Simulations with Dynamical Domain Wall Fermions

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(Dated: March 28, 2007)

We propose to use USQCD resources at BNL, JLab or FNAL for the generation of lattice configurations using 2+1 flavors of domain wall dynamical fermions. This work would provide two new streams of configurations with size $32^3 \times 64$, lattice spacing $a = 0.093$ fm and light quark masses of 1/5 and 1/7 of the strange quark mass. We also describe further generation of lattice configurations with smaller quark masses and appropriately larger volumes which would provide an important extension to this work and could be carried out on additional resources expected to become available at other DOE facilities. In addition to this configuration generation,

we also propose to use a modest fraction (20%) of this time to calculate a series of "standard" fermion propagators measured with a smeared Gaussian source and quark masses which match those used in generating the configurations. Our complete proposal requests 60 million QCDOC processor hours (eight of the twelve QCDOC racks at BNL) or the equivalent spread across the various available resources.

I. INTRODUCTION

Lattice fermion formulations which preserve chiral symmetry even at non-zero lattice spacing provide a critical opportunity to study the chiral and continuum limits independently. With the usual Wilson and staggered fermion formulations finite lattice spacing errors become more serious as the chiral limit is approached, requiring that the very difficult limit of vanishing lattice spacing be performed at the smallest quark masses. In contrast, with the domain wall or alternative chiral formulations, these two sources of errors can be studied independently.

For many quantities of physical interest chiral symmetry plays a vital role. The challenging task of computing nucleon structure functions or kaon decay matrix elements becomes substantially more practical if chiral symmetry can be used to limit the number of operators which must be studied. In fact, many calculations in these areas cannot even be attempted without a chirally symmetric fermionic formulation. While interesting work can be done using chiral valence quarks and lattice configurations generated with a different, non-chiral fermion formulation, the ultimate goal must be a fully unitary calculation with the accompanying clear control of systematic errors. This requires that gauge configurations be generated using lattice chiral fermions.

Aided by the recent advances in algorithms and the large capabilities of the QCDOC machines, the RBC and UKQCD collaborations have been generating a series of such gauge configurations using domain wall fermions. As is described in greater detail below, this has resulted in a series of lattice configurations with two lattice volumes and a single lattice spacing. This work has now expanded to include a second lattice spacing and it is these very demanding smaller lattice spacing calculations that we propose to extend in this proposal.

Given the importance of chiral fermions to nucleon physics which is a major goal of the

LHPC collaboration, it is natural for LHPC to play a central role in this effort. As a result, this present proposal is being made jointing by the LHPC and RBC collaborations. As is discussed below, this proposal is carefully coordinated with the configuration generation and calculation of physical observables that is underway in the UK. Substantial additional configurations are expected to be created using UK resources, further extending the physics reach of the project proposed here.

An important additional component of this proposal is the calculation of a series of fermion propagators using the lattices that are being generated. State-of-the-art calculations of the weak matrix elements that enter kaon decay or the matrix elements of 2-quark operators between nucleon states needed to calculate form factors or structure functions require specialized techniques with highly refined sources, tailored to the problem at hand. While these propagators could be made generally available, they are of limited utility beyond the specific project for which they were computed. Even when two groups intend to study the same physics, their choices for these specialized propagators are often quite different.

However, there is a clear need for what might be called “standard” propagators computed with a smeared Gaussian source with good overlap with meson and nucleon ground states. These propagators are typically computed by any group working on a given set of lattices and are used to compute the hadron spectrum and simple matrix elements. The results provide immediate estimates of the lattice scale and the quark masses. These propagators are often also woven into the more complex calculations of other more difficult quantities. We propose to calculate such propagators for the configurations which are part of this proposal. These will be of immediate use to the LHPC, RBC and UKQCD collaborations. In addition, by making them available with the lattice configurations, we will enable other groups or individuals to easily carry out basic measurements on these configurations with the use of little additional resources.

