large collaborative projects such as the Los Alamos Computer Science Institute and SciDAC PERI, only direct collaborators and co-authors are cited.)

Graduate and Post-doctoral Advisors/Advisees

Dissertation Advisor (pre-2004): Richard Ladner, University of Washington.

Ph.D. Advisees (pre-2004): Povl Koch (DIKU, Denmark), Jack Veenstra (Rochester), and Alan L. Cox (Rochester). G. Todd Gamblin (2009), University of North Carolina (*de facto* advisor in Dan Reed's absence). Post-doctoral advisees: James Horey (ORNL), Min Yeol Lim (UNC), and Michael Siegel (UNC). Other graduate students: Roberto Rodriguez, Yusuf Simonson.

Curriculum Vitae FRITHJOF KARSCH

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Professional Preparation

Dr. rer. nat. Physics, Bielefeld University, Germany, 1982 (Advisor, H. Satz)
Diplom Physics, Bielefeld University, Germany, 1979 (Advisor, H. Satz)

Appointments

2005–present, Sr. Scientist, Brookhaven National Laboratory, USA
1990–present, Professor for Theoretical Physics, Bielefeld University, Germany
1990–1993, Head of the particle physics group at HLRZ, HLRZ-Jülich, Germany
1986–1990, Staff Member, Theory Division, CERN, Geneva, Switzerland
1984–1986, Research Associate, University of Illinois at Urbana-Champaign, USA
1982–1984, Research Fellow, CERN, Geneva, Switzerland

Visiting Positions: Visiting Scientist, University of Tsukuba, Tsukuba, Japan, May-July 1999; CERN, Geneva, Switzerland, August 1999 - April 2000

Synergetic Activities

Member, Editorial Board of *The European Physical Journal C*

Member, USQCD Executive Committee, 2011–present

Member, USQCD Scientific Program Committee, 2009–present; chair, 2010–present

Member, Advisory Board, New York Center for Comp. Science, 2007–present

International Advisory Committees:

- a) International Symposia on Lattice Field Theory: Lattice 2008, William and Mary, USA; Lattice 2009, Beijing, China; Lattice 2010, Villasimius, Italy; Lattice 2011, Squaw Valley, USA
- b) International Conference on Ultrarelativistic Nucleus-Nucleus Collisions: Quark Matter 2008, Knoxville, USA; Quark Matter 2011, Annecy, France; Quark Matter 2012, Washington DC
- c) International Conference on 'Critical Point and Onset of Deconfinement': CPOD 2009, BNL, USA, CPOD 2010, Dubna, Russia; CPOD 2011, Wuhan, China; CPOD 2013, Berkeley, USA.

Organizing Committee:

Lattice 06, Tucson, 2006; Lattice 94, Bielefeld 1994; Strong and Electroweak Matter 2006, BNL 2006; Critical Point and Onset of Deconfinement 2009, BNL 2009; Extreme QCD 10, Bad Honnef, Germany 2010

Coordination of research programs:

Coordinator of the interdisciplinary research project *Multiscale Phenomena and their Simulation on Massively Parallel Computers*, Center for Interdisciplinary Research, Bielefeld University Germany, 8/1996-12/1998
Coordinator of the European research network *Finite Temperature Phase Transitions in Particle Physics*, 12/1997 - 12/2001

Graduate and Postdoctoral Advisor: Prof. H. Satz, Bielefeld University

Graduate and Postdoctoral Advisees: P. Hegde (BNL), S. Datta (TIFR), H.-T. Ding (BNL), C. Schmidt (Bielefeld), W. Söldner (Regensburg),

Selected Publications: Frithjof Karsch

202 publications in refereed journals; total of 13500 citations (SPIRES)

- 1.) A. Bazavov, T. Bhattacharya, M. Cheng, N. H. Christ, C. DeTar, S. Ejiri, S. Gottlieb and R. Gupta, U.M. Heller, K. Huebner, C. Jung, F. Karsch, E. Laermann, L. Levkova, C. Miao, R.D. Mawhinney, P. Petreczky, C. Schmidt, R.A. Soltz, W. Soeldner, R. Sugar, D. Toussaint, P. Vranas [HotQCD Collaboration], Equation of state and QCD transition at finite temperature, *Phys. Rev. D* **80**, 014504 (2009) [arXiv:0903.4379 [hep-lat]] (252 citations).
- 2.) A. Bazavov, T. Bhattacharya, M. Cheng, C. DeTar, H. T. Ding, S. Gottlieb, R. Gupta and P. Hegde, U. M. Heller, F. Karsch, E. Laermann, L. Levkova, S. Mukherjee, P. Petreczky, C. Schmidt, R. A. Soltz, W. Soeldner, R. Sugar, D. Toussaint, W. Unger, P. Vranas [HotQCD Collaboration], The chiral and deconfinement aspects of the QCD transition, arXiv:1111.1710 [hep-lat] (4 citations).
- 3.) M. Cheng, N. H. Christ, M. Li, R. D. Mawhinney, D. Renfrew, P. Hegde, F. Karsch and M. Lin, R. D. Mawhinney, D. Renfrew, P. Vranas, The finite temperature QCD using 2 + 1 flavors of domain wall fermions at $N(t) = 8$, *Phys. Rev. D* **81**, 054510 (2010) [arXiv:0911.3450 [hep-lat]] (28 citations).
- 4.) C. R. Allton, S. Ejiri, S. J. Hands, O. Kaczmarek, F. Karsch, E. Laermann, C. Schmidt and L. Scorzato, The QCD thermal phase transition in the presence of a small chemical potential, *Phys. Rev. D* **66**, 074507 (2002) [hep-lat/0204010] (389 citations).
- 5.) C. R. Allton, M. Doring, S. Ejiri, S. J. Hands, O. Kaczmarek, F. Karsch, E. Laermann and K. Redlich, Thermodynamics of two flavor QCD to sixth order in quark chemical potential, *Phys. Rev. D* **71**, 054508 (2005) [hep-lat/0501030] (263 citations).
- 6.) M. Cheng, P. Hendge, C. Jung, F. Karsch, O. Kaczmarek, E. Laermann, R. D. Mawhinney and C. Miao, P. Petreczky, C. Schmidt, W. Soeldner, Baryon Number, Strangeness and Electric Charge Fluctuations in QCD at High Temperature, *Phys. Rev. D* **79**, 074505 (2009) [arXiv:0811.1006 [hep-lat]] (84 citations).
- 7.) O. Kaczmarek, F. Karsch, E. Laermann, C. Miao, S. Mukherjee, P. Petreczky, C. Schmidt and W. Soeldner, W. Unger, Phase boundary for the chiral transition in (2+1) -flavor QCD at small values of the chemical potential, *Phys. Rev. D* **83**, 014504 (2011) [arXiv:1011.3130 [hep-lat]] (26 citations).
- 8.) S. Datta, F. Karsch, P. Petreczky and I. Wetzorke, Behavior of charmonium systems after deconfinement, *Phys. Rev. D* **69**, 094507 (2004) [hep-lat/0312037] (300 citations)
- 9.) H. -T. Ding, A. Francis, O. Kaczmarek, F. Karsch, E. Laermann and W. Soeldner, Thermal dilepton rate and electrical conductivity: An analysis of vector current correlation functions in quenched lattice QCD, *Phys. Rev. D* **83**, 034504 (2011) [arXiv:1012.4963 [hep-lat]] (14 citations).
- 10.) G. Boyd, J. Engels, F. Karsch, E. Laermann, C. Legeland, M. Lutgemeier and B. Petersson, Thermodynamics of SU(3) lattice gauge theory, *Nucl. Phys. B* **469**, 419 (1996) [hep-lat/9602007] (636 citations)

