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. It 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 the Standard Model 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 allocations to develop an improved action (improved 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 available to lattice gauge theorists, and major improvements in the performance of our code, have enabled us to make important progress in our research. During the coming year our work will be greatly enhanced through access to the QCD on a Chip (QCDOC) computer that has recently been constructed at Brookhaven National Laboratory with funding from the Department of Energy. The QCDOC was custom designed for the study of QCD by a collaboration centered at Columbia University, and will be dedicated to our field. Our group has been allocated approximately 50% of the time on the QCDOC during its first year of operation to generate gauge configurations (snapshots of the system we are simulating) using the improved Asqtad action. These configurations or lattices will be made available immediately to the entire U.S. lattice gauge theory community, and with a modest delay to the international community. The bulk of the computer time in any lattice QCD calculation goes into the generation of gauge configurations, which are saved and then used to calculate a wide variety of physical quantities. The configurations we plan to generate during the coming year will significantly reduce the two largest sources of error in our calculations: extrapolations to the continuum (zero lattice spacing) and chiral (physical masses of the up and down quarks) limits. The QCDOC is ideally suited for the generation of gauge configurations. If it performs as anticipated, we will move all of this component of our work to it. On the other hand, the computers provided by the NSF centers are far better suited for the extraction of physics from stored configurations than the QCDOC, because of their greater programing and communications flexibility, and their superior I/O characteristics. Therefore, in this proposal we request time only to perform physics analysis on configurations already in hand or planned to be produced with the QCDOC. By making use of each type of computer for the component of our work for which it is best suited, we will optimize our scientific output, and greatly enhance the return on the long term investment the NSF has made in our 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 gauge configurations we have already generated and those we are planning to generate. The portion of the study relevant to this proposal is contained in the attachment titled Impact of the Asqtad Gauge Configurations. One notes that in all cases analyzed in this study for which experiments have been performed, the current lattice error is significantly larger than the experimental one. Our objective is to reduce the lattice errors so that they are less than or comparable to the experimental ones. The importance of doing so 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.

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 some quantities whose values are well known experimentally. Since these calculations make use of the same configurations 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 carried out such a study working in collaboration with several other groups that are making use of our configurations [3]. Some of our results are shown in Figure 1 of the Progress Report contained in an attachment. 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].

More recently the HPQCD and UKQCD Collaborations have used our configurations to make the first determination of the strong coupling constant in full QCD [8]. Their result is in agreement with the world average from other approaches compiled by the Particle Data Group, but has somewhat smaller errors. There have also been a number of important predictions made with our configurations that have subsequently been confirmed by experiments. These include our joint work with the Fermilab Lattice Collaboration predicting the leptonic decays constants of the $D$ and $D_s$ mesons [9], and the form factors describing the semileptonic decays of these particles [10]. They also include the Fermilab Lattice and UKQCD Collaborations’ prediction of the mass of the $B_c$ meson [11]. This work indicates that we are in a position to determine a wide range of physical quantities of great importance to the phenomenology of high energy and nuclear physics.

In Section II, we describe our code and recent work that has improved its performance. 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 justification for our resource request. We request a one year allocation with a total of 6,068,500 service units. A breakdown of our request by projects and computing platforms is given in the attachment titled Resource Request by Projects. Our request is to support the work of six principal investigators, their postdoctoral research associates and graduate students. Thus, it comes to 1,011,417 service units per principal investigator. A description of our local computing environments, current and pending allocations of supercomputing time, and the qualifications of the principal investigators is given in the attachment titled Computer Resources. A complete list of of publications of our collaboration, the current members of our group, and the vita of the principal investigators are provided in the attachment Publications and People.

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

**Generation of gauge configurations with improved gauge and quark actions:** The ensembles of gauge configurations that we have generated are the basis for a wide variety of physics calculations by our group and by others; but, as is discussed below, in order to determine some of the most interesting quantities we are studying to an accuracy required by experiment, it is necessary to push our simulations to smaller lattice spacings and quark masses. We therefore plan to continue to generate gauge configurations. However, by the start of this grant, we expect to move all of our configuration generation to the QCDOC.

Configurations are being generated 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. We are working 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. We currently have ensembles at three different lattice spacings, $a \approx 0.18$ fm, 0.12 fm and 0.09 fm. Since the leading discretization errors are of order $a^2/\log(a)$, they are expected to be in the ratio 1.00/0.40/0.18 for these three ensembles. Measuring physical quantities in all three ensembles enables us to estimate the size of systematic errors arising from finite lattice spacing, and to perform extrapolations to the continuum limit. By the end of August 2005, we expect to complete generation of and make some basic measurements on ensembles with $a \approx 0.15$ fm, which should further help us to better understand the lattice spacing dependence of physical quantities. Of course, vastly greater computer resources will be needed to extend our calculations to smaller lattice spacing, which is essential for controlling 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 other formulations. 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 tastes 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 [12]. Furthermore, one of us (CB) has developed techniques, based on the pioneering work of Lee and Sharpe [13] for incorporating the effects of taste symmetry breaking into chiral perturbation theory [14, 15, 16], thereby significantly improving our ability to make extrapolations to the chiral and continuum limits.

Another difficulty with staggered quarks is that each Kogut-Susskind field represents four tastes of quarks with discretization errors included ("staggered chiral perturbation theory" [13, 14, 15, 16] — S$^4$PT). The latter allows us to fit the lattice data accurately, including the effects of $O(a^2)$ lattice spacing errors, and then

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 check our lattice methods to high ($\approx 2$ to 3%) precision, and to 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 [20]. This formalism has been extended to the "partially quenched" case [21], where valence and sea quark masses are different, and, further, to the case of staggered quarks with discretization errors included ("staggered chiral perturbation theory" [13, 14, 15, 16] — S$^4$PT). 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 \(m_l\)) followed by a controlled continuum extrapolation.

Using the above method, we have computed the leptonic decay constants of the \(\pi\) and \(K\) mesons, \(f_\pi\) and \(f_K\), with total errors 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. A calculation of \(f_K/f_\pi\) enables one to determine the CKM matrix element \(V_{us}\). Our current value is \(|V_{us}| = 0.2219(26)\), which is consistent with the world average value \(|V_{us}| = 0.2200(26)\) [22] determined from alternative methods.

The same computational method, coupled with perturbative calculation of the mass renormalization constant, has allowed us to determine quark masses (the mass of the strange quark, \(m_s\), the average mass of the \(u\) and \(d\) quarks, \(m_t\), and the ratio \(m_u/m_d\)) and several of the so-called Gasser-Leutwyler parameters, \(L_i\) [20]. 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 \(\epsilon'/\epsilon\) [23]. Determination of \(m_u/m_d\) addresses the long standing proposal [24] that \(m_u = 0\). A massless up quark could have solved the “Strong CP Puzzle” [25]; however, our results rule that possibility out at the 10\(\sigma\) level. Our current results [3, 26, 27] 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 masses and fine lattice spacing. We estimate that the configurations with lattice spacing \(a \approx 0.09\) fm and light quark mass \(m_l = 0.1m_s\), along with those at lattice spacing \(a \approx 0.06\) fm, will allow us to reduce the systematic errors on \(f_\pi\) and \(f_K\) to 2% or better, which would be an important milestone for lattice QCD calculations. We expect corresponding improvements in other physical quantities of interest. In particular, our evaluation of \(|V_{us}|\) should become more accurate than the current world average. 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 of the section *CKM Matrix Elements* in the attachment *Impact of the Asqtad Gauge Configurations*, would have a broad impact on the study of the Standard Model.