II. PRESENT DWF CONFIGURATIONS

We will now briefly outline the DWF lattice configurations that have already been generated by the RBC and UKQCD collaborations using their own resources as well as past USQCD allocations. This configuration generation began with an exploration of parameter space in the Spring of 2005. As a result of this work, it was decided to use the Iwasaki gauge action to provide reasonable suppression of explicit chiral symmetry breaking and adequate tunneling between topological charge sectors. An appropriate gauge coupling (to yield a lattice spacing of ∼1.6 GeV) and bare strange quark mass were also determined. This preliminary work is described in Ref. [1]

Actual production running on $16^3 \times 32$ configurations was then begun with first preliminary results reported in the Dublin meeting in August 2005 [2–8] and a complete description of these results is presented in Ref. [9]. The lattice volumes were then expanded to $24^3 \times 64$ and important algorithmic improvements implemented and tuned in the fall and winter of 2005. Production runs were completed for three light quark masses on the $16^3 \times 32$ volumes and corresponding runs carried out on $24^3 \times 64$ as listed in Table I. This table also shows a new set of configurations generated with a lighter, 0.005 quark mass corresponding to a 305 MeV pion.

	Run #	Volume	m_l/m_s	m_π(MeV)	Time units
RBC	1	$24^3 \times 64$	0.005/0.04	305	3805
UKQCD	2	$16^3 \times 32$	0.01/0.04	389	4000
UKQCD	3	$24^3 \times 64$	0.01/0.04	389	3735
UKQCD	4	$16^3 \times 32$	0.02/0.04	518	4000
RBC	5	$24^3 \times 64$	0.02/0.04	518	2850
UKQCD	6	$16^3 \times 32$	0.03/0.04	620	4000
RBC	7	$24^3 \times 64$	0.03/0.04	620	2813

TABLE I: Current dynamical domain wall fermion production runs with $1/a = 1.62$ GeV. These all use the Iwasaki gauge action with $\beta = 2.13$ and an extent in the fifth dimension of $L_s = 16$. Here the run lengths are specified in time units. The contribution of the residual mass, $m_{\rm res} \approx 0.003$, is not included in quark masses listed in column 4 but, of course, is reflected in the measured pion masses shown in the fifth column.

While the $m_l = 0.02$ and 0.03 runs are now considered complete, additional configurations will be collected for the $m_l = 0.01$ and 0.005, $24^3 \times 64$ runs, extending them to perhaps twice their present length. This will be done using a portion of the remaining USQCD DWF allocation and RBC resources.

As presented in the 2006-2007 RBC proposal for USQCD computer time, we have begun generation of configurations at a second, smaller lattice spacing with $1/a = 2.16$ GeV at two reasonably small light quark masses, 0.004 and 0.006, corresponding to approximately 1/7 and 1/5 of the strange quark mass. One of these streams is being generated on the US DOE 4K QCDOC machine recently made available. The other is being carried out in the UK. These two runs are listed Table II.

	Run #	Volume	m_l/m_s	m_π(MeV)	Time units
RBC	8	$32^3 \times 64$	0.004/0.03	315	1400
UKQCD	9	$32^3 \times 64$	0.006/0.03	261	1400

TABLE II: Current dynamical domain wall fermion production runs with $1/a = 2.16$ GeV. These all use the Iwasaki gauge action with $\beta = 2.25$ and an extent in the fifth dimension of $L_s = 16$. Here the run lengths are specified in time units. The contribution of the residual mass, $m_{\rm res} \approx 0.0004$, is not included in quark masses listed in column 4 but, of course, is reflected the measured pion masses shown in the fifth column. The number of time units collected as of this writing are 174 and 500 for rows 8 and 9 respectively. The time units shown in the table are the numbers expected to be completed by June 2007, the end of the current allocation period.

III. PROPOSED CONFIGURATIONS

These new $32^3 \times 64$, $a = 0.093$ fm lattice configurations play a critical role in the domain wall fermion program of the LHPC, RBC and UKQCD collaborations. They represent a second lattice spacing, permitting tests of scaling and a bound on finite lattice spacing errors to be determined when combined with the earlier $24^3 \times 64$, $a = 0.123$ fm ensembles. Since the residual chiral symmetry breaking decreases rapidly with decreasing lattice spacing, these $a = 0.093$ ensembles, generated with the same $L_s = 16$, fifth-dimensional extent as the earlier lattice configurations are expected to have substantially smaller residual chiral symmetry breaking. By comparing detailed fits to the chiral limit and the chiral symmetry breaking seen in off-shell Rome-Southampton Green's functions between these two lattice spacings we will obtain important estimates of the errors associated with our treatment of this residual chiral symmetry breaking.

These smaller lattice spacing runs come at a significant cost. In addition to the obvious factors of volume and volume-dependent required step size, there is an expected increase in critical slowing down that accompanies such a smaller lattice spacing. Since there is always uncertainty that a given Monte Carlo run is of sufficient length to properly estimate the autocorrelation time and hence the true statistical errors, this uncertainty is even larger for these new configurations. As a result, we believe it is very important to collect adequate statistics and RBC-UKQCD plans to extend both the $m_l = 0.004$ and 0.006 runs currently underway by adding an additional 3,100 and 3,200 time units respectively producing ensembles of total length 4,500 and 4,600 times units. Since these runs are both shorter than the coarser $24^3 \times 64$ ensembles, our proposal for the use of USQCD resources is to collect two independent streams at identical parameters of 2,400 and 2,500 time units each. Thus, the total number of time units, including all of the planned RBC, UKQCD and USQCD runs will be 6,900 and 7,100 respectively for the 0.004 and 0.006 ensembles. By making independent starts we will learn more about the equilibration and long term autocorrelations and nearly double the statistics. These four runs, planned to begin in July of 2007, are listed in Table III.

	Run #	Volume	m_l/m_s	m_π(MeV)	Time units	M QCDOC hours
RBC	10	$32^3 \times 64$	0.004/0.03	261	3100	31.83
UKQCD	11	$32^3 \times 64$	0.006/0.03	315	3200	31.26
USQCD-DOE	12	$32^3 \times 64$	0.004/0.03	261	2400	24.64
USQCD-DOE	13	$32^3 \times 64$	0.006/0.03	315	2500	24.42

TABLE III: Planned dynamical domain wall fermion production runs with $1/a = 2.16$ GeV. These all use the Iwasaki gauge action with $\beta = 2.25$ and an extent in the fifth dimension of $L_s = 16$. Here the run lengths are specified in time units. The contribution of the residual mass, $m_{\rm res} \approx 0.0004$, is not included in quark masses listed in column 4 but, of course, is reflected the measured pion masses shown in the fifth column. The RBC and UKQCD runs are planned for machines at the RBRC and Edinburgh. The USQCD-DOE runs are those proposed to be carried out using USQCD QCDOC machines at BNL. The proposed runs listed here total ~50M processor hours. When the additional 20% required for propagator generation is added, we arrive at our total 60M QCDOC processor hour request.

We will use the doubled streams of ensembles in two ways. First we can make a simple combination of the thermalized configurations to give reduced (and better controlled) statistical errors. Second we can compare complete analyses carried out on these equivalent ensembles to check that our statistical errors correctly describe the variance between the two independent results.

A further motivation for collecting these extended statistics derives from the changing balance between the resources needed to generate these configurations and those required for the actual calculation (measurement) of physical observables on these lattices. With the spectacular improvements in algorithms we are now in the situation that more computer resources are required for the measurements than for the generation of the ensembles. Important physics measurements, whether they be nucleon matrix elements, weak kaon decay amplitudes or heavy quark matrix elements must typically be performed on hundreds of lattice configurations. If the underlying ensembles are short, these measurements must be performed on closely spaced configurations and will suffer from significant autocorrelations. By performing the longer runs, we allow these measurements to be made on more nearly independent lattices and substantially increase the value of these very expensive measurements.

As the BlueGene/P machine at Argonne turns on during the 7/2007-6/2008 period, an important objective is to substantially expand these fine, $a = 0.093$ fm lattices by studying light quarks with even smaller masses. While the direct cost of decreasing the light quark mass is small with present algorithms, controlling finite volume errors requires that we work on larger volumes and collect even longer ensembles to compensate for the increased spatial correlation lengths and accompanying increased autocorrelation time. Possible runs that are of substantial interest to the LHPC, RBC and UKQCD collaborations are listed in Table IV. Here we exploit the large capability of the BlueGene/P computer to collect large ensembles composed of a single Monte Carlo stream. While the runs listed in this table are of great physics benefit, it is important that the corresponding specialized and expensive measurements (presented in separate proposals from the LHPC and RBC collaborations) also be planned for these machines so that substantial physics results can be quickly derived from these ensembles.

It should be emphasized that the specific direction examined above shows concretely how much benefit can be derived by extending this project to the Argonne BlueGene/P

	Run #	Volume	m_l/m_s	m_π(MeV)	Time units	Tflops-years
Argonne BG/P	14	$48^3 \times 64$	0.0016/0.03	176	9200	14
Argonne BG/P	15	$48^3 \times 64$	0.0028/0.03	223	7300	10
Argonne BG/P	16	$48^3 \times 64$	0.0040/0.03	261	6200	8

TABLE IV: Dynamical domain wall fermion production runs with $1/a = 2.16$ GeV and small light-quark masses proposed for the Argonne BlueGene/P computer. These will create companion ensembles to those described in Tables II and III using the same parameters but here extending to substantially lighter quark masses.

machine. As we begin to collect information from the just-begun $32^3 \times 64$, $a = 0.093$ runs over this spring and early summer, it is quite possible that these plans may be modified. For example, if it becomes clear that the errors associated with extrapolating to the continuum limit dominate quantities of physical importance, we may recognize that this substantial increase in computing capability should be directed to studying a smaller lattice spacing rather than exploring the chiral limit. Such a change would have to be agreed to by our larger collaboration and the Scientific Program Committee would be kept informed.

IV. PROPOSED PROPAGATORS

As outlined above we propose to use an additional 20% of the configuration generation time for the calculation of fermion propagators. This computation time will permit these propagators to be computed for four independent sources every 10 times units. (This amounts to 48 Dirac operator inversions per lattice configuration: 4 sources, 3 colors and 4 spins.) Only unitary propagators will be computed, *i.e.* those with equal valence and sea quark masses. The propagators will be stored according to a QIO standard to be adopted before this work begins. This frequent measurement will permit both statistically accurate measurement ($\sim$1%) of ρ and nucleon propagators but also create a collection of propagators which can be used in later, more demanding matrix element calculations.

V. CONFIGURATION AVAILABILITY

At present all of the initial $16^3 \times 32$ runs with $L_s = 8$ and the DBW2 gauge action have been posted on the BNL web site `http://lattices.qcdoc.bnl.gov/` and are publically available. In addition, the complete set of $16^3 \times 32$ Iwasaki gauge action lattices which represent the first part of the 2+1 flavor, RBC-UKQCD configuration generation effort have been posted in the same place. Finally, the present $24^3 \times 64$, $L_s = 16$ lattices are expected to be posted within the next few weeks, making the entire ensemble of configurations listed in Table I available.

For future configurations, this proposal specifies an equal generation of gauge configurations on the USQCD-DOE resource as we expect to produce using RBC and UKQCD computers. Following past agreements between the USQCD Executive Committee and UKQCD, these USQCD-DOE resources which are being made available to UKQCD will be matched by an equal number of non-USQCD lattice configurations that will be provided "as generated" for use by the US community. Given the balance between proposed USQCD and planned RBC-UKQCD resources, this implies that all of the $32^3 \times 64$ configurations generated on UKQCD and RBC computers will be available to the US community, providing a complete common set of DWF lattice configurations. (To the extent that the timely release of UKQCD lattices exceeds this reciprocity arrangement, these contributions will be "banked" in the sense that later USQCD configurations will be made available to UKQCD. It seems fair that these will be valued not in teraflops hours but according to the fraction of current USQCD computer resources which they represent when made available by UKQCD and when returned in kind by USQCD, thereby accounting for "Moore inflation".

Finally it should be recognized that while the plans presented here have been formulated during detailed discussions with members of UKQCD, they have not been officially approved by the UKQCD collaboration. We expect that these plans will be formally discussed by the UKQCD collaboration within the next few weeks and that we will provide any needed changes to this proposal to the Scientific Program Committee in a timely fashion.

VI. ACCOUNTING OF U.S. RESOURCES

As in the proposal submitted to the Scientific Program Committee for the period July 2006-June 2007, we find this an appropriate place to detail the sharing of DWF lattices between UKQCD and USQCD. That earlier proposal described the exchange of gauge configurations which occured on or before February 2006. In exchange for the 10M QCDOC processor hours of USQCD-DOE allocation to the RBC collaboration whose equivalent value in configurations was made available to UKQCD (prorated to 6.7M hours for the July 2005 through February 2006 period), UKQCD (and RBC on their behalf) made available to the US community, 52% beyond the required 6.7M QCDOC hours.

The remaining 3.3M QCDOC processor hours, completing the 2005-2006 allocation, have been provided in the form of the 12K time units of $16^3 \times 32$, $a = 0.123$ fm lattices that were posted in December 2006. Given the performance of the code with which these were generated, they represent 25M QCDOC processor hours. These lattices are intended to correspond to the value of the actual QCDOC time made available to the RBC (which was to be used to generate lattices open to the USQCD community) and to the matching required of UKQCD for their access to these resources. Thus, these 25M QCDOC processor hours exceed the required 3.3M + 3.3M QCDOC processor hours by 280%.

The USQCD allocation of 26.23M QCDOC processor hours to the RBC collaboration for the July 2006 - June 2007 period has only begun being used since it was decided to provide the bulk of the QCDOC running time to MILC for the beginning of the proposal period. At present this RBC allocation is being provided as a 4K QCDOC partition which is now generating run 8 in Table II. We expect to gain access to a second 4K QCDOC partition to complete this period's allocation in a month or so. This second 4K node partition will be used to extend run 3 in Table I.

VII. SOFTWARE AND COMPUTER REQUIREMENTS

Since domain wall fermion code exists that will run efficiently on both QCDOC and clusters, the program of configuration generation proposed here can be carried out on either the QCDOC machine a BNL or the clusters at JLab or FNAL. However, there are significant reasons for carrying out this program on the QCDOC machine at BNL. First we recognize that it is important that all of the proposed configurations be run with the same algorithm to insure that the autocorrelation time is the same for all runs performed with the same parameters.

Since components of the highly tuned RHMC algorithm which are being used in the CPS code are not presently available in Chroma this suggests that at least initially CPS code be used. However, CPS has not be optimized for running on Intel or AMD processors so using CPS on clusters would result in an unacceptable loss in performance. Of course, these two obstacles (lack of the full suite of RHMC components in Chroma and Intel optimization for CPS) can be overcome with some additional effort. Thus, if the US program requires it, this DWF configuration generation could be split between BNL, JLab and FNAL. Given the current state of our optimized cluster software and the expertise available within our collaboration, we are confident that we can make the needed changes between the all-hands meeting and the July 1, 2007 beginning of this allocation period. If the requested resources are allocated on clusters, we will commit to making the necessary software changes.

In order to accommodate the large QCDOC allocation that would be required if this entire configuration generation proposal is run at BNL, the large, class A, RBC proposal to compute kaon decay matrix elements is being proposed to run at JLab or FNAL. As is described in that proposal, Chroma would be used for the expensive propagator calculation and the somewhat elaborate but less demanding matrix elements would be constructed from these propagators using CPS code on RBC or UKQCD QCDOC resources.

The complete RHMC DWF configuration generation code currently runs with a reasonable ∼15% efficiency on 512-node (or larger) BlueGene/L partitions. Thus, it should be straight-forward to move the configuration generation program proposed here to the Argonne machine. This also provides motivation for making the final improvements to Chroma so that code base as well can be used for this project at Argonne. Additