Hadron Structure at Light Quark Masses

March 13, 2006

Abstract

We propose the next step in a comprehensive set of full QCD calculations of hadron structure extending to the chiral regime of light quark masses, using a hybrid combination of chiral domain wall valence quarks and dynamical improved staggered sea quark configurations provided by the MILC collaboration. Physical observables will include moments of nucleon structure functions, nucleon electromagnetic and generalized form factors, the nucleon sigma term, the neutron electric dipole moment, nucleon density-density correlation functions, hadron wave functions, hadron quark distribution amplitudes, nucleon electric and magnetic polarizabilities, the nucleon to Delta transition form factors, pentaquark observables, spectroscopic quantities, and the pion electromagnetic and generalized form factors. Perturbative operator renormalization will be checked non-perturbatively in selected cases. Based on experience during the past year, additional calculations are proposed at lattice spacing $a = 0.125$ fm using lattices with $\frac{m_l}{m_s} = 0.6, 0.4, 0.2, 0.14, \text{ and } 0.1$ to improve statistics and to include more observables. High statistics calculations are proposed at $a = 0.09$ fm with $\frac{m_l}{m_s} = 1, 0.4, 0.2, \text{ and } 0.1$; and initial exploratory calculations of spectroscopic quantities are proposed for $a = 0.06$ fm at $\frac{m_l}{m_s} = 0.4$ and 0.2.

Total Request: 16.29 million processor hours in units of JLab 4g cluster

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1 Physics Goals

Our physics goals are twofold: 1) to quantitatively calculate the experimentally observable properties of the nucleon and other hadrons from first principles and, 2) to obtain insight into how QCD actually works in producing the rich and complex structure of hadrons.

The physical observables we propose to calculate include electric and magnetic form factors, generalized form factors, the spin structure of the nucleon, and the nucleon to delta transition form factors that lie at the core of the DOE experimental nuclear physics program at JLab and RHIC-spin. Beyond simply calculating numbers that agree with experiment, we also seek to answer basic questions concerning hadron structure. For example, what are the dominant components of the nucleon wave function? How does the total spin of the nucleon arise from the spin and orbital angular momentum of its quark and gluon constituents? How does the nucleon quark and gluon structure produce the observed scaling behavior of form factors? What is the transverse, as well as longitudinal structure of the nucleon light-cone wave function? As the quark mass is continuously decreased from a world in which the pion mass is 1 GeV to the physical world of light pions, how does the physics of the quark model and adiabatic flux tube potentials evolve into the physics of chiral symmetry breaking, where instantons, quark zero modes, and the associated pion cloud play a dominant role? What is the role of diquarks in conventional hadrons and exotic states such as pentaquarks? Essential aspects of the proposed research bear on these questions as well as quantitative comparison with experiment.

The dynamical QCD configurations with improved staggered quarks that the MILC collaboration is generating and making available to the national lattice QCD community provide us with an unprecedented opportunity to lead the exploration of the chiral regime of hadron structure. With last year’s allocation of US LQCD resources, utilizing the computational techniques and software our collaboration has developed during the last seven years, and using a hybrid strategy combining the chiral symmetry of domain wall valence quarks and the cost-effectiveness of improved staggered sea quarks, we have made an important entree into the chiral regime. The good news from this effort can be seen in our recent calculation\cite{1} of $g_A$ shown in Fig. 1, where we were the first to perform a chiral extrapolation in both mass and volume in the chiral regime and thereby calculated $g_A$ with 6.8% errors and in agreement with experiment.