Collaborators and Co-editors: A. Bazavov (BNL), P. Braun-Munzinger (GSI), T. Bhattacharya (Los Alamos), M. Cheng (Boston U.), N. H. Christ (Columbia U.), C. DeTar (Utah U.), H. -T. Ding (BNL), S. Ejiri (Niigata), J. Engels (Bielefeld U.), A. Francis (Mainz U.), B. Friman (GSI), R. Gupta (Los Alamos), P. Hegde (BNL), U.M. Heller (APS), K. Huebner, C. Jung (BNL), O. Kaczmarek (Bielefeld U.), D. Kharzeev (Stony Brook), M. Kitazawa (Osaka U.), E. Laermann (Bielefeld U.), L. Levkova (Utah U.), C. Miao (Mainz U.), R.D. Mawhinney (Columbia U.), S. Mukherjee (BNL), C. Pica (Southern Denmark U.), P. Petreczky (BNL), K. Redlich (Wroclaw U.), H. Satz (Bielefeld U.), B.-J. Schaefer (Giessen U.), C. Schmidt (Bielefeld U.), S. Scheredin (Bielefeld U.), V. Skokov (BNL), R.A. Soltz (LLNL), W. Soeldner (Regensburg U.), R. Sugar (Santa Barbara), K. Tuchin (Iowa State U.), D. Toussaint (Tucson), W. Unger (ETH Zürich), M. Wagner (Bielefeld U.), J. Wambach (Darmstadt U.)

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Professional Preparation

Ph.D. Theoretical Physics, Cornell University, 1969, (advisor, Hans A. Bethe)
B.S. Engineering Sciences, Purdue University, 1965, With Highest Distinction

Appointments

1991 - present, William A. Coolidge Professor of Physics, MIT
1989 - 1998, Director, Center for Theoretical Physics, MIT
1988 - 1998, Head, Theoretical Division of Department of Physics, MIT
1979 - present, Professor of Physics, MIT
1972 - 1979, Associate Professor of Physics, MIT
1971 - 1972, Assistant Professor of Physics, MIT
1970 - 1971, Visiting Assistant Professor of Physics, MIT
1970 - 1971, Postdoctoral Fellow, Niels Bohr Institute, Copenhagen, Denmark

Publications relevant to this proposal

- 1.) C. Alexandrou, E. B. Gregory, T. Korzec, G. Koutsou, J. W. Negele, T. Sato and A. Tsapalis, “The $\Delta(1232)$ axial charge and form factors from lattice QCD,” Phys. Rev. Lett. **107**, 141601 (2011) [arXiv:1106.6000 [hep-lat]].
- 2.) C. Alexandrou, G. Koutsou, J. W. Negele, Y. Proestos, A. Tsapalis, “Nucleon to Delta transition form factors with $N_F = 2 + 1$ domain wall fermions,” Phys. Rev. **D83**, 014501 (2011). [arXiv:1011.3233 [hep-lat]].
- 3.) B. U. Musch, P. Hagler, J. W. Negele, A. Schafer, “Exploring quark transverse momentum distributions with lattice QCD,” Phys. Rev. **D83**, 094507 (2011). [arXiv:1011.1213 [hep-lat]].
- 4.) J.D. Bratt, R.G. Edwards, M. Engelhardt, Ph. Hagler, H.W. Lin, M.F. Lin, H.B. Meyer, B. Musch, J.W. Negele, K. Orginos, A.V. Pochinsky, M. Procura, D.G. Richards, W. Schroers, and S.N. Syritsyn [LHPC Collaboration], “Nucleon structure from mixed action calculations using 2+1 flavors of asqtad sea and domain wall valence fermions,” Phys. Rev. **D82**, 094502 (2010). [arXiv:1001.3620 [hep-lat]].
- 5.) S. N. Syritsyn, J. D. Bratt, M. F. Lin, H. B. Meyer, J. W. Negele, A. V. Pochinsky, M. Procura, M. Engelhardt *et al.*, “Nucleon Electromagnetic Form Factors from Lattice QCD using 2+1 Flavor Domain Wall Fermions on Fine Lattices and Chiral Perturbation Theory,” Phys. Rev. **D81**, 034507 (2010). [arXiv:0907.4194 [hep-lat]].
- 6.) C. Alexandrou, T. Korzec, G. Koutsou, C. Lorce, J. W. Negele, V. Pascalutsa, A. Tsapalis, M. Vanderhaeghen, “Quark transverse charge densities in the Delta(1232) from lattice QCD,” Nucl. Phys. **A825**, 115-144 (2009). [arXiv:0901.3457 [hep-ph]].
- 7.) A. Walker-Loud, H. -W. Lin, D. G. Richards, R. G. Edwards, M. Engelhardt, G. T. Fleming, P. Hagler and B. Musch, M.F. Lin, H. Meyer, J.W. Negele, A.V. Pochinsky, M. Procura, S. Syritsyn, C.J. Morningstar, K. Orginos, D.B. Renner, and W. Schroers, “Light hadron spectroscopy using domain wall valence quarks on an Asqtad sea,” Phys. Rev. D **79**, 054502 (2009) [arXiv:0806.4549 [hep-lat]].

- 8.) Ph. Hägler, W. Schroers, J. Bratt, J.W. Negele, A.V. Pochinsky, R.G. Edwards and D.G. Richards, M. Engelhardt, G.T. Fleming, B. Musch, K. Orginos, and D.B. Renner [LHPC Collaboration], “Nucleon Generalized Parton Distributions from Full Lattice QCD,” Phys. Rev. **D77**, 094502 (2008) [arXiv:0705.4295 [hep-lat]].
- 9.) H. B. Meyer and J. W. Negele, “Gluon contributions to the pion mass and light cone momentum fraction,” Phys. Rev. D **77**, 037501 (2008) [arXiv:0707.3225 [hep-lat]].
- 10.) R.G. Edwards, G.T. Fleming, Ph. Hägler, J.W. Negele, K. Orginos, A.V. Pochinsky, D.B. Renner, D.G. Richards, and W. Schroers [LHPC Collaboration], “The Nucleon axial charge in full lattice QCD,” Phys. Rev. Lett. **96**, 052001 (2006). [hep-lat/0510062].

Synergistic Activities

National Committees

USQCD Executive Committee 1999-present, Program Committee, 1999 – 2008
 DOE Advanced Scientific Computing Advisory Committee (ASCAC), 2009 – present
 Executive Committee, APS Topical Group on Computational Physics, 1990 – 91
 Chair, American Physical Society Division of Computational Physics, 1992
 National Advisory Committee, Institute for Nuclear Theory, Seattle, 1990 – 94,
 Chair 1992 – 94

Conference Organization

Chair, Nuclear Structure Gordon Research Conference, 1982
 Co-Organizer, Nuclear Many-Body Theory Program, ITP Santa Barbara, 1982
 Co-Organizer, NATO Advanced Study Institute, “Hadrons and Hadronic Matter”, Cargese, 1989
 Co-Organizer, Seattle ITP programs “Phenomenology and Lattice QCD”, 1993 and “Exploration of Hadron Structure and Spectroscopy using Lattice QCD”, 2006
 Chair of Organizing Committee, Lattice 2002

Collaborators and Co-editors

C. Alexandrou (U. Cyprus), Douglas Beck, Univ. Illinois: R. Brower (Boston U.), J. Bratt (Huntington Coll.), M Di Pierro (De Paul U.), J. Green (MIT), E Gregory (U. Cyprus), R. G. Edwards (Jefferson Lab), M. Engelhardt (U. New Mexico), P. Faccioli (U. Trento), G.T. Fleming (Yale U.), Ph. Hägler (Munich), T. R. Hemmert (Regensburg), O. Jahn (MIT), E. Jenkins (UCSD), T Korzek (Humboldt U.), G Koutsou (Cyprus Institute), H. W. Lin (U. Washington), M.-F Lin (Yale University), C. Lorce (Gutenberg U.), A. Manohar (UCSD), H. Meyer (U Mainz), B. Musch (Jefferson Lab), C. Morningstar (Carnegie Mellon U), K. Orginos (William and Mary), V. Pascalutsa (Gutenberg U.), A. Pochinsky (MIT), M. Procura (Munich), Y. Proestos (Cyprus Institute), D. B. Renner (Jefferson Lab), D. G. Richards (Jefferson Lab), T Sato (Osaka U), A. Schafer (Regensburg), W. Schroers (DEAY), D. Sigaev (Goldman Sachs), S. Syritsyn (LBL), M. Thies, (U. Erlangen), A. Tsapalis (U. Athens), A. Walker-Loud (William and Mary), M Vanderhaeghen (U. Mainz)

Graduate students and postdoctoral associates

J. Bratt (Huntington Coll.), J. Green (MIT), O. Jahn (MIT), F.-J. Jiang (National Taiwan U.), M.-F Lin (Yale University), H. Meyer (U Mainz), M. Procura (Munich), D. Sigaev (Goldman Sachs), B. C. Tiburzi (City College of New York), S. Syritsyn (LBL)

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Education and Training

Ph.D. Theoretical Physics, University of Cambridge, 1984.
B.A. Mathematics, University of Cambridge, First Class Honours, 1980.