**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 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.

Our group and the Fermilab Lattice Collaboration are involved in an extensive joint study of the decays of pseudoscalar mesons with one light and one heavy quark. The main objects of our work are \(B\) (with a heavy \(b\) quark and light \(u\) or \(d\) antiquark), \(B_c\) (\(b\) quark and \(s\) antiquark), \(D\) (\(c\) quark and \(u\) or \(d\) antiquark) and \(D_s\) (\(c\) quark and \(s\) antiquark). We are studying both leptonic and semileptonic decays. Strong interaction effects in leptonic decays are characterized by the decay constants \(f_B, f_{B_c}, f_D, f_{D_s}\). Semileptonic decays are characterized by various form factors \(F(q^2)\), where \(q\) is the momentum transfer carried by the leptons. CLEO-c is providing precise measurements of the \(D\) and \(D_s\) leptonic and semileptonic decays. Comparisons of lattice and experimental results offer a unique opportunity to validate our approach, and insure that we do, in fact, have full control over systematic errors. The successful predictions of the leptonic decay constants [9] and the shape and normalization of the semileptonic form factors [10] for \(D\) mesons by us and our Fermilab collaborators is a first step in this process. We are now in a position to carry out similar calculations for the \(b\)-quark system, where the corresponding quantities have not been measured, and are unlikely to be in the near future. 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 \(V_{ub}\) 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 \(V_{ub}\). These calculations are in progress [28]. 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 are doing this with the same techniques that are being employed for our studies of the \(D\) mesons.

To achieve an accurate determination of the CKM matrix elements, it is essential that all sources of sys-
tematic error in the lattice calculations be overcome and controlled—more so than in any previous attempt [29, 30, 31, 32, 33, 34, 35, 36]. 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 our goal over the next two years, thanks to the following developments: (1) our generation of an extensive archive of gauge configurations incorporating the effects of dynamical up, down and strange quarks; (2) the availability of the QCDDOC, which will enable the generation of gauge configurations at a lattice resolution of $a \approx 0.06$ fm with reasonably light quark masses, and the enhancement of NSF computing facilities to the level needed to analyze these configurations; (3) the use of the improved Asqtad action for light valence, as well as sea quarks, which enables us to work with significantly lighter valence quarks than was previously possible; (4) the development of an improved formulation of heavy quarks on the lattice by the Fermilab group; (5) an extension of staggered chiral perturbation theory to decays of $B$ and $D$ mesons that determines both the dependence on light quark masses and the leading discretization errors [16]; and (6) automated perturbation theory [37] to compute the renormalization factors. Development (4) makes possible a significant reduction in systematic errors associated with Compton wavelengths that are comparable to the lattice spacing, and (2), (3) and (5), a reduction in errors associated with the light quark mass (chiral) and continuum extrapolations.

**Hadron mass spectrum with the improved action:** Calculation of the spectrum of the light hadrons is an essential test of lattice simulations. The nucleon and $\Omega^-$ masses are precisely known, and can be computed accurately on the lattice, making them trenchant tests of our techniques. 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 customarily 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.

An accurate determination of the mass of the nucleon has been a long term problem for lattice gauge theorists. The major difficulty has been the extrapolation to the physical value of $m_l$. We expect to improve the accuracy of this extrapolation through the use of our new light quark mass, fine lattice spacing configurations, coupled with a staggered chiral perturbation theory calculation of the dependence of the nucleon mass on $m_l$ being carried out by a graduate student, Jon Bailey. In addition to better fitting and extrapolation techniques, we also expect to improve our results by simultaneous fitting to nucleon and delta propagators, since the delta appears as an excited state in nucleon propagators with Kogut-Susskind quarks. We have calculated the $\Delta$ and $\Omega^-$ masses on all of the gauge configurations generated to date, and propose to do so on the ones we create during the coming year. We are also investigating improved sources and sinks for the nucleon and other light baryons.

**Partially quenched baryon masses:** In collaboration with Matthew Wingate and Andre Walker-Loud, we plan to apply the partial quenching technique that was so important for the study of light pseudoscalars to the study of baryons. As with the pseudoscalars, having a large number of data points with different valence quark masses should allow us to determine the many parameters that appear in chiral perturbation theory, be it staggered (as under investigation by Bailey) or in the continuum [38].