However, there was also bad news from our effort last year. In our proposal last year, to try to be as accommodating as possible in using US LQCD resources, we agreed to run a major fraction of our allocation on the QCDOC, using estimated performance cited for domain wall fermions. In response to our request for 7.7 M processor hours on clusters, we agreed to an allocation of 3.5 M hours on clusters and 8.7 M hours on the QCDOC. Unfortunately, despite impressive efforts by members of our collaboration and by Columbia and BNL colleagues, due to the inefficiency of putting $28^3$ lattices on the QCDOC, the inefficiency of IO, and the inefficiency of the global sums required for calculating Fourier transforms, we obtained only a tiny fraction of the useful production we would have achieved on a cluster. Although this QCDOC effort led to some useful incremental developments of QCDOC software, it was a substantial setback for our physics objectives, and seriously delayed our schedule for publishing comprehensive hadron structure results during the window of
Figure 1: Nucleon axial charge $g_A$ as a function of the pion mass. The left plot compares our calculations including pion masses down to 350 MeV with all other existing calculations[2, 3], showing how much further into the chiral regime the MILC lattices have enabled us to calculate. The right plot shows how the present data extend sufficiently into the chiral regime to enable us to perform the first chiral extrapolation in both mass and volume. Squares and triangles denote lattice volumes $L^3$ with $L = 3.5$ and 2.5 fm respectively. The heavy solid line and shaded error band show the $\chi$PT fit to the finite volume data evaluated in the infinite volume limit, and the lines below it show the behavior of this chiral fit in boxes of finite volume $L^3$, as $L$ is reduced to 3.5, 2.5, and 1.6 fm respectively.

opportunity provided by the MILC lattices before a number of other groups have full QCD configurations in the same regime. In particular we were unable to complete calculations at pion masses of 300 MeV and 250 MeV or to calculate any observables at smaller lattice spacings.

An important lesson from Fig. 1 that strongly influences our proposal for the coming year is the growth of the statistical errors as the pion mass decreases. In order to obtain statistical errors providing effective constraints at pion masses of 350 MeV and below, we need to increase our statistics. Accordingly, as described in section 2 on Computational Strategy, we have developed and tested a new method which will enable us to utilize different space-time regions of the MILC lattices to obtain 8 times as many statistically independent measurements as previously at 5$\frac{1}{3}$ times the previous cost. Hence, the goal of our request this year is to complete our coordinated program of measurements of a broad range of physical observables at lattice spacings $a = 0.125$ fm and $a = 0.09$ fm with high statistics, and begin exploratory calculations at $a = 0.06$ fm. The multiple use of MILC lattices for calculation of both weak matrix elements and hadron structure is a significant success of the national SciDAC collaboration, and the requested allocation will provide an important opportunity for the US community to play a world-leading role in hadronic physics, and will enable us to fulfill the first phase of the commitment we made in the white paper [4] written to motivate nuclear physics support of the national lattice QCD effort.
Research Topics

A central feature of the LHPC hadron structure research program is the coordination of a large number of separate research projects to calculate a minimal common set of propagators and operator building blocks for all the required observables as efficiently as possible. In this proposal, we are focussing on the connected contributions relevant to flavor non-singlet observables, and comment on a separate proposal to investigate some disconnected diagrams below. Here we summarize the basic physical quantities of interest, with reference to figures in the appendix for readers who are interested in details. Section 4 presents a table of all the propagators and building blocks we propose, and Section 6 lists the project leaders for each research topic. Alternatively, one could imagine 14 separate proposals to address each of the 14 research topics, but we believe our single coordinated proposal has compelling advantages of economy and efficiency.

1. Moments of Structure Functions

Nucleon matrix elements of the twist-2 operators

\[ \langle PS|O^{\mu_1 \cdots \mu_n}|P'S'\rangle \quad \text{with} \quad O^{\mu_1 \cdots \mu_n} = \bar{\psi}\Gamma_i D^{\mu_1} \cdots i D^{\mu_n}\psi \]  

(1)

specify moments of the parton distributions and generalized parton distributions that have been measured extensively in high energy scattering experiments. Diagonal matrix elements, \( P = P' \), correspond to the moments of the light cone quark distribution, longitudinal spin distribution, and transversity distribution for \( \Gamma = \gamma_\mu, \gamma_5\gamma_\mu \), and \( \sigma_{\mu\nu} \) respectively, and will be calculated using the methodology we developed in Ref. [5]. As seen in Fig. 2, understanding the chiral behavior of the momentum fraction, \( \langle x \rangle \), corresponding to the first moment of the quark distribution, will be an important challenge. The zeroth moment of the spin dependent structure function, \( \langle 1 \rangle_{\Delta q} \), specifies the contribution of the quark spin to the total nucleon spin, and thus lies at the heart of the proton "spin crisis".