Research and Professional Experience

2009-present, JLab, Senior Staff Scientist; Acting Associate Director for Theoretical and Computational Physics 10/2009-9/2010
2002-2009, JLab, Staff Scientist
1999-2002, JLab/Old Dominion University joint Assistant Professor
1993-1999, University of Edinburgh, PPARC Advanced Fellow
1988-1993, University of Edinburgh, Postdoctoral Fellow
1986-1988, Argonne National Laboratory, Postdoctoral Fellow
1984-1986, Southampton University, Postdoctoral Fellow

Ten Publications Relevant to This Proposal

- J. J. Dudek, R. G. Edwards, B. Joo, M. J. Peardon, D. G. Richards, C. E. Thomas, “Isoscalar meson spectroscopy from lattice QCD,” Phys. Rev. **D83**, 111502 (2011). [arXiv:1102.4299].
- R. G. Edwards, J. J. Dudek, D. G. Richards, S. J. Wallace, “Excited state baryon spectroscopy from lattice QCD,” Phys. Rev. **D84**, 074508 (2011). [arXiv:1104.5152].
- J. J. Dudek, R. G. Edwards, M. J. Peardon, D. G. Richards, C. E. Thomas, “Highly excited and exotic meson spectrum from dynamical lattice QCD,” Phys. Rev. Lett. **103**, 262001 (2009). [arXiv:0909.0200].
- M. Peardon, J. Bulava, J. Foley, C. Morningstar, J. Dudek, R.G. Edwards, B. Joo, H.-W. Lin, D.G. Richards, K. Jimmy Juge, “A Novel quark-field creation operator construction for hadronic physics in lattice QCD,” Phys. Rev. D **80**, 054506 (2009) [arXiv:0905.2160 [hep-lat]].
- H.-W. Lin, S.D. Cohen, J. Dudek, R.G. Edwards, B. Joo, D.G. Richards, J. Bulava, J. Foley, C. Morningstar, E. Engelson, S. Wallace, K. Jimmy Juge, N. Mathur, M. Peardon, S.M. Ryan, “First results from 2+1 dynamical quark flavors on an anisotropic lattice: Light-hadron spectroscopy and setting the strange-quark mass,” Phys. Rev. D **79** (2009) 034502 [arXiv:0810.3588 [hep-lat]].
- Ph. Hägler, W. Schroers, J. Bratt, J.W. Negele, A.V. Pochinsky, R.G. Edwards, D.G. Richards, M. Engelhardt, G.T. Fleming, B. Musch, K. Orginos, D.B. Renner, “Nucleon Generalized Parton Distributions from Full Lattice QCD”, Phys. Rev. D **77**, 094502 (2008) [arXiv:0705.4295].
- A. Walker-Loud, H.-W. Lin, D.G. Richards, R.G. Edwards, M. Engelhardt, G.T. Fleming, Ph. Hagler, B. Musch, M.F. Lin, H. Meyer, J.W. Negele, A.V. Pochinsky, M. Procura, S. Syritsyn, C.J. Morningstar, K. Orginos, D.B. Renner, W. Schroers, “Light hadron spectroscopy using domain wall valence quarks on an Asqtad sea”, Phys. Rev. D **79**, 054502 (2009) [arXiv:0806.4549].
- J. J. Dudek, R. G. Edwards and D. G. Richards, “Radiative transitions in charmonium from lattice QCD,” Phys. Rev. D **73**, 074507 (2006) [hep-ph/0601137].

- R.G. Edwards, G.T. Fleming, Ph. Hagler, J.W. Negele, K. Orginos, A.V. Pochinsky, D.B. Renner, D.G. Richards, W. Schroers, “The Nucleon axial charge in full lattice QCD,” Phys. Rev. Lett. **96** (2006) 052001 [hep-lat/0510062].
- C. R. Allton, C.T. Sachrajda, R.M. Baxter, S.P. Booth, K.C. Bowler, S. Collins, D.S. Henty, R.D. Kenway, B.J. Pendleton, D.G. Richards, J.N. Simone, A.D. Simpson, B.E. Wilkes, C. Michael, Christopher, “Gauge invariant smearing and matrix correlators using Wilson Phys. Rev. D **47** (1993) 5128 [hep-lat/9303009].

Synergistic Activities

- Member, USQCD Executive Committee, 2004-present
- Local Organizing Committees: Lattice 2008, College of William and Mary, July 2008; MENU 2010, College of William and Mary, June 2010; NStar 2011, Jefferson Laboratory, May 2011.
- Co-organizer of INT Program “Exploration of Hadron Structure and Spectroscopy using Lattice QCD, March 6 - May 26, 2006
- Co-convenor, panel on Cold QCD, Extreme Scale Computing Workshop “Forefront Questions in Nuclear Science and the Role of High-Performance Computing”, Washington DC, January 26-28, 2009

Collaborators and Co-editors

D. Armstrong (WM), J. Bratt (MIT), J. Bulava (DESY), V. Burkert (JLab), J-P. Chen (JLab), S. Cohen (UW), W. Detmold (WM), J. Dudek (JLAB), R.G. Edwards (JLAB), M. Engelhardt (NMSU), E. Engleson (UMD), G.T. Fleming (Yale), J. Foley (Utah), Ph. Hagler (Mainz), M. Jones (JLab), B. Joo (JLAB), J. Juge (Univ. Pacific), H-W Lin (Washington), M.F. Lin (Yale), P.B. Mackenzie (FNAL), N. Mathur (Tata Institute), H. Meyer (Regensburg), W. Melnitchouk (JLab), C. Morningstar (CMU), B. Musch (JLab), J.W. Negele (MIT), K. Orginos (JLAB), M. Peardon (TCD), M. Pennington (JLab), A. Pochinsky (MIT), M. Procura (MIT), D.B. Renner (JLab), S. Ryan (TCD), W. Schroers (NuAS, Berlin), S. Syritsyn (LBNL), A. Tsapalis (Cyprus), A. Thomas (Adelaide), C. Thomas (JLab), A. Walker-Loud (LBNL), S. Wallace (UMD), W. Watson (JLab), R. Wong (UCSD).

Graduate Advisors and Postdoctoral Sponsors

Peter Landshoff (Cambridge), James Stirling (Cambridge), Chris Sachrajda (Southampton), Dennis Sivers (Portland Physics Institute), Ken Bowler (Edinburgh).

Thesis Advisor and Postgraduate-Scholar sponsor

Chris Scott (Southampton, 1985)

Chris Maynard, Paul Rowland (Edinburgh, 1999)

Katia Mastropas (College of William and Mary, current).

Total graduate students advised: 4. Total post-doctoral scholars sponsored: 5.

Curriculum Vitae
MARTIN J. SAVAGE

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Professional Preparation

Ph.D., Physics, Caltech, 1990 (Advisor, Mark B. Wise)
M.Sc., Physics, University of Auckland, 1985
B.Sc., Physics and Mathematics, University of Auckland, 1984

Appointments

2003-present, University of Washington, Professor
1999-2003, University of Washington, Associate Professor
1996-1999, University of Washington, Assistant Professor
1993-1996, Carnegie Mellon University, Assistant Professor
1991-1993, University of California, San Diego, Postdoctoral Fellow
1990-1991, Rutgers University, Postdoctoral Fellow

Visiting Positions

MIT, 8/2004-1/2005
Caltech, 1/2005-7/2005

Honors and Awards

Fellow, American Physical Society, 2002
DOE OJI, 1995-1997
SSC Fellow, 1992-1993
New Zealand Post Graduate Scholar, 1985-1988
Commonwealth Scholar, 1985

Outside Activities

Associate Editor of *Physical Review C*, 2011-present
Member, USQCD Scientific Program Committee, 2009-present.
Member, Organizing Committee, SciDAC 2009.
International Advisory Committee, International Symposia on Lattice Field Theory: Lattice 08, Williamsburg, 2008.
Co-Chair of the Grand Challenges Workshop *Forefront Questions in Nuclear Science and the Role of High Performance Computing*, January 26-28 2009.
Associate Editor of *Nuclear Physics A*, 1999-2010.
Numerous Review Committees.
Numerous INT programs and Workshops.
Numerous International Advisory Committees.
Co-leader of b-baryon working group for the C0-detector at Fermilab, 1996.

Selected Publications
MARTIN J. SAVAGE

167 publications in refereed journals; total of 7531 citations (SPIRES)

- 1.) Nucleon-nucleon scattering from fully-dynamical lattice QCD. S.R. Beane, P.F. Bedaque, K. Orginos, M.J. Savage, [NPLQCD Collaboration]. Published in Phys.Rev.Lett.97 (2006) 012001, e-Print: hep-lat/0602010
- 2.) Evidence for a Bound H-dibaryon from Lattice QCD. S.R. Beane, E. Chang, W. Detmold, B. Joo, H.W. Lin, T.C. Luu, K. Orginos, A. Parreno, M.J. Savage, A. Torok, A. Walker-Loud, [NPLQCD Collaboration], Published in Phys.Rev.Lett. 106 (2011) 162001, e-Print: arXiv:1012.3812 [hep-lat]
- 3.) A method to study complex systems of mesons in Lattice QCD. W. Detmold and M. J. Savage, Published in Phys.Rev. D82 (2010) 014511, e-Print: arXiv:1001.2768 [hep-lat]
- 4.) High Statistics Analysis using Anisotropic Clover Lattices: (III) Baryon-Baryon Interactions. S. R. Beane, W. Detmold, H.-W. Lin, T. C. Luu, K. Orginos, M. J. Savage, A. Torok, A. Walker-Loud [NPLQCD Collaboration], Published in Phys.Rev. D81 (2010) 054505 e-Print: arXiv:0912.4243 [hep-lat]
- 5.) High Statistics Analysis using Anisotropic Clover Lattices. II. Three-Baryon Systems. S. R. Beane, W. Detmold, T. C. Luu, K. Orginos, A. Parreno, M. J. Savage, A. Torok, A. Walker-Loud [NPLQCD Collaboration], Published in Phys.Rev. D80 (2009) 074501 e-Print: arXiv:0905.0466 [hep-lat]
- 6.) Kaon Condensation with Lattice QCD. W. Detmold, K. Orginos, M. J. Savage, A. Walker-Loud [NPLQCD Collaboration], Published in Phys.Rev. D78 (2008) 054514 e-Print: arXiv:0807.1856 [hep-lat]
- 7.) Multi-Pion Systems in Lattice QCD and the Three-Pion Interaction. S. R. Beane, W. Detmold, T. C. Luu, K. Orginos, M. J. Savage, A. Torok [NPLQCD Collaboration], Published in Phys.Rev.Lett. 100 (2008) 082004 e-Print: arXiv:0710.1827 [hep-lat]
- 8.) Precise Determination of the $I = 2 \pi\pi$ Scattering Length from Mixed-Action Lattice QCD. S. R. Beane, T. C. Luu, K. Orginos, A. Parreno, M. J. Savage, A. Torok, A. Walker-Loud [NPLQCD Collaboration], Published in Phys.Rev. D77 (2008) 014505 e-Print: arXiv:0706.3026 [hep-lat]
- 9.) BB Potentials in Quenched Lattice QCD. W. Detmold, K. Orginos, M. J. Savage [NPLQCD Collaboration], Published in Phys.Rev. D76 (2007) 114503 e-Print: hep-lat/0703009 [HEP-LAT]
- 10.) Hyperon-Nucleon Scattering from Fully-Dynamical Lattice QCD. S. R. Beane, P. F. Bedaque, T. C. Luu, K. Orginos, E. Pallante, A. Parreno, M. J. Savage [NPLQCD Collaboration], Published in Nucl.Phys. A794 (2007) 62-72 e-Print: hep-lat/0612026

Collaborators

S. Beane (University of New Hampshire), W. Detmold (College of William and Mary), T.C. Luu (LLNL), K. Orginos (College of William and Mary), A. Parreno (University of Barcelona), E. Chang (University of Barcelona), A. Walker-Loud (LBNL), H.-W. Lin (UW), S. Cohen (UW), Z. Davoudi (UW), R. Briceno (UW), D. B. Kaplan (INT), M.B. Wise (Caltech), A. Manohar (UCSD), M. Luke (University of Toronto), E. Jenkins (UCSD), G. Rupak (Mississippi State) J.-W. Chen (University of Taiwan)

Curriculum Vitae ANDREAS STATHOPOULOS

Contact Information

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Education

Ph.D. Computer Science, Vanderbilt University, Nashville, TN, 1995
M.S. Computer Science: Vanderbilt University, Nashville, TN, 1991
B.S. Mathematics: University of Athens, Athens, Greece, 1989

Appointments

2008–present, Professor, Computer Science Department, College of William and Mary
2002–2008, Associate Professor, Computer Science Department, College of William and Mary
1997–2002, Assistant Professor, Computer Science Department, College of William and Mary
1995–1997, NSF Postdoctoral Research Associate, Computer Science Department, University of Minnesota

Visiting Positions:

2010–2011, Visiting Scientist, IBM Research, Zurich Lab, Switzerland
1993, Summer Visiting Researcher, Army High Performance Computing Research Center, Minneapolis

Synergetic Activities

- Co-developed Incremental-EigCG which finds and deflates eigenvectors while solving linear systems with multiple right hand sides. The code is available in the DOE's QCD package Chroma.
- Developed PRIMME, PReconditioned Iterative MultiMethod Eigensolver, with Ph.D. student James McCombs. This is a comprehensive, flexible, efficient and robust software for Hermitian eigenvalue problems. As of January 2006, PRIMME is available at www.cs.wm.edu/~andreas/software.
- Developed DVDSON, a Davidson eigenvalue code, which has been used extensively in the atomic physics community, throughout the US and Europe. In addition, it has been used as kernel application for studying I/O performance at CMU and other research groups.
- Member of the Computational Sciences Cluster at William and Mary. Helped develop the curriculum requirements for a campus wide, computational science program. Also, helped develop several Computer Science graduate courses in support of this curriculum.
- Editorial board of ISRN Applied Mathematics Journal
- Co-organizer for workshop "Building Bridges between Computational Mathematics and Electronic Structure", UIUC, June 16–17, 2008
- Co-organizer of several minisymposia at various conferences.

Graduate Advisor: Professor Charlotte F. Fischer, Vanderbilt University.

Postdoctoral Advisor: Professor Yousef Saad, University of Minnesota.

Graduate Advisees: Dr. James R. McCombs, Dr. Richard Mills (currently scientist at ORNL).

Postdoctoral Advisee: Dr. Abdou M. Abdel-Rehim.

Selected Publications: Andreas Stathopoulos

1. A. Stathopoulos and K. Orginos, “Computing and deflating eigenvalues while solving multiple right hand side linear systems in Quantum Chromodynamics”, *SIAM Journal on Scientific Computing*, Vol. 32, No. 1, (2010), 439–462.
2. A. Stathopoulos and J. R. McCombs, “PRIMME: PREconditioned Iterative MultiMethod Eigensolver: Methods and software description”, *ACM Transactions on Mathematical Software*, Vol. 37, No. 2, (2010), 21:1–21:30.
3. A. M. Abdel-Rehim, K. Orginos and A. Stathopoulos, “Extending the eigCG algorithm to non-symmetric linear systems with multiple right-hand sides”, in proceedings of “The XXVII International Symposium on Lattice Field Theory - LAT2009”, PoS (LATTICE 09) 036.
4. A. Stathopoulos, “Nearly optimal preconditioned methods for hermitian eigenproblems under limited memory. Part I: Seeking one eigenvalue”, *SIAM Journal on Scientific Computing*, Vol. 29, No. 2, (2007), 481–514.
5. A. Stathopoulos and J. R. McCombs, “Nearly optimal preconditioned methods for Hermitian eigenproblems under limited memory. Part II: Seeking many eigenvalues”, *SIAM Journal on Scientific Computing*, Vol. 29, No. 5, (2007), 2162–2188.
6. J. R. McCombs and A. Stathopoulos, “Iterative Validation of Eigensolvers: A Scheme for Improving the Reliability of Hermitian Eigenvalue Solvers”, *SIAM Journal on Scientific Computing*, Vol. 28, No. 6, (2006), 2337–2358.
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Collaborators: C. Bekas (IBM Research), James R. Chelikowsky (U. Texas), D. Nikolopoulos (U. Crete), A. Heindl (U. Erlangen), K. Orginos (College of W&M), A. Rehim (College of W&M), E. Smirni (College of W&M), C. Yue (W&M), Q. Zhang (Microsoft).

5 Description of Facilities and Resources

The research on software development for lattice QCD simulations in Nuclear Physics that is proposed here will largely benefit from the infrastructure of the participating institutions, in particular the three DOE laboratories, BNL, TJNAF and LLNL. The project is embedded in the activities of the national lattice gauge theory consortium – USQCD. Through this the participating institutions have access to the computer hardware operated by USQCD at BNL, TJNAF and FNAL. Furthermore, as members of USQCD the participating teams also have access to computing resources which USQCD receives through an INCITE grant. This grant provides access to the national computing centers at Argonne (ALCF) and Oak Ridge (NCCS).

In detail, the participating teams currently have granted computing time on the following computers:

- At TJNAF USQCD operates a 144 node cluster equipped with 480 NVIDIA GPUs. This includes 128 Fermi Tesla (NVIDIA C2050) cards with error correction. This cluster will be extended in 2012.
- At FNAL USQCD operates a 421 node cluster equipped with 2 GHz Quad CPU Eight Core Opteron and an older 856 node cluster equipped with 2.1 GHz Dual CPU Quad Core Opteron. The FNAL installation will be extended with a 65 node cluster equipped with 2 NVIDIA C2050 GPUs per node.
- At BNL three prototype racks of BlueGene/Q are currently being installed which will be operational early in 2012. One rack is owned by RIKEN/BNL the other two racks are owned by BNL. USQCD has been granted access to the latter for software development projects for upcoming BlueGene/Q installations at ALCF and at LLNL.
- BNL operates a 18432 node BlueGene/L (18 racks) for the New York Center for Computational Sciences (NYCCS) and a 2048 node BlueGene/P (2 racks). On these machines about half of the available CPU time is devoted to lattice QCD applications.
- MIT has a 2048 processor BlueGene/L rack and a 130 Terabyte storage system dedicated to lattice QCD software development and lattice QCD physics research. This facility was funded by ASCR and NNSA with operations support by MIT.
- USQCD holds an INCITE grant which in 2012 will provide 30 M core-hours on the BlueGene/P at ALCF and 20 M core-hours on the Cray XT4 and XT 5 (Jaguar) at NCCS.
- An Early Science Grant of USQCD provides computing time on the BlueGene/P at ALCF which is dedicated to the algorithm development and tuning of future applications on the BlueGene/Q. This grant also will provide time on the upcoming new BlueGene/Q at ALCF.
- Through collaborations with colleagues at LLNL (HotQCD collaboration, LPQCD collaboration) we have access to the BlueGene/P at LLNL (ubgl) and will be able to work also on the upcoming BlueGene/Q installation.
- At W&M, Prof. Orginos has built and maintains a cluster with Pentium 2.5Ghz quad core (Pernyn) dual socket compute nodes for a total of 864 compute cores. This cluster uses Infiniband interconnect and has about 75 terabytes of disk space. It delivers about 1TFlops of sustained performance for QCD applications using the SciDAC QCD software stack. This machine is shared with a group of high energy physics experimentalists. It was acquired with funds from NSF Major Research Instrumentation grant, funds from the College of William and Mary vice dean of research and a DOE OJI grant that Orginos received. We also have an 8 node test system equipped with 32 Nvidia GPUs and an Infiniband interconnect that enables us to develop codes for such heterogeneous architectures. The SciDAC lattice QCD software Chroma is optimized for such machines as well as the QUDA Lattice QCD optimized software for GPU enabled clusters are installed on our systems. Prof. Orginos, as a senior staff member

of the JLab theory group, has access also to the JLab lattice QCD computers, where larger scale experiments can be performed. Finally, Prof. Orginos has access to significant allocations on NSF (XSEDE), DoE national supercomputing centers, and machines operated under the auspices of the USQCD LQCD infrastructure project.

In addition, the W&M PIs have access to SciClone, a heterogeneous cluster of six clusters of workstations (<http://www.compsci.wm.edu/SciClone/>), which has been funded by SUN and by an NSF Major Research Instrumentation grant. The facility has peak a performance of 700 GFlops.

- At UNC/RENCI there exists hardware for code development and tuning. At present this is a cluster of 128 node of Dell M610 blades (2 x 2.8 GHz Intel xeon 5560) and four R710 Nehalem nodes, each with four Nvidia S1070s.

The SUPER group maintains a set of stand alone development systems running experimental performance and energy monitoring. Currently, these are:

- One Dell R910 with four Nehalem EX7560 chips and 128 GB of memory.
- A “white box” dual-Westmere (X5670, 2.93GHz, 6 core) chips, 24 GB of memory, four Nvidia M2050 Tesla accelerators, and one Nvidia GeForce 480 accelerator.
- One Dell M905 quad socket AMD Istanbul (8425 HE, 2.1 GHz, 6 cores) system with 32 GB of memory.

Through collaborations we furthermore make use of computing resources accessible to our colleagues world wide.

8.2 Letter from NVIDIA

On the next page we reproduce a letter from Dr. David Luebke, Director of Research at NVIDIA Corporation, to Dr. Paul Mackenzie, the Chair of the USQCD Executive Committee, expressing his companys commitment to work with USQCD on the GPU codes discussed in this proposal. Dr. Luebke sets out the joint goals and milestones of NVIDIA and USQCD for this work, and the resources that NVIDIA will contribute to this effort.



December 6, 2012

Paul Mackenzie, Ph.D.
Theoretical Physics Department
Fermilab
MS 106
P.O. Box 500
Batavia, IL 60510 USA

Dear Paul,

On behalf of NVIDIA Corporation, I'm pleased to voice our enthusiastic support for the USQCD collaboration's SciDAC-3 proposals.

As you know, NVIDIA and the LQCD community have had a close but informal collaboration dating back as far as 2006 when the physics community first began researching the use of commodity GPUs for QCD. Since that time the community has created a rich set of open source software assets (e.g. the QUDA library¹) and an effective software framework for the international community to build application suites that exploit GPU computing (including Chroma, MILC, and CPS).

Although the USQCD community has already achieved a great deal of groundbreaking success using GPUs, we have clearly only scratched the surface. Far greater opportunities to exploit the potential of GPUs lie ahead, with vast implications for research into the fundamental nature of matter. Furthermore, NVIDIA anticipates that the lessons learned in numerical algorithms, software infrastructure, and hardware design, will benefit not only the LQCD community, but the greater scientific community as well.

¹ <http://lattice.github.com/quda>

Goals

The collaboration between NVIDIA and USQCD will have a number of goals:

1. World-class sustained performance for gauge generation on the order of hundreds of TFLOP/s, scaling to the order of thousands of GPUs.
2. World-class efficiency for the analysis of gauge configurations on the order of tens of TFLOP/s, scaling to the order of hundreds of GPUs.
3. State-of-the-art multigrid-based Dirac inverters that run efficiently on single and multi GPU systems.
4. Complete implementation of GPU support in a domain specific language (e.g. QDP++)
5. Add multi-GPU support for additional fermion formulations, such as domain-wall fermions (DWF).
6. A roadmap for future GPU hardware and software that continues to address the goals of the QCD community.
7. A roadmap for a GPU programming model that continues to address the goals of the QCD community.

Proposed Milestones

Vast GPU installations are becoming increasingly common in NSF and DOE leadership class facilities, notably the Titan system at Oak Ridge National Laboratory, and more recently the Blue Waters system at the National Center for Supercomputing Applications (NCSA). The proposed collaboration between NVIDIA and USQCD should strive to be prepared to exploit these systems as soon as they become available.

NVIDIA and USQCD should target the following high-level milestones:

- 2012 – Refine domain-decomposition algorithms in QUDA & Chroma
- 2012 – Improve scaling through more efficient use of shared memory
- 2012 – Demonstrate Lattice ensemble generation (e.g. full Hybrid Monte Carlo) on GPUs in MILC
- 2013 – Demonstrate adaptive multigrid solver in Chroma ($O(10)$ -fold performance improvement over current QUDA solvers)
- 2013 – Demonstrate adaptive multigrid combined with hybrid Monte Carlo

Resources

NVIDIA is extremely pleased to have the world's two foremost experts in using GPUs for QCD on staff, Dr. Mike Clark and Dr. Ron Babich.

Mike Clark will focus the majority of his time in the near term to supporting the USQCD community to develop software assets that exploit GPUs. He will also work closely with the community to disseminate skills and practical lessons learned so that the community can develop a larger pool of capable resources for this collaboration.

Ron Babich will be responsible for leveraging the lessons learned during this collaboration to guide the design of next-generation GPU architectures from NVIDIA.

Jonathan Cohen manages the Emerging Applications group, an applied research group in GPU computing. Jonathan will support Mike as they explore refinements to domain decomposition algorithms, adaptive multigrid solvers, and scalable hybrid Monte Carlo methods for gauge generation. There are opportunities for adding additional members to the Emerging Applications team, depending on needs, schedule, and suitable candidates.

Finally, Jerry Chen manages NVIDIA's strategic partnership with the QCD community. Jerry will provide program management and strategic alignment between this collaboration and NVIDIA's broader organization.

We look forward to the opportunity to extend our collaboration with the QCD community. Please do not hesitate to contact me with any questions.

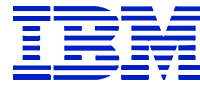
Sincerely,



David Luebke, Ph.D.
NVIDIA Distinguished Inventor
Director of Research
NVIDIA Corporation
dluebke@nvidia.com

8.3 Letter from IBM

On the next page we reproduce a letter from Dr. George Chiu, Senior Manager, Advanced Server Systems, IBM, to Paul Mackenzie, the Chair of the USQCD Executive Committee, expressing his companys plans to continue to work with members of USQCD on the optimization of USQCD codes to run efficiently on the Blue Gene/Q, and on the development of new algorithms that will more effectively exploit this computer.



International Business Machines Corporation

*Thomas J. Watson Research Center
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914-945-2436*

December 19, 2011

Dr. Paul Mackenzie,
Chair, USQCD Executive Committee
Theoretical Physics Department, MS 106
Fermilab
P. O. Box 500
Batavia, IL 60510 USA

Dear Paul,

Lattice QCD (Quantum Chromodynamics) is an important target application for the Blue Gene Research Project at IBM and for future IBM high performance machines. This is both because of the exciting fundamental science discoveries and the challenges for software and hardware design that must be met to achieve high performance for lattice QCD.

The Blue Gene research group at the Watson Research Center plans to continue its fruitful, 10+ year collaboration with USQCD scientists and particularly the groups at Columbia and Edinburgh Universities and the Brookhaven National Laboratory. We expect to work closely together on many of the research topics addressed by this USQCD SciDAC proposal. This includes both the continued optimization of USQCD codes to run efficiently on the Blue Gene/Q architecture as well as the development of new algorithms which more effectively exploit the heterogeneous architectures built from powerful many-pipe floating point units, embedded in complex multi-thread, many-core nodes which are then replicated tens of thousands of times.

I and my colleagues at Watson look forward to working with those in USQCD on these critical challenges.

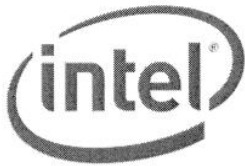
Yours truly,

George Chiu
IEEE Fellow,
Senior Manager, Advanced Server Systems, IBM

8.4 Letter from Intel

On the next page we reproduce a letter from Joseph Curley, Director of Marketing of the Technical Computing Group, Intel, expressing the desire of the Company to partner with USQCD on the development of LQCD software for emerging many-core architectures, and of the strategic value to Intel of such a partnership.

Intel Corporation
2200 Mission College Blvd.
Santa Clara, CA 95054



Chip Watson
Group Lead and Deputy CIO, High Performance Computing
Jefferson Lab
12000 Jefferson Avenue
Newport News, VA 23606

January 2, 2011

Dear Chip:

Intel Corporation is pleased to support JLAB and the USQCD grant proposals. We recognize that optimizing and scaling Lattice QCD on new technologies, tools and architectures as we move towards Exascale computing is a significant challenge for the USQCD collaboration team. Intel is excited to be considered such a strategic partner as you tackle Lattice QCD technical challenges through the USQCD collaboration team.

As a strategic investment for Intel, we have accepted JLAB into Intel's early software development program for Intel Many Integrated Core (Intel MIC) Architecture.

We look forward to the opportunity to proceed on collaborative interactions.

Sincerely,

A handwritten signature in dark ink, appearing to read "Joseph Curley". The signature is fluid and cursive, with a large, sweeping initial "J".

Joseph Curley,
Director of Marketing, Technical Computing Group
Intel Corporation