**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 [40]. Recent work is reviewed in the progress report. During the past year we have completed a study of the equation of state of high temperature QCD at zero baryon density. In the coming year we plan to extend this work to the small baryon densities relevant to the relativistic heavy ion collision experiment experiments in progress at Brookhaven National Laboratory. We plan to make use of the Bielefeld-Swansea Taylor series method for this phase of our work [41].

II. Code Maturity and Development

We have developed a family of highly portable codes for the study of QCD with conventional and improved Kogut-Susskind dynamical quarks, improved Wilson (Clover) dynamical quarks, and in the quenched approximation. Compilation options allow one to choose among different architectures, different formulations of lattice QCD, and different algorithms for carrying out simulations. Version 7 of the code is currently under development. 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. It has been our policy for some time to make our code and the large gauge configurations we generate with it publicly available. Most of our configurations are available from the NERSC Gauge Connection http://qcd.nersc.gov. A list of papers based on our configurations, and a table enumerating them is given in the attachment Impact of the Asqtad Gauge Configurations. We estimate about 15 downloads of the code per month, and we field several questions per month about it.

We continue to put significant effort into improving the performance and flexibility of our code. Several of us participate in the DOE-funded SciDAC project for lattice gauge theory, which, over the past 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, Version 7 of the MILC code interoperates with SciDAC modules and incorporates SciDAC optimization strategies. We have already seen considerable improvement in our production code. For example, 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 580 Mflop/s per processor in dual-node, single-precision production runs with 32 processors on the NCSA Tungsten cluster. The comparable figure for the NCSA Teragrid machine is 680 MFlop/s. The corresponding Lemieux figure is 340–350 MFlop/s.

At PSC, we have been working with staff to shake down the new Cray XT3, and have recently started to work with Cray to improve the Streaming SIMD Extension (SSE) coded kernels that work so well for our code on the Pentium 4 architecture, but do not seem to do as well on the AMD Opteron.

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, list papers that were published or submitted for publication during that period, and show figures illustrating some of our recent work. Results from most of the projects discussed in the Progress Report will be presented at Lattice 2005 in July.

IV. Resource Justification

A breakdown of our request by projects and computing platforms is given in the attachment Resource Request by Projects. We request 2,577,000 processor-hours on the NCSA Tungsten Cluster, 1,891,500 processor-hours on the PSC Cray XT3, and 1,500,000 processor-hours on the Teragrid Itanium Clusters. Our code performs similarly on a per processor basis on each of these platforms, so our projects can be moved among them if that would help with load balancing. The timing estimates below refer to these three machines, and unless otherwise noted come from benchmarks on one or more of them. On the PSC Alpha-Server Lemieux, our code runs at approximately 60% the speed obtained on the above machines, so if part of our request is moved to Lemieux, we ask that the number of transferred service units be increased by a factor of 1.67. We are eager to try the SDSC BlueGene/L and request an allocation of 100,000 processor-hours on it to adapt our code and run benchmarks on production sized jobs. Although we have not requested time for production work on DataStar at SDSC, we do ask that our accounts on DataStar be kept open, as they have been for the last two years, so that we can continue to access the large amount of data we have in archival
Generation of lattices with improved gauge and quark actions: Our major lattice generation efforts in the next year will be the extension of the $m_l = 0.1 m_q$, $a \approx 0.09$ fm run, and a series of simulations at $a \approx 0.06$ fm. We plan to do these runs on the QCDOC, and then move the configurations to NSF centers for physics analysis.

Hadron mass spectrum and decays of light pseudoscalar mesons: We calculate the masses of the simplest light hadrons, the heavy quark potential and the partially quenched light pseudoscalar masses and decay constants as soon as we generate the lattices. We request resources to analyze 200 new $a \approx 0.09$ fm, $m_l = 0.1 m_q$ configurations during the coming year. On the NCSA Tungsten cluster each such lattice requires 1,200 processor-hours for the light hadron spectrum, 530 hours for the $\Omega^-$ propagators, 920 hours for the Delta baryon, and 800 hours for the partially quenched pseudoscalar masses and decay constants. Thus, the total time for these calculations will be $200 \times 3,450 = 690,000$ processor-hours. For the lattice with $a \approx 0.06$ the grid size is $48^4 \times 144$. Taking into account the number of conjugate gradient iterations needed for convergence for $m_l = 0.4 m_q$, we find that on the Tungsten cluster each such lattice requires 2,200 processor-hours for the light hadron spectrum, 420 hours for the smeared potential, 2040 hours for the $\Omega^-$ and Delta propagators, and 3600 hours for the partially quenched pseudoscalars. Thus, computation of the spectrum on 200 of these configurations will require $200 \times 8,260 = 1,650,000$ processor-hours. We had not yet produced any $m_l = 0.2 m_q$ configurations, but we can estimate the change in the number of CG iterations. (For the partially quenched pseudoscalars there is no quark mass factor in the rescaling, since we will still need to run with light ($\geq 0.1 m_q$) valence quarks.) We estimate the following requirements: 4,400 processor-hours for the light hadron spectrum, 420 hours for the smeared potential, 3,060 hours for the $\Omega^-$ and Delta propagators, and 3,600 hours for the partially quenched pseudoscalars. For the 125 configurations we expect to generate on the QCDOC, the total requirement is $125 \times 11,480 = 1,435,000$ processor-hours. Thus, are total request for the spectrum calculations, and decays of light pseudoscalar mesons is 3,777,000 processor-hours, which we propose to divide between the Teragrid and Tungsten Clusters.

Weak decays of particles containing heavy quarks: Analysis of the leptonic decay constants of $B$ and $D$ mesons on our $28^3 \times 96$ $a \approx 0.09$ fm lattices is nearly complete. Essential goals for the coming year are to analyze the $40^3 \times 96$, $a \approx 0.09$ fm configurations that are still being generated and to make substantial progress on the $a \approx 0.06$ configurations just being started. (This is a joint project with Fermilab and we have been allocated 3,000,000 node-hours on a SciDAC funded cluster for this work.) In this proposal we request time to analyze 200 of the $40^3 \times 96$, $a \approx 0.09$ fm, $m_l = 0.1 m_q$ lattices, and 100 of the $48^3 \times 144$, $a \approx 0.06$ fm, $m_l = 0.4 m_q$ lattices. Working in double precision for light quark masses down to $0.1 m_q$ 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 Cray TX3. So, the total cost will be $200 \times 2,245 = 449,000$ processor-hours. The larger configurations will require 2.6 times as many floating point operations because of the larger volume, as well as an addition factor of $(0.031/0.018)$ because the inversions will require more iterations for lighter quark mass. This amounts to a factor of 4.5 or 10,100 hours per configuration. To analyze 100 configurations will require 1,010,000 cpu-hours. Thus, we request a total of 1,460,000 cpu-hours for the study of weak decays.

Partially quenched baryon masses: We propose to begin the partially quenched baryon study by analyzing our $a \approx 0.12$ fm configurations with light quark masses $m_l = 0.1 m_q$, 0.2$m_q$, and our $a \approx 0.09$ fm configurations with $m_l = 0.2 m_q$ and 0.4$m_q$. This project will require some code modification, so we do not yet have an exact timing. However, the computation is comparable to that for the $\Delta$ baryon calculation, so we base our timing estimates for this calculation on it. We conclude that the analysis of each $a \approx 0.12$ fm configuration will require 77 processor-hours on Tungsten, and each $a \approx 0.09$ fm configuration will require 316 processor-hours. Thus, the total time required for the 1,500 coarse configurations we propose to analyze is $1,500 \times 77 = 115,500$ processor-hours, and that for the 1,000 fine configurations is $1,000 \times 316 = 316,000$ processor-hours. So the total for the project is 431,500 processor-hours.

High temperature QCD with three flavors of quarks: The computational methodology at nonzero density is very similar to that at zero density. The necessary observables have not been coded yet, so there are no timing figures, but based on time required on Tungsten and the NCSA Teragrid for our just-completed zero-density project we estimate we will need 300,000 processor-hours in the latter half of the coming year to begin this two-year effort.
References