2. Form Factors and 3. Generalized Form Factors

Off-diagonal matrix elements of the twist-two operators given in Eq.(1) for \( P \neq P' \) yield a hierarchy of generalized form factors \( A_{nm}(t) \), \( B_{nm}(t) \), and \( C_n(t) \) for the spin independent case and \( \bar{A}_{nm}(t) \), \( \bar{B}_{nm}(t) \) for the spin-dependent case, where \( n - 1 \) equals the number of covariant derivatives. The form factors \( A_{10}(t) \) and \( B_{10}(t) \) correspond to the familiar electromagnetic form factors \( F_1 \) and \( F_2 \), which are of great interest as a result of the \( F_2 \) measurements and apparent early onset of scaling in recent JLab experiments, as well as strangeness form factors studied extensively at Bates and JLab. Figure 5 shows our preliminary calculations of the ratio \( F_2/F_1 \) which is in excellent qualitative agreement with the recent Jlab spin transfer measurements.

The total quark contribution to the nucleon spin is given by the extrapolation to \( t = 0 \) of \( A_{20}^{\text{ind}}(t) \) and \( B_{20}^{\text{ind}}(t) \) shown in Fig. 3. Combined with \( \langle 1 \rangle_{\Delta q} \), one can decompose the nucleon spin into the contributions from quark spin and orbital angular momentum, with the remainder arising from gluons. The right portion of Fig. 3 shows the results of our earlier calculations at large quark masses using SESAM configurations[7] and again, one expects a dramatic change in the physics as the quark spin contribution decreases from the quark model value toward the experimental value in the chiral limit.

Generalized parton distributions explore the quark distribution in three dimensions, \( q(x, \vec{r}_\perp) \),
as a function of the longitudinal momentum fraction $x$ and the transverse spatial coordinate $\vec{r}_\perp$. It turns out that several of the generalized form factors, which can be calculated on the lattice, measure moments of the Fourier transform of $q(x, \vec{r}_\perp)$:

$$A_{n0}(-\Delta_\perp^2) = \int d^2r_\perp \int dx \, x^{n-1} q(x, \vec{r}_\perp) \, e^{i\vec{r}_\perp \cdot \Delta_\perp}.$$  

Fig. 6 shows the striking variation in the slope, and therefore the rms radius, as the moment increases from $n = 1$ to $n = 3$ using our results with SESAM lattices[8], indicating how the transverse size of the nucleon decreases as the momentum fraction $\langle x \rangle$ increases, and Fig. 4 shows preliminary results with MILC lattices. With this methodology, we expect to measure the transverse structure of the nucleon in the chiral regime.

4. Nucleon Sigma Term Low-energy pion-nucleus scattering data allow one to determine the $\pi - N$ sigma term, $\sigma = \frac{1}{2}(m_u + m_d) \langle P|\bar{u}u + \bar{d}d|P \rangle$. Combined with chiral perturbation theory analysis of the baryon octet mass splitting, the $\sigma$ term implies that a large fraction of the nucleon mass arises from the strange quark mass term: $m_s \langle P|\bar{s}s|P \rangle$. A definitive lattice calculation will be quite valuable in clarifying whether this matrix element is indeed large, or if the experimental analysis is flawed.

5. Neutron Electric Dipole Moment The neutron electric dipole moment places a fundamental limit on the strong CP $\Theta$-angle, so it is of great interest to have a first principles calculation of it. Since the unambiguous topology associated with domain wall fermions enables a conceptually clean calculation and the MILC lattices provide unique access to light pion masses, this calculation has the potential for significant physics impact.

6. Nucleon Electric and Magnetic Polarizability Electric and magnetic intrinsic polarizabilities characterize the deformability of both charged and neutral hadrons in external fields and are important fundamental properties of particles. They are most directly measured by Compton scattering, and lattice calculations using external fields have the potential to equal or exceed current experimental precision.

7. Density-Density Correlation Functions and Hadron Wave Functions Density-density correlation functions[9] provide a useful tool to examine the ground state structure of hadrons calculated on the lattice, and to explore physical questions such as the role of diquarks in hadrons. Calculation of the overlap between the state created by an interpolating field acting on the vacuum and the lattice eigenstate provides a variational tool for exploring a hadron wave function. In addition, an appealing definition of a hadron wave function is the overlap between the hadron ground state and an adiabatic ground state with a corresponding number of static quarks and antiquarks at specified locations[10, 11].

8. Quark Distribution Amplitudes According to perturbative QCD, the form factors at asymptotic $Q^2$ are determined by quark distribution amplitudes. The moments of these amplitudes involve nucleon-to-vacuum matrix elements,

$$\langle 0|\epsilon^{ijk} u_i \gamma_\mu D^{\alpha_1} \cdots D^{\alpha_n} u_j D^{\alpha_{n+1}} \cdots D^{\alpha_\ell} \gamma_5 \gamma^\mu d_k |P \rangle,$$

which can be calculated in terms of two-point functions. Given the widely differing models prevalent in the literature, definitive lattice calculations will be quite useful.
9. **N - Δ Transition Form Factors** The experimental method of choice to reveal the presence of deformation in the low-lying baryons is measuring the N - Δ transition amplitude, where the dominant transition is the magnetic dipole (M1) and non-vanishing electric quadrupole (E2) and Coulomb quadrupole (C2) amplitudes are a signature of deformation in the nucleon, Delta, or both. Extensive measurements have been completed at Bates and JLab. Figure 7 shows quenched results in which we developed a new lattice method that for the first time has the precision to measure non-vanishing $R_{EM}$ and $R_{SM}$ ratios[12, 13]. Linear extrapolation of these quenched results yields results qualitatively similar to experiment, raising the expectation that the proposed chiral calculations will produce a definitive result.

10. **Pion Form Factor and 11. Pion Generalized Form Factors** The pion form factor is the simplest of all hadronic form factors, and its recent measurement at JLab renders it an important target of opportunity. Initial calculations using MILC lattices in Fig 8 show promising consistency with experiment for light quark masses[14], so we have included precision measurements of the pion form factor and generalized form factors revealing its transverse structure with the other hadronic form factors we propose to investigate.

12. **Pentaquark Structure** Recently, exploratory quenched calculations of possible pentaquark states have been reported [15] using the most general combination of the nineteen linearly independent local sources, as well as with a non-local source of the form advocated by Jaffe and Wilczek[16]. These calculations show substantially smaller overlap between the sources and possible pentaquark states than those arising between mesons or nucleons and their corresponding sources, suggesting that, at least in the domain of heavy quarks, the state differs substantially from the simple quark-model inspired sources. Accurate determination of the lowest states in the negative and positive parity pentaquark channels requires time extents longer than the $N_T = 32$ lattices with Dirichlet boundary conditions used last year, so the propagators calculated with the new source technique described in the next section will be used to extend the pentaquark calculation into the chiral regime.

13. **Spectroscopy** An obvious component of this project is careful extraction of hadron masses, quark masses and the decay constants $f_\pi$ and $f_K$. Comparison with MILC results with staggered valence quarks is an important test of our hybrid approach. In addition, since a single valence pion cannot simultaneously cancel the four different-mass pions arising from the staggered sea, the lattice $a_0$ propagator goes negative and provides an important test of our ability to extract the proper physical result using chiral perturbation theory for our hybrid action.

14. **Nonperturbative Renormalization** The relevant twist-2 quark bilinear operators have been renormalized perturbatively at one-loop level[17]. It is valuable to check the accuracy of perturbative renormalization constants in accessible cases, and we have already done so for the axial and vector currents using the 5-dimensional Noether current. We now propose to calculate the twist-2 operators with a single covariant derivative non-perturbatively in selected cases, which will require a set of 5 additional forward propagators.
2 Computational Strategy

Lattice action  The proposed calculations will continue use of a hybrid combination of chiral domain wall valence fermions calculated on HYP smeared improved sea quark configurations calculated by the MILC collaboration. The Asqtad action is described in Refs. [18, 19] and we used HYP smearing as described in Ref. [20] with the standard non-perturbative parameters. The domain wall fermions are calculated with $M = 1.7$ and studies at $a = 0.125$ fm showed[21] that $L_5 = 16$ yields $m_{res}$ an order of magnitude smaller than $m_{quark}$ for $m_l/m_s$ down to 0.2. We also calculated nucleon and pion masses as a function of $L_5$ and verified that no statistically significant changes occurred in these masses when $L_5$ was increased from 16 to 32 and 48. The domain wall quark masses are tuned to reproduce the (Goldstone) pion masses measured by MILC with staggered quarks. The values of $L_5$ for other quark masses and lattice spacings in Table 1 are determined to ensure that $m_{res}$ is less than 10 % of the quark mass.

Hadron Observables  The strategy for computing hadronic matrix elements has been continually developed and tested by our collaboration over the past seven years, and is briefly summarized below.

In past calculations, because the time extent between hadron source and sink is of the order of 1.2 fm, it was useful to bisect the MILC lattices in the time direction, apply Dirichlet boundary conditions, and calculate propagators that were a factor of 2 cheaper than with the full lattice. As described in Ref. [5], we use Wuppertal smeared sources and sinks, with the degree of smearing optimized to yield an overlap with the nucleon of order 50%. Forward propagators are used to construct the sink, which is typically projected onto 2 distinct momenta. A set of forward propagators from the source and backward propagators from the sink are then combined to calculate a set of building block operators for the tower of twist-2 operators. These building block operators consist of all relevant gamma matrices multiplied by zero, one, two, or three link variables and are Fourier transformed with each of the values of the momentum transfer that will be used to calculate form factors. These building blocks are stored and used to calculate all the nucleon matrix elements and generalized form factors described in Section 1. To economize, since the sources and sinks we use have a non-relativistic limit, it is adequate to retain only the upper two Dirac components, decreasing the number of propagators by a factor of 2. In addition, by carefully analyzing the operators for generalized form factors, it is possible to calculate all the operators of interest with the nucleon source and sink having the same spin orientation, saving another factor of 2.

Because of the need for higher statistics, we have recently developed and tested a new method in which 12 component forward propagators are calculated from 4 sources on equally separated time slices on the full MILC lattices, sampling essentially statistically independent regions of space-time. Four nucleon sinks 1.2 fm from each source are constructed from the forward propagators from the nearest source, and one set of 6 component backward propagators is calculated from the set of four sinks and used with the four sets of forward propagators to form 4 independent sets of building blocks for operators. A
second set of four antinucleon sinks, 1.2 fm from each sink in the other time direction is constructed, and one set of 6 component backward propagators is calculated from this set of sinks and used to form a set of 4 independent sets of building blocks for the antinucleons, which are physically equivalent to but statistically independent from the nucleon building blocks. The single calculation of backward propagators created by 4 sources differs from 4 separate calculations of backward propagators from each source by terms that average to zero in the functional integral. Tests show that the new procedure is statistically equivalent to the original procedure on bisected lattices, but provides 4 times the statistics at \( 2^{\frac{2}{3}} \) the cost. An additional factor of 2 in statistics will be achieved by no longer skipping alternate lattices.

Generalized parton distributions are calculated using the overdetermined analysis described in Ref. [7]. For many observables of interest, the straightforward method of calculating a single lattice operator that yields the matrix element of interest requires such high statistics for a useful degree of precision that it is computationally impractical. Hence, we identify the largest set of physically equivalent but statistically independent operators we can calculate, and simultaneously least squares fit this overdetermined set. As shown in Figure 9 the error bars are reduced by up to a factor of 5 relative to the naive method.

The nucleon to Delta transition form factor is also calculated from an overdetermined analysis using a set of forward and backward propagators from a smeared nucleon source and a smeared Delta sink as described in Ref. [12]. In this case, to obtain an optimal signal, three different sinks are calculated, optimized for calculating the M1, C2, and E2 form factors respectively.

The pion form factor is calculated using the method described in Ref [14]. To obtain accurate measurements over a range of momentum transfer, it is useful to use several different sink operators and momenta.

**Renormalization**  Perturbative 1-loop renormalization factors have now been calculated for the twist-two bilinear operators used for moments of structure functions and generalized form factors[17]. By virtue of the HYP smearing, the \( Z \) factors are close to 1, and higher order corrections are expected to be small. The proposed non-perturbative calculation of renormalization factors for operators with a single derivative will be a useful check.

**Disconnected Diagrams**  A separate proposal is being submitted by James Osborn et. al. for stochastic calculation of disconnected contributions to strange quark form factors. We will collaborate with that project in two ways. First, we will provide the relevant nucleon two point functions needed in that calculation. Secondly, using other resources, we will explore truncated eigenmode expansions for the necessary all-to-all propagators[22]. In the future, we plan to combine the truncated eigenmode expansion with stochastic evaluation of the contribution from the omitted space, but no resources are being requested for this calculation as part of this present proposal.
3 Software

The proposed calculations will utilize Andrew Pochinsky’s highly optimized SciDAC Level 3 domain wall inverter, and the time requests in Table 1 are based on production or test runs with this inverter. Analysis software has been developed for all the major physics components of this proposal.

4 Resources Requested

The computational resources requested for the hadron structure calculations described above are summarized in Table 1. Almost all of the computer time is used for calculating domain wall valence quark propagators on HYP smeared MILC lattices, with the order of 5% being used to calculate operator building blocks from forward and backward propagators. All timing measurements were made using the 4g 384 node GigE cluster at JLab, and the times are listed as processor hours on this machine.

To display how the cost is distributed between various projects and different lattices, we have separated out the forward propagators (F) required for all projects, the sequential (backward) propagators from a nucleon (N), a pion (π), and a Delta (∆), the propagators required for nonperturbative renormalization (NP) and the propagators required for nucleon polarization (Pol). Although for economy, we are able to restrict nucleon sinks to upper components only, requiring only 6 instead of 12 propagators per set, we have expressed all propagators sets in terms of 12 component sets for simplicity. So, for example, for the nucleon sink that contains contributions from four distinct space-time sites, we calculate 6 components for each of 2 flavors and 2 momenta, equivalent to 2 12-component propagators. Doing the same for an antinucleon sink requires another 2 12-component propagators, so we have listed a total of 4 12-component propagators for this calculation in the table.

The times for domain wall conjugate gradient inversions in Table 1 are based on interpolation between measured values using the relation

\[ T = (A \frac{1}{m_l/m_s} + C)N_L^2N_TN_5 \]

Inversion was timed for \( a = 0.125 \) and 0.09 lattices to determine \( A \) and \( C \) in each case, and the \( a = 0.06 \) estimate was obtained by scaling according to the volume from the \( a = 0.09 \) case.

To keep the overall request within reasonable bounds, we have deferred until next year the full analysis of the MILC \( a = 0.06 \) lattice.
Table 1: Resources requested, in processor hours on JLab 4g 384 node GigE Cluster. The processor hours for convergence of the domain wall conjugate gradient inverter on one set of propagators are denoted p-h/CG and all sets of propagators refer to 12 Dirac/color components. F denotes the number of sets of forward propagators, and the number of sets of backward propagators for nucleon, pion, and Delta sinks are denoted by N, \( \pi \), and \( \Delta \) respectively. The number of propagators for non-perturbative renormalization calculations is denoted by NP and the number of propagators for nucleon polarization is denoted Pol. All propagators are calculated for the listed number of configurations except for NP, which use 100, and Pol, which use 200. The time required to calculate operator building blocks is denote BB pr hrs.

\[
\begin{array}{cccccccccccc}
\text{m} / m_s & N_L & N_5 & m_\pi & \text{configs avail} & \text{pr hrs} & F & N & \pi & \Delta & NP & Pol & BB & \text{Total pr hrs} \\
0.6 & 20 & 16 & 605 & 200^a & 41.9 & 0 & 0 & 0 & 5 & 6 & 0 & 0.07M \\
0.4 & 20 & 16 & 498 & 200^b & 57.4 & 0 & 0 & 0 & 0 & 6 & 0 & 0.07M \\
0.2 & 20 & 16 & 359 & 695 & 104 & 4 & 4 & 3 & 3 & 5 & 6 & 52K & 1.24M \\
0.2 & 28 & 16 & 359 & 275 & 285 & 4 & 4 & 3 & 3 & 0 & 6 & 57K & 1.50M \\
0.14 & 20 & 16 & 300 & 650 & 144 & 4 & 4 & 3 & 3 & 5 & 6 & 49K & 1.60M \\
0.1 & 24 & 16 & 254 & 529 & 1022 & 4 & 4 & 0 & 0 & 0 & 0 & 69K & 4.39M \\
\end{array}
\]

Total processor hours (Millions) 8.88M

\[
\begin{array}{cccccccccccc}
\text{m} / m_s & N_L & N_5 & m_\pi & \text{configs avail} & \text{pr hrs} & F & N & \pi & \Delta & NP & Pol & BB & \text{Total pr hrs} \\
1 & 28 & 12 & 775 & 500 & 61.9 & 4 & 4 & 2 & 0 & 5 & 6 & 103K & 0.52M \\
0.4 & 28 & 12 & 498 & 514 & 136 & 4 & 4 & 2 & 0 & 5 & 6 & 106K & 1.04M \\
0.2 & 28 & 12 & 359 & 512 & 259 & 4 & 4 & 2 & 0 & 5 & 6 & 105K & 1.87M \\
0.1 & 40 & 12 & 254 & 200^c & 1475 & 4 & 4 & 0 & 0 & 0 & 0 & 120K & 2.48M \\
\end{array}
\]

Total processor hours (Millions) 5.91M

\[
\begin{array}{cccccccccccc}
\text{m} / m_s & N_L & N_5 & m_\pi & \text{configs avail} & \text{pr hrs} & F & N & \pi & \Delta & NP & Pol & BB & \text{Total pr hrs} \\
0.4 & 48 & 8 & 498 & 530^d & 685 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0.73M \\
0.2 & 48 & 8 & 359 & 300^d & 1306 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0.78M \\
\end{array}
\]

Total processor hours (Millions) 1.51M

Total processor hours for all lattices (Millions) 16.29M

\(^a\) Using 200 of 559, \(^b\) Using 200 of 485, \(^c\) Using 200 of 550, \(^d\) Expected to be available from MILC after 6 months
Table 2: Domain wall inverter performance on US LQCD clusters. Multiplying our time estimates on the Jlab 4g cluster by the performance factor in the last column converts them to each of the other clusters.

<table>
<thead>
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<th>Cluster</th>
<th>Gflop/node</th>
<th>Gflop/processor</th>
<th>Perf. Factor</th>
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<td>1.2</td>
<td>1</td>
</tr>
<tr>
<td>JLab 6n 256 node Infiniband</td>
<td>2.2</td>
<td>1.1</td>
<td>1.09</td>
</tr>
<tr>
<td>Fermilab 128 node Myrinet</td>
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<td>1.08</td>
<td>1.11</td>
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<tr>
<td>Fermilab 512 node Infiniband</td>
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<td>1.80</td>
<td>0.73</td>
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<tr>
<td>Fermilab 500 node dual core/dual proc</td>
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<td>N/A</td>
<td>N/A</td>
</tr>
</tbody>
</table>

**Request Summary**  The total time enumerated in Table 1 in processor hours on the JLab 4g 384 node GigE cluster is 16.29 million processor hours. Cluster time on any of the JLab or Fermilab US LQCD clusters is acceptable, when adjusted appropriately for performance relative to the JLab 4g cluster. To convert between the various clusters, we have benchmarked our code at the appropriate lattice sizes on various US LQCD clusters, with the results shown in Table 2. Performance on the new Fermilab dual core, dual processor 500 node cluster will be provided as soon as it is available.

5  Data Sharing

All the domain wall propagators will be made available to the entire SciDAC collaboration as they are produced for use in projects other than the exclusive calculations listed below. For practical purposes and quality control, we expect to wait until all runs at a given mass, lattice size and lattice spacing are complete and tested before making them publicly available.

6  Exclusive Calculations

As explained above in the Physics Goals, this proposal combines 14 distinct research projects being carried out by different subgroups of investigators into a single unified request that seeks to maximize the efficiency and reuse of common propagators, sources, and operator building blocks. Each project is led by one of our junior collaborators, who is taking the lead in formulating the calculation, overseeing the production and data analysis, coordinating the writing of publications of the work, and will normally be the first author on the publications. In terms of credit and external visibility, we believe this is essential for the career advancement of young theorists in our collaboration. Because of the importance of each of these projects to the theorists involved, we believe that each project should be
treated as exclusive. Our intent is to make the relevant propagators available within six months of the publication of the first paper using them.

We list below each of the thirteen research topics, and the corresponding Project Leader.

1. Moments of Structure Functions (Dru Renner)
2. Nucleon Form Factors (George Fleming)
3. Nucleon Generalized Form Factors (Philipp Haegler)
4. Nucleon Sigma Term (Kostas Orginos)
5. Neutron Electric Dipole Moment (Kostas Orginos)
6. Nucleon Electric and Magnetic Polarizability (Michael Engelhardt)
7. Hadron Wave Functions and Density-Density Correlation Functions (Jonathan Bratt)
8. Quark Distribution Amplitudes (Michael Engelhardt)
9. Nucleon-Delta Transition Form Factors (Wolfram Schroers and senior collaborator Constantia Alexandrou)
10. Pentaquark Structure (Dmitry Sigaev)
11. Spectroscopy including hadron and quark masses, decay constants, and $a_0$ propagator (Kostas Orginos and Dru Renner)
12. Nonperturbative Renormalization (Kostas Orginos)
13. Pion Form Factors (George Fleming)
14. Pion Generalized Form factors (Philipp Haegler)

References


Figure 2: Chiral extrapolation of the quark momentum fraction, $\langle x \rangle$, using a phenomenological form that interpolates between the correct chiral limit and lattice data in the heavy quark regime[23] (left panel) and preliminary measurements on MILC lattices (open circle and solid diamond, square, and triangle on right panel).

Figure 3: Generalized form factors $A_{20}, B_{20}$ determining the total quark contribution to the nucleon spin (left panel) and the fraction of the nucleon spin arising from the quark spin, $\Delta \Sigma$, and quark orbital angular momentum, $2L_q$, (right panel).
Figure 4: Preliminary calculations of spin-independent generalized form factors $A_{10}$ and $A_{20}$ (left panel) and of spin-dependent generalized form factors $\tilde{A}_{10}, \tilde{A}_{20},$ and $\tilde{A}_{10}$ on $28^3 \times 32$ MILC lattices at $M_\pi = 359$ MeV.

Figure 5: Preliminary results for the ratio of the electromagnetic form factors $F_2/F_1$ as a function of momentum transfer using MILC lattices, showing qualitative agreement with the JLab experimental result denoted by the solid curve.
Figure 6: The left panel shows normalized generalized form factors $A_{n,0}^{u-d}(t)$ for $n=1$ (diamonds), $n=2$ (triangles), and $n=3$ (squares). The right panel shows the transverse rms radius of the proton light cone wave function as a function of the average quark momentum fraction, $x_{av}$, for each measured moment.

Figure 7: The left panel shows the magnetic dipole nucleon-to-Delta transition form factor calculated in quenched QCD at three heavy quark masses, the linear extrapolation to the chiral limit, and a phenomenological fit to experiment. The right panel shows the ratio of Coulomb to magnetic form factors, $R_{SM}$. The upper curves show quenched calculations at several pion masses and their chiral extrapolation, and the lower curves compare the extrapolated result with experimental data.
Figure 8: Pion form factor calculated with domain wall fermions and MILC configurations.

Figure 9: Generalized form factor $C_{20}$ obtained by simultaneous fits to $N$ external momentum combinations having a common virtuality $t$. The $N = 0$ point, denoted by a triangle, uses three operators and a single external momentum to determine three form factors $A_{20}, B_{20}$, and $C_{20}$. The remaining points, designated by squares, use six operators and $N$ external momentum combinations to determine the three form factors. The improvement in accuracy by a factor of 5 indicates the effectiveness of this technique.