I. Research Objectives

We propose to continue the broad research program in Quantum Chromodynamics (QCD) that we have been engaged in for a number of years. This research addresses fundamental questions in high energy and nuclear physics, and is directly related to major experimental programs in these fields. It includes studies of the mass spectrum of strongly interacting particles, the weak interactions of these particles, and the behavior of strongly interacting matter under extreme conditions.

The Standard Model of High Energy Physics consists of two quantum field theories: the Weinberg-Salam Theory of the electromagnetic and weak interactions, and QCD, the theory of the strong interactions. The Standard Model has been enormously successful in explaining a wealth of data produced in accelerator and cosmic ray experiments over the past twenty-five years. However, our knowledge of it is incomplete because it has been difficult to extract many of the most interesting predictions of QCD, those that require non-perturbative calculations. Although there is little doubt that QCD is the correct theory of the strong interactions, non-perturbative QCD calculations are crucial for testing the weak interaction part of the Standard Model: In the absence of such calculations the strong effects completely obscure the weak physics one is trying to study. At present the only means of carrying out non-perturbative QCD calculations from first principles and with controlled errors is through large scale numerical simulations. These simulations are needed to obtain a quantitative understanding of the physical phenomena controlled by the strong interactions, to determine a number of the basic parameters of the Standard Model, and to make precise tests of the Standard Model’s range of validity. Despite the many successes of the Standard Model, it is believed by high energy physicists that to understand physics at the shortest distances a more general theory, which unifies all four of the fundamental forces of nature, will be required. The Standard Model is expected to be a limiting case of this more general theory, just as classical mechanics is a limiting case of the more general quantum mechanics. A central objective of the experimental program in high energy physics, and of lattice QCD simulations, is to determine the range of validity of the Standard Model, and to search for new physics beyond it. Thus, QCD simulations play an important role in efforts to obtain a deeper understanding of the fundamental laws of physics.

Several years ago we used our NRAC allocation to develop an improved action (improved lattice discretization) for lattice QCD [1], which significantly increases the accuracy of our simulations for a given amount of computing resources. This improved Asqtad action, coupled with increases in computing resources within the NSF program and major improvements in the performance of our code, are enabling us to make important progress in our research. The bulk of our allocation goes into the generation of lattices (snapshots of the systems we are simulating) using the improved Asqtad action. These lattices are saved, and then used to calculate a wide variety of physical quantities. In order to maximize the physics output from the large investment of the NSF program in the generation of these lattices, we are making them available to other lattice gauge theorists for their research.

The level of accuracy we seek in our calculations is determined in large part by our studies of the weak interactions of strongly interacting particles. An international effort is in progress to determine the elements of the Cabibbo-Kobayashi-Maskawa (CKM) matrix, which determines how quarks, the fundamental strongly interacting particles, couple to the weak interactions. In most cases both an accurate experiment and lattice calculation are needed. By determining individual elements of the CKM matrix from different experiments and lattice calculations, one can place powerful constraints on the range of validity of the Standard Model. The Lattice QCD Executive Committee, which is leading an effort to develop computational infrastructure for our field, has recently made a detailed analysis of the impact of improved lattice calculations on constraints on the Standard Model [2]. This study is based in large part on the lattices we have or are planning to generate. Table 1 summarizes the portion of the study relevant to this proposal. The first column indicates the quantity measured experimentally, the second column the effected CKM matrix
element, and the third column the hadronic matrix element which must be calculated on the lattice. The fourth column shows the current non-lattice errors, which are primarily experimental, and the fifth the current lattice errors. The column labeled Lattice Errors Phase I shows the expected lattice errors once the analysis has been completed on our existing lattices, and the column labeled Lattice Errors Phase II shows the expected lattice errors once analysis has been completed on the lattices currently being generated or planned for the near future. One notes that in all cases for which experiments have been performed, the current lattice error is significantly larger than the experimental one, and that is also likely to be the case for the third row once $\Delta M_s$ has been measured. However, once the Phase II analysis has been completed, the lattice errors will be less than or comparable to the experimental ones. The importance of this can be seen from the fact that a significant fraction of the $750,000,000 per year that the United States spends on experimental high energy physics is devoted to the study of the weak decays of strongly interacting particles. It is clear that to fully capitalize on this investment, the lattice calculations must keep pace with the experimental measurements. The impact of reducing lattice errors on the determination of CKM matrix elements is illustrated in Figure 1 of the attachment titled Figures Illustrating Recent Progress. Finally, we note that in addition to generating the lattices, we are engaged in the analysis effort for the last three rows of this table in collaboration with the Fermilab group, while the Los Alamos, Ohio State, Washington and UKQCD groups are carrying out the analysis for the first row.

Because lattice gauge theory calculations have rarely reached the level of accuracy required by the weak interaction studies, it is important to verify that we have control over all sources of systematic errors by calculating quantities whose values are well known experimentally. Since these calculations make use of the same lattices employed in our weak interaction studies, they consume a small fraction of the resources of our project; however, they provide an important validation of our approach. We have recently carried out such a study working in collaboration with several other groups that are making use of our lattices [3]. Some of our results are shown in Figure 2 of the attachment titled Figures Illustrating Recent Progress. In each case the calculations agree with experiment within statistical and systematic errors of 3% or less. This work was described in a News and Views article in Nature [4], as well as in a News Focus article in Science [5]. Within the high energy community, it has been featured in FermiNews Today [6] and in a cover article in the CERN Courier [7].

In Section II, we describe our computational methodology, and recent work that has improved the performance of our code. In Section III, we present brief highlights of progress made during the past year. A detailed progress report is contained in an attachment. In Section IV we give the

<table>
<thead>
<tr>
<th>Measurement</th>
<th>CKM Matrix Element</th>
<th>Hadronic Matrix Element</th>
<th>Non-Lattice Errors</th>
<th>Current Lattice Errors</th>
<th>Lattice Errors Phase I</th>
<th>Lattice Errors Phase II</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\varepsilon_K$</td>
<td>Im$V_{td}^2$</td>
<td>$\hat{B}_K$</td>
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<td>20%</td>
<td>12%</td>
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<tr>
<td>$(\bar{K}K$ mixing)</td>
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<tr>
<td>$\Delta M_d$</td>
<td>$</td>
<td>V_{td}</td>
<td>^2$</td>
<td>$f_{B_d}^2 B_{B_d}$</td>
<td>6%</td>
<td>30%</td>
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<td>$(\bar{B}B$ mixing)</td>
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<tr>
<td>$\Delta M_d/\Delta M_s$</td>
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<td>V_{td}/V_{ts}</td>
<td>^2$</td>
<td>$\xi^2$</td>
<td>---</td>
<td>12%</td>
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<tr>
<td>$B \to (\pi^0)_\nu$</td>
<td>$</td>
<td>V_{ub}</td>
<td>^2$</td>
<td>$\langle 0_\pi</td>
<td>(V - A)_\mu</td>
<td>B \rangle$</td>
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Table 1: Impact of Asqtad lattices on the determination of CKM matrix elements.
justification for our resource request. We request a one year allocation with a total of 3,848,200 service units. A breakdown of our request by projects and computing platforms is given Table 2, which can be found in Section IV. Our request is to support the work of six principal investigators, their postdoctoral research associates and graduate students. Thus, it comes to 641,367 service units per principal investigator.

We understand that our request is large, so we think it is important to point out that our allocation is having an impact well beyond our own research. Physicists outside our collaboration at Boston U., Brookhaven National Laboratory, CalTech, U. of Connecticut, Cornell U., DePaul U., U. of Edinburgh, Fermi National Accelerator Laboratory, U. of Glasgow, U. Illinois, Thomas Jefferson National Accelerator Facility, MIT, Ohio State U., Oxford U., Simon Fraser U and U. of Washington, are currently using our lattices. Their research covers a broad range of topics including determinations of the strong coupling constant, the masses of the strange, charm, and bottom quarks, quarkonium spectroscopy and decay widths, the weak decays of mesons containing heavy quarks, the quark and gluon structure of hadrons, and hadronic contributions to the muon anomalous magnetic moment. In preparing our last two NRAC proposals we asked some of the physicists making use of our lattices to comment on the impact they are having. Since these comments were quite uniform, this year we have simply reproduced those from last year in the attachment titled Impact of Asqtad Lattices. Here we provide two quotes which directly address the impact our lattices are having. Peter Lepage: “The gluon configurations being produced by MILC are critically important to the research of several collaborations, including my own... MILC’s configurations are uniquely valuable, and MILC has been unusually generous in sharing them with other collaborations. The continued production of MILC configurations is of the utmost importance to my collaboration’s research, and to the entire field of lattice QCD.” Junko Shigemitsu: “my own research program, together with that of many other lattice groups, has benefited enormously from MILC’s program to create state-of-the-art dynamical gauge configurations and make them generally available to the lattice community. I cannot think of another development in recent years that has had more impact or contributed more to progress in lattice gauge theory than these efforts by the MILC collaboration... The MILC dynamical configurations are currently the most realistic configurations in the world.”

In the remainder of this section we describe our research objectives in greater detail.

**Generation of lattices with improved gauge and quark actions:** As is clear from the above discussion, the lattice ensembles that we generate are the basis for a wide variety of physics calculations by our group and by others. The results of Ref. [3] indicate that the approach we are pursuing is producing calculations of a wide variety of quantities of great importance to current experiments. However, as is discussed below, in order for the determination of some of the most interesting quantities we are studying to reach an accuracy required by experiment, it is necessary for us to push our simulations to smaller lattice spacings and quark masses.

We therefore propose to continue to generate zero-temperature lattices with three flavors of dynamical sea quarks: up, down and strange. These three flavors of quarks are the only ones with masses comparable to the energy scale of QCD. They are therefore the only ones light enough so that their virtual loops have a significant impact on realistic calculations. Despite their importance, strange sea quarks have typically been neglected in large scale simulations of QCD. Their inclusion is an important feature of our work, as is the use of large enough spatial sizes to accurately include the effects of light pions.

The lattices are being generated with a one-loop Symanzik improved gauge action and the Asqtad staggered quark action [1]. Both the gauge and quark actions have all lattice artifacts removed through order $a^2$ ($a$ is the lattice spacing) at the tree level, and are tadpole improved. This action appears to have the best scaling properties in the lattice spacing of any QCD action currently being applied to large scale simulations [8]. We are currently generating lattices at two different
lattices spacings, $a \approx 0.12$ fm and $a \approx 0.09$ fm. Since the leading discretization errors are of order $a^2 / \log(a)$, the finer grained ($a \approx 0.09$ fm) lattices have finite lattice spacing artifacts approximately half the magnitude of those of the coarse ($a \approx 0.12$ fm) lattices, allowing us to estimate the size of these systematic errors, and to perform extrapolations to the continuum limit.

We are working with the Kogut-Susskind (staggered) formulation of lattice quarks because at present they enable dynamical simulations with significantly smaller quark masses than the Wilson formulation. A problem with Kogut–Susskind quarks is the breaking of taste symmetry. (“Taste” refers to the different ways one can construct the same physical particle in the Kogut-Susskind formalism. Although particles with different taste become identical in the continuum limit, their masses can differ at finite lattice spacing.) However, the Asqtad action has significantly better rotational and taste symmetry than the conventional Kogut–Susskind action [9]. Furthermore, one of us (CB) has developed techniques, based on the pioneering work of Lee and Sharpe [10] for incorporating the effects of taste symmetry breaking into chiral perturbation theory [11, 12, 13], thereby significantly improving our ability to make extrapolations to the chiral limit.

For both lattice spacings we are studying, we attempt to keep the mass of the strange quark fixed at its physical value, $m_s$. We take the masses of the up and down quarks to be equal, which has a negligible effect (< 1%) on isospin-averaged quantities. A table showing the current status of our lattice generation is provided in the attachment titled Impact of Asqtad Lattices. We have completed work on an extensive set of $20^3 \times 64$ lattices with $a \approx 0.12$ fm and $m_{u,d}$ in the range $0.14 m_s \leq m_{u,d} \leq m_s$, and a set of $28^3 \times 96$ lattices with lattice spacing $a \approx 0.09$ fm and $m_{u,d} = m_s$, 0.4 $m_s$ and 0.2 $m_s$. These are the Phase I lattices of Table 1.

The average light quark mass, which we denote by $m_{u,d}$, is much smaller than other energy scales in QCD. Since the computing resources required to carry out a simulation scale approximately as $m_{u,d}^{-3}$, it is presently too expensive to perform simulations at the physical value of $m_{u,d}$. Instead one works with a range of values for $m_{u,d}$ which are small enough so that one can perform extrapolations to its physical value with the aid of chiral perturbation theory. This chiral extrapolation is the largest source of error in our current calculations. For this reason, a major part of our current work is the generation of lattices with $m_{u,d} = 0.1 m_s$, which yields a $\pi$ to $\rho$ mass ratio of approximately 0.298, the lowest value achieved to date in a study with dynamical quarks. These lattices play a major role in anchoring the chiral extrapolations, thereby significantly reducing systematic errors in a wide range of physical quantities. By the beginning of the next grant period we expect to have completed a run at $a = 0.12$ fm with $m_{u,d} = 0.1 m_s$, and the lattice size increased to $24^3 \times 64$ in order to avoid finite size effects, which increase as the pion mass is decreased. Our major continuing simulation is an ensemble of $40^3 \times 96$ lattices at lattice spacing 0.09 fm with $m_{u,d} = 0.1 m_s$. We expect to have 120 equilibrated lattices in hand by the end of our current allocation, and propose to generate at least 80 additional ones in the coming year using resources outside the NSF program.

To avoid finite size effects, this ensemble has a spatial size of 3.6 fm, instead of the 2.5 fm used at larger quark masses. Since the pion mass in lattice units is about $am_{\pi} = 0.104$ in this run, we have $m_{\pi} L \approx 4.2$. Finite size effects are expected to be proportional to $\exp(-m_{\pi} L)$, so these effects should be small. The 3.6 fm box size should be sufficient for studies of effects that depend on the “pion cloud” around hadrons. Of course, the three times larger spatial volume means that a molecular dynamics trajectory takes about three times as long as on a 2.5 fm box. However, for most of the quantities we study, including hadron masses, decay constants, the static quark potential and others, the statistics obtained from each lattice is approximately proportional to the volume, so fewer equilibrated time units will be required to obtain results of comparable accuracy.

Further increases in accuracy require decreasing the lattice spacing. In particular, with the current lattice spacing of 0.09 fm and lightest quark mass of $0.1 m_s$, the “taste splittings,” or discretization artifacts, in the pion masses are comparable to the masses themselves. Therefore we need to decrease the lattice spacing before pushing closer to the physical up and down quark masses. This
project will require several years, and will involve resources other than NSF centers. However, it is essential that we begin the preparatory "tuning runs" needed to find the values of the gauge coupling and input quark mass that correspond to the desired lattice spacing and physical strange and light quark masses. This tuning will be guided by extrapolation from our extensive data at larger lattice spacings, so we may reasonably expect that a single tuning run at each light quark mass will suffice. Once the couplings are fixed, we propose to begin a simulation on a $40^3 \times 144$ lattice with $a = 0.06$ fm and $m_{u,d} = 0.4 m_s$. While we cannot finish this run during the oncoming year, we will get enough statistics to obtain accurate results for quantities such as the static quark potential and the pseudoscalar mesons. Results for the pseudoscalar mesons will greatly improve the accuracy of our fits to chiral perturbation theory, improving our results for the light and strange quark masses and the low energy constants (Gasser-Leutwyler parameters) in the effective chiral lagrangian. As statistics increase, this first $a = 0.06$ run will enable us to check and better control the continuum extrapolation of the topological susceptibility and the heavy-light form factors and decay constants which are important to the determination of the CKM matrix elements. Of course, in the long run these very fine simulations must be extended to smaller light quark masses. We will seek resources beyond the NSF program, perhaps even in international collaborations, for the bulk of these runs.

**Physics of light pseudoscalars:** Lattice computation of the properties of light pseudoscalar mesons ($i.e.$, $\pi$, $K$ and $\eta$ mesons) offers a unique opportunity to (1) check our lattice methods to high ($\approx 2$ to 3\%) precision, and (2) calculate phenomenologically important physical quantities that are difficult or impossible to obtain with controlled errors by other methods. The advantages of this system stem firstly from the fact that we are able to compute quantities such as the $\pi$ and $K$ masses and decay constants at fixed lattice spacing and (larger than physical) quark mass with extremely high statistical accuracy: 0.1\% to 0.7\%, depending on the quark masses. Secondly, the dependence of these quantities on quark masses is governed by the formalism of chiral perturbation theory [14]. This formalism has been extended to the “partially quenched” case [15], where valence and sea quark masses are different, and, further, to the case of staggered quarks with discretization errors included (“staggered chiral perturbation theory” [10, 11, 12, 13] — SXPT). The latter allows us to fit the lattice data accurately, including the effects of $O(a^2)$ lattice spacing errors, and then make a controlled chiral extrapolation (extrapolation to the physical value of $m_{u,d}$) followed by a controlled continuum extrapolation. Note that a further systematic error of previous lattice calculations — having either the wrong number of dynamical (sea) quarks or no sea quarks at all — is absent from ours, since we simulate with the physical number of light dynamical quarks.

Using the above method, we can currently compute the leptonic decay constants of the $\pi$ and $K$ mesons, $f_\pi$ and $f_K$, with a total error of under 3\% (see the attached progress report). The results agree with experiment at this level, providing good evidence that we understand and can control our errors. The same computational method, coupled with perturbative calculation of the mass renormalization constant, allows us to extract quark masses (the mass of the strange quark, $m_s$, the average mass of the $u$ and $d$ quarks, $m_{u,d}$, and the ratio $m_u/m_d$) and several of the so-called Gasser-Leutwyler parameters, $L_i$ [14]. Two of these quantities, in particular, urgently require precise lattice QCD evaluations: Uncertainty in $m_s$ severely limits the theoretical precision of various phenomenological studies, including the important CP-violating quantity $\epsilon'/\epsilon$ [16]. Determination of $m_u/m_d$, either indirectly through the combination $2L_8 - L_5$ of Gasser-Leutwyler parameters, or from the $K^+ - K_0$ mass difference with electromagnetic effects accounted for can answer the question of whether a vanishing $u$ quark mass is possible — which would be a solution of the strong CP problem [17]. Our current results [18, 3, 19] for decay constants, quark masses, and $L_i$ are presented in the attachment titled Progress Report.

To go further, we need to have more lattice data at small quark mass and fine lattice spacing. We estimate that the running proposed here at lattice spacing $a \approx 0.09$ fm and light quark mass $m_{u,d} \approx 0.1 m_s$, together with recent runs with an unphysically light strange quark mass, will allow
us to reduce the systematic errors on $f_\pi$ and $f_K$ to 2% or better, with corresponding improvements on the other physical quantities of interest. A 2% determination of light decay constants would be an important milestone for lattice QCD calculations. Applying this approach to the computation of decay constants of mesons containing a heavy quark to reach the level of precision indicated in the last column of Table 1, would have a broad impact on the study of the Standard Model and the physics beyond it.

**Weak decays of particles containing heavy quarks:** At the SLAC and KEK B-factories, and facilities at Fermilab and Cornell, a concerted experimental effort is under way to determine elements of the CKM matrix through studies of the mixings and decays of B mesons. In addition, the properties of D mesons are being measured to high accuracy in the CLEO-c Program at Cornell. The CLEO-c measurements can provide powerful constraints on the CKM matrix, both directly (on matrix elements involving $c$ quarks) and indirectly (through implications for $b$ quark systems). Indeed, one hopes that by tightly over-constraining these CKM matrix elements, the range of validity of the Standard Model will be determined, and new physics beyond it will be discovered. However, the experimental results do not in general determine the CKM parameters without theoretical calculations of the effects of the strong interactions. At present, lattice QCD provides the only known approach to evaluate these effects from first principles.

For the past several years we have been involved in a study of the decays of pseudoscalar mesons with one light and one heavy quark. The main objects of our study are $B$ (with a heavy $b$ quark and light $u$ or $d$ antiquark), $B_s$ ($b$ quark and $s$ antiquark), $D$ ($c$ quark and $u$ or $d$ antiquark) and $D_s$ ($c$ quark and $s$ antiquark). We are studying two types of decays: purely leptonic decays, e.g., $B \rightarrow \ell \nu_\ell$, and semileptonic decays, e.g., $B \rightarrow \pi \ell \nu_\ell$. Results of experimental measurements from these decays, combined with results from lattice calculations will provide crucial information about CKM matrix elements.

Strong interaction effects in leptonic decays are characterized by the decay constants $f_B$, $f_{B_s}$, $f_D$ and $f_{D_s}$. Semileptonic decays are characterized by various form factors $F(q^2)$, where $q$ is the momentum transfer carried by the leptons. A number of these constants and form factors have not yet been measured, so our calculations constitute predictions that will be tested by future experiments. CLEO-c will provide precise measurements of the $D$ and $D_s$ leptonic and semileptonic decays. If lattice computations can reach a precision of a few percent, comparisons of lattice and experimental results will offer an unprecedented opportunity to validate our approach, and insure that we do in fact have full control over systematic errors as we proceed to similar calculations for the $b$-quark system, where the corresponding quantities have not been measured experimentally, and are unlikely to be in the near future. After confirmation from these $c$-quark systems, lattice results for $f_B$ and $f_{B_s}$ with comparable precision would have a major impact on determination of the poorly known CKM matrix element $V_{td}$ from experimental measurements of $B$-$\bar{B}$ and $B_s$-$\bar{B}_s$ mixing. Similarly, accurate lattice determinations of semileptonic form factors for $B$ and $B_s$ would provide a new window on the CKM matrix element $V_{ub}$.

Clearly, to make the most of the forthcoming high precision experimental measurements, we must provide simulation results with at least a comparable accuracy. Inspired by recent successes in computing decay constants of pseudoscalar mesons with light quarks and antiquarks [18, 3], *our goal in the next few years is to determine $f_B$ and the corresponding semileptonic form factors to an accuracy of 5% to 10%*. We will do this with new techniques that significantly reduce errors arising from the extrapolation to physical up and down quark masses, and from the treatment of heavy quarks. The new lattices which we propose to generate are critical for this project. Over the past year we have joined forces with the Fermilab theory group in this effort.

To achieve an accurate determination of the CKM matrix elements, it is essential that all sources of systematic error in the lattice calculations be overcome and controlled—more so than in any previous attempt [20, 21, 22, 23, 24, 25, 26, 27]. Errors in earlier work arose from (1) the neglect
of dynamical quark loops (sea quarks), (2) the presence of large lattice discretization errors, (3) an inability to reach sufficiently light up and down quark masses, (4) an inaccurate treatment of heavy quark propagation, and (5) perturbative errors in the renormalization of lattice currents.

We are in a unique position to reach this goal over the next two years, thanks to the following timely developments: (1) our generation of an extensive archive of gauge configurations incorporating the effects of dynamical up, down and strange quarks which is to be augmented under this proposal; (2) the enhancement of NSF computing facilities to the level needed to perform calculations at a lattice resolution of $a = 0.09$ fm with reasonably light quark masses, enabling extrapolations to the continuum limit and to the physical values of the up and down quark masses; (3) the development of a new heavy quark formulation by the Fermilab group; (4) the use of the improved Asqtad action for light valence, as well as sea, quarks; (5) a recent formulation of the chiral extrapolation in light quark masses to their physical values that takes into account discretization errors [13]; and (6) automated perturbation theory [28] to compute the renormalization factors. Development (3) makes possible a significant reduction in systematic errors associated with Compton wavelengths that are comparable to the lattice spacing, and (4) and (5), a reduction in errors associated with the light quark mass (chiral) and continuum extrapolations. In addition, A. El-Khadra, M. Nobes and collaborators [29] have recently completed a calculation of the relevant renormalization constants for our determination of heavy-light decay constants and form factors. Fortunately, the Fermilab trick [20] that relates needed renormalization constants to others that can be evaluated non-perturbatively plus perturbative corrections, works better than expected. The perturbative corrections are small and therefore have small errors.

It has recently been suggested that the size of the systematic errors associated with the chiral extrapolation in heavy-light systems may be considerably larger than previously believed [30]. To study this effect one needs lighter quark masses, so that the chiral logarithm terms can actually be observed and included in a controlled way in the fits. Since we use improved staggered dynamical quarks, it is very likely the masses of the sea quarks available to us are light enough. Up to now, our valence quarks have used the tadpole-improved “clover” formulation, which constrains them to be relatively heavy by the existence of exceptional configurations [31]. The use of the Asqtad action for the light valence quarks solves this problem.

The heavy valence quarks must be clover quarks in order to apply the Fermilab formalism [32]. However, the standard heavy quarks may be combined with light staggered quarks [33], making it possible to construct mesons with light $u$ and $d$ quarks. In collaboration with the Fermilab group, we are in the process of computing heavy-light decay constants with staggered light valence quarks on both the coarse and fine lattice sets. Completion of this study will be one of our major goals under this grant. We plan to combine our NRAC allocation with cluster resources at Fermilab to accomplish this. In order to control the extrapolation to physical light quark mass in these simulations, we require precise information about the chiral logarithms at finite lattice spacing with staggered dynamical quarks. In other words, we need $S\chi PT$ for heavy-light mesons, just as we already have for light mesons [10, 11, 12]. Such calculations have been completed [13]. Combined with the lattice data being generated, we expect that this will make possible results for the decay constants of heavy-light mesons with the errors indicated in Table 1.

As in the case of the decay constants, it is important to determine the effects of the dynamical quarks on the semileptonic form factors, and perform extrapolations to the physical mass of the up and down quarks, and to the continuum limit. These calculations are demanding because, in order to make contact with experiment, we must evaluate the form factors over a large range of momenta, $q^2$. This requires that we vary the masses of three participating quarks, and study a range of incident three-momenta and three-momentum transfers.

Because form factor calculations are very expensive, this will be a multi–year project. However, given the critical importance of these calculations to the analysis of results from experiments cur-
rently underway, we believe the expense is justified at this time.

**Hadron mass spectrum with the improved action:** Calculation of the spectrum of the light hadrons is an essential test of lattice simulations. Moreover, lattice computations can shed light on some of the open questions regarding the nature of the light hadrons. For example, the nature of the \( a_0(980) \) is still somewhat controversial — to what extent is it a quark-antiquark state, and to what extent a \( K - \bar{K} \) molecule? Also, the quark model assignments of many of the excited states are not well established, and lattice computations should be used to help nail them down. Lattice calculations are also important for understanding hadrons that are not explained by the naive quark model, namely hybrids and glueballs. These hadrons, especially those with exotic quantum numbers, are an important part of the experimental program at Jefferson Laboratory.

We have computed the masses of the simplest hadrons, which can be produced from a point-like operator with staggered quarks, as we have generated the lattices. This “point source” spectrum gives us the masses of the \( \pi, \rho, a_0, a_1, b_1 \) and nucleon, together with the corresponding states containing strange quarks. We will continue calculating these hadron masses in parallel with our lattice generation. In addition to being important in its own right, the light hadron spectrum is important in monitoring the progress of these runs.

The decuplet baryons (\( \Delta, \Omega^- \), etc.) require a more complicated set of propagators. The \( \Delta \) mass is interesting because the \( N - \Delta \) mass splitting, like the \( \pi - \rho \) splitting, is due to hyperfine interaction in the quark model, and lattice calculations with unimproved actions and at larger lattice spacings have historically had trouble matching the experimental results. The \( \Omega^- \) mass is interesting because it is stable under the strong interactions, and is therefore one of the quantities which should be calculable to high accuracy in lattice simulations. We have calculated the \( \Delta \) and \( \Omega^- \) masses on all of the coarse lattices and three of the fine lattice runs. We propose to calculate the \( \Delta \) mass on the remaining data set and extend our computations \( \Omega^- \) mass as more lattices become available.

Although it is technically difficult, we have been looking at the masses of excited states in our propagators, and expect to continue this effort in the next year. One promising avenue for improving these calculations is to use different operators to create and destroy the particles, with operators that are engineered to minimize overlap with the ground state. (Ironically, our usual operators are engineered to give good ground state masses, so they minimize overlap with the excited states!) Designing and testing such operators is an exploratory project that we wish to pursue during this grant period. In the real world most of the strongly interacting particles decay via the strong interaction. When the quark masses in a lattice simulation with dynamical quarks are made small enough and the box size large enough that these decays are kinematically possible, the lightest state with given quantum numbers, which is the state whose energy is found in a conventional lattice spectrum calculation, will not be the desired particle mass, but instead the energy of the multiparticle state to which it decays. Our three flavor simulations are now reaching the point where many of the mesons can decay, and a major project for the next few years is to develop the techniques to extract physics from propagators in this regime.

**High temperature QCD with three flavors of quarks:** At very high temperatures one expects to observe a phase transition or crossover from ordinary strongly interacting matter to a plasma of quarks and gluons. A primary motivation for the construction of the Relativistic Heavy Ion Collider (RHIC) at Brookhaven National Laboratory was to observe the quark–gluon plasma and determine its properties. The plasma was the state of matter in the early development of the Universe, and may be a central component of neutron stars today. The behavior of strongly interacting matter in the vicinity of the phase transition or crossover is inherently a strong coupling problem, which can only be studied from first principles through lattice gauge theory calculations. Among the issues that can uniquely be addressed by lattice calculations are the nature of the transition, the properties of the plasma, including strange quark content, and the equation of state. We are engaged in a multi–year effort to carry out detailed studies of these issues using the improved Asqtad action.
In the first phase of this project we have been studying the phase diagram of high temperature QCD and a variety of phenomenologically important quark-number susceptibilities [34]. The second phase of this project is a calculation of the equation of state (energy density, pressure, and entropy vs. temperature), including strange quark fluctuations. These are highly important for the modeling and understanding of heavy ion collisions. The equation of state is central to hydrodynamic models of plasma evolution, and excess strangeness production and strangeness fluctuations have been proposed as a signature for plasma production. However, a first principles quantification is needed for the experimental confirmation of plasma formation. Measurements of the equation of state are expensive, because all thermodynamic quantities are measured relative to the QCD vacuum, and they suffer from ultraviolet divergences. Thus, it is necessary to subtract quantities obtained at zero temperature from results at nonzero temperature. The computational effort therefore scales with the lattice spacing as $a^{-12}$, placing a high premium on algorithmic improvements that permit reliable calculation at moderate $a$. We believe our improved action is ideally suited for this calculation.

We are carrying out our studies of high temperature QCD with resources outside the NSF program, but mention it here and in our progress report, because it constitutes an important part of our research program that was begun with NSF resources.

II. Computational Methodology

We have developed a family of codes for the study of QCD with conventional and improved Kogut-Susskind dynamical quarks, Wilson and Clover–Wilson dynamical quarks, and in the quenched approximation. The dynamical quark codes have compilation options which allow one to choose between the hybrid Monte Carlo and hybrid molecular dynamics algorithms. The quenched approximation code employs the over-relaxed/quasi heatbath algorithm. In all lattice gauge theory calculations, a very significant fraction of the computer time is spent inverting the lattice Dirac operator. Compilation options allow one to choose among the conjugate gradient, stabilized biconjugate gradient (for Wilson quarks) and minimum residual algorithms for this purpose. A manual describing our code in detail can be found at the URL http://www.physics.utah.edu/~detar/milc. The code itself can also be obtained at this URL. We have already described lattice sharing. We estimate about 15 downloads of the code per month. We have, however, no convenient way to judge actual usage, but we do field several questions per month about the code.

We continue to put significant effort into improving the performance of our code. Several of us participate in the DOE-funded SciDAC project for lattice gauge theory, which, over the past three years, has been developing a software framework for the US community of lattice gauge theorists. To take advantage of the considerable optimization effort of that project, we are now incorporating SciDAC modules and optimization strategies in our code. We have already seen considerable improvement in our production code. The performance of the conjugate gradient subroutine for the inversion of large sparse matrices, which uses the bulk of the floating point operations in any lattice gauge theory calculation, increased from 408 to 471 Mflop/s per processor in production runs with 32 processors on the NCSA Tungsten cluster. Given the extensive work that has gone into optimizing this subroutine in the past, and the large number of floating point operations it consumes, we were very pleased by this 15% improvement. The calculation of the fermion force uses the second greatest number of floating point operations in our code. Over the past year its performance in production runs with 32 processors on the Tungsten cluster improved by 50% from 360 to 538 Mflop/s per processor. Working on the Fermilab Xeon cluster, which is similar in architecture to the Tungsten cluster, but has slower processors, we improved the performance of our double-precision multi-mass conjugate gradient inverter by 97%. This subroutine will play an important role in our studies of the weak decays of strongly interacting particles during the coming year. The fermion force and multi-mass inverter subroutines are newer and have received
less attention in the past than the standard conjugate gradient subroutine, so they have gained far more from our optimization efforts.

At PSC we have been working with staff to improve performance through testing on Lemieux and Tcsini. On Lemieux, we have provided detailed performance data from production runs and histogrammed the variation during our runs. After an OS upgrade this Spring, we tested the new system and demonstrated increased performance from about 300–325 Mflop/s per processor to 340–350 Mflop/s per processor. A great deal of effort had previously gone into optimizing the code running on Lemieux, so we regard this improvement as significant. We have also provided performance data from production runs to help track down network hardware problems. On Tcsini, we have done extensive running on an experimental OS.

III. Progress to Date

In the attachment titled Progress Report, we review the research we have carried out at the NSF Centers since submitting our last NRAC proposal, and list papers that were published or submitted for publication during that period. Results from most of the projects discussed in the Progress Report were presented at Lattice 2004 in June. The attachment titled Figures Illustrating Recent Results shows some of this work. The figures referred to in this section are found in that attachment. Major results include the evaluation of the decay constants for $\pi$ and $K$ mesons to an accuracy of better than 3% (Figures 3 and 4); the first determination of the up, down and strange quark masses in full QCD in the continuum limit (Figure 5); progress towards high precision calculations of decay constants and form factors for $D$ and $B$ mesons (Figures 6 and 7); progress in the study of the light hadron spectrum, including the evaluation of the mass of the $\Omega^-$ (Figures 2 and 10); progress in mapping the phase diagram for three-flavor QCD (Figure 11); the first determination of the baryon, isospin and hypercharge density susceptibilities in full QCD (Figure 12); and improved evaluation of the topological susceptibility for light quark masses (Figure 13).

IV. Resource Justification

A breakdown of our request by projects and computing platforms is given in Table 2. We request a total 2,105,000 processor-hours on the PSC Alpha-Server, Lemieux, and 1,743,200 processor-hours on the NCSA Xeon cluster, Tungsten. Note, that in our NRAC allocation that began on October 1, 2003, we were awarded 2,829,200 processor-hours on Tungsten. However, because of the delay in Tungsten going into production use, this allocation was moved to the period April 1, 2004 to March 31, 2005. So our request for time on Tungsten in this proposal covers the period April 1, 2005 to September 30, 2005. Although we have not requested time for production work at SDSC, we do ask that our accounts on DataStar be kept open, as they have been this year, so that we can continue to access the large amount of data we have in archival storage at SDSC.

<table>
<thead>
<tr>
<th>Project</th>
<th>Lemieux</th>
<th>Tungsten Cluster</th>
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<tbody>
<tr>
<td>Lattice Generation</td>
<td>2,105,000</td>
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<tr>
<td>Light Pseudoscalars</td>
<td></td>
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<td>Leptonic Decay Constants</td>
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<td>449,000</td>
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<td>Semileptonic Form Factors</td>
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<tr>
<td>Light Hadron Spectrum</td>
<td></td>
<td>286,300</td>
</tr>
<tr>
<td>Totals</td>
<td>2,105,000</td>
<td>1,743,200</td>
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Generation of lattices with improved gauge and quark actions: Our major lattice generation efforts in the next year will be the extension of the $m_{u,d} = 0.1 m_s$, $a = 0.09$ fm run, and the beginning of a series of simulations at $a \approx 0.06$ fm. We hope to do the first of these with non-NSF machines, using NSF resources for the analysis of these configurations and for the 0.06 fm run.

Time estimates for the $a = 0.06$ fm simulation at $m_{u,d} = 0.4 m_s$ can be obtained by scaling up the timings for a trial trajectory run on the NCSA Tungsten cluster. This trajectory used 900 Xeon processor-hours to run one time unit on a $28^3 \times 96$ lattice. We therefore need $900 \times (40^3 \times 144)/(28^3 \times 96) = 3940$ Xeon processor-hours per time unit. Since the Xeon and Lemieux processor give very similar performance for this sized lattice, we estimate that running for 500 time units on the PSC Alpha-Server, Lemieux will require $500 \times 3940 = 1,970,000$ processor-hours.

In addition we need a short “tuning” run to prepare for a simulation at $m_{u,d} = 0.2 m_s$. Again scaling up from the time used by the test run, this will take 135,000 processor hours on Lemieux. So, our total request for lattice generation is 2,105,000 processor-hours on Lemieux.

Hadron mass spectrum with the improved action: We are calculating the masses of the simplest light hadrons, the heavy quark potential and the partially quenched light pseudoscalar masses and decay constants as we generate the lattices. We propose to continue the $a = 0.09$ fm, $m_{u,d} = 0.1 m_s$ simulation with non-NSF resources, and hope to have a minimum of 200 equilibrated lattices by October 1, 2005. We expect have analyzed 100 of these lattices by the end of our current grant period. On the NCSA Tungsten cluster each such lattice requires 1250 processor-hours for the light hadron spectrum, 250 hours for the $\Omega^-$ propagators, and 1500 hours for the partially quenched pseudoscalars. Thus, computation of the spectrum on these lattices will require $100 \times (1250 + 250 + 1500) = 300,000$ processor-hours.

We will also need to compute the spectrum, static potential, and light pseudoscalar decay constants on the first $a = 0.06$ fm run. We propose to simulate 500 time units at $m_{u,d} = 0.4 m_s$, of which we estimate 150 will be required for equilibration. We are computing these quantities every six time units, so we will have 58 equilibrated lattices. Time estimates for the spectrum and light decay constant calculations are obtained by scaling up the above numbers by the ratio of the volumes. In the case of the light hadron spectrum, we also scale by the inverse ratio of the light quark masses, since the heavier $u$ and $d$ quarks in this run will require fewer conjugate gradient iterations. For the partially quenched pseudoscalars there is no quark mass factor in the rescaling, since we will still need to run with light ($\geq 0.1 m_s$) valence quarks. Thus, the analysis of a single lattice requires $1250 \times (40^3 \times 144)/(28^3 \times 96) \times (0.0031/0.0072) = 2,350$ processor-hours for the light hadron spectrum and static potential, and $1500 \times (40^3 \times 144)/(28^3 \times 96) = 6550$ processor-hours for the partially quenched pseudoscalars. Therefore the analysis of these quantities for the anticipated 58 equilibrated lattices requires $58 \times (2,350 + 6,550) = 516,200$ processor-hours on the Tungsten cluster.

Weak decays of particles containing heavy quarks: Analysis of the leptonic decay constants and semileptonic form factors of $B$ and $D$ mesons on our $a = 0.12$ fm lattices is nearly complete, and time is available for this analysis on our $a = 0.09$ fm lattices with $m_{u,d} = 0.4 m_s$ and $0.2 m_s$ in our current allocation on the Tungsten cluster and a joint allocation with our Fermilab collaborators on the SciDAC FNAL Xeon cluster. In this proposal we request time for the most important and difficult ensemble of $40^3 \times 96$, $a = 0.09$ fm, $m_{u,d} = 0.1 m_s$ lattices, which is currently being generated. We request time to analyze 200 of these lattices.

We can estimate the time required for the calculation of leptonic decay constants based on our current running. To permit a controlled extrapolation to zero lattice spacing, our parameter choices and ensemble selection for the $a = 0.09$ fm lattices must match the choices we have made for the nearly completed analysis of the $a = 0.12$ fm lattices. Working in double precision for light quark masses down to $0.1 m_s$ and using four source planes per lattice and two heavy quark masses (charm
and bottom) will require approximately $2,245$ processor-hours per $40^3 \times 96$ lattice on the NCSA Tungsten cluster. So, the total cost will be $200 \times 2,245 = 449,000$ processor-hours.

The semileptonic form factor project on the $a = 0.09$ fm lattice ensembles will reuse the quark propagator files generated in the leptonic form factor project. One calculation will be carried out for the case that the virtual quarks and valence quarks are of equal mass and one for which they have unequal masses. Based on our current runs, the cost per lattice is $2,390$ processor-hours on Tungsten. So, $200 \times 2,390 = 478,000$ processor-hours are requested for the analysis of 200 lattices.

V. Local Computing Environment

The bulk of our code development, debugging and data analysis is done on collaboration-member workstations. They are, of course, inadequate for carrying out all but our smallest simulations, or for storing the large lattices generated in our work. Some of us have access to larger local campus resources for code testing, and small to moderate sized projects; through the University of Utah Center for High Performance Computing, CD has modest allocations on a 256-node Linux Opteron cluster; at Indiana University, SG has access to an IBM SP Power 3, two 32 node Linux clusters and two 96-node dual-cpu Xeon clusters; at UCSB RS has access to a 128 node Xeon cluster.

VI. Current and Pending Allocations of Supercomputer Time

Our current NRAC grant, MCA93S002, provides a total of 1,677,000 service units on Lemieux and the Teragrid for the period October 1, 2003 to September 30, 2004. This grant originally contained an allocation of 2,829,200 service units on the Tungsten Cluster for the same period. However, because of the delay in Tungsten going into production use, this allocation has been moved to the period April 1, 2004 to March 31, 2005. We also have an allocation of 2,525,000 processor-hours on the NERSC IBM SP, which is being used for the generation of $40^3 \times 96$ lattices at $a \approx 0.09$ fm and $m_{u,d} = 0.1 m_s$. This allocation runs through November 30, 2004. We are preparing a proposal for a new allocation in which we will request resources to extend this run. We have a joint allocation with our collaborators at Fermilab of 830,000 processor-hours on the SciDAC FNAL cluster for the study of the weak decays of particles containing heavy quarks. Most of this time will be used for the analysis of the $a = 0.09$ fm, $m_{u,d} = 0.4 m_s$ and $0.2 m_s$ lattices. We have an allocation of 250,000 processor-hours on the SciDAC Jefferson Laboratory cluster for the study of high temperature QCD. We are part of an effort by the U.S. lattice gauge theory community to obtain computational resources for our field. In response to this effort, Department of Energy has recently announced plans to fund a special purpose computer for the study of lattice gauge theory, the QCDOC. Construction of this computer, which is expected to have a total throughput of 3 to 5 Tflop/s depending on the specific application, is scheduled for completion in the spring of 2005. We hope to gain access to it in order to accelerate and enhance the research program set out in this proposal. By the end of the proposal period we hope to move our lattice generation to the QCDOC, and devote our use of the more flexible NSF computers to extracting physics from the lattices. We believe that this approach will optimize our use of both types of machines. Finally, as members of the Lattice Gauge Theory SciDAC Project, we have access to computing facilities Oak Ridge National Laboratory, which we are using to generate additional coarse lattices.

VII. Qualifications of the Principal Investigators

The principal investigators have had extensive experience in lattice gauge theory. Our research has covered a broad range of topics in this field, including high temperature QCD, the hadron mass spectrum, and weak decays of strongly interacting particles. It has involved the development of new algorithms and calculational techniques, small exploratory calculations, and very large simulations. A list of the publications of our collaboration, the current members of our group, and the vita of the principal investigators are provided in an attachment.
References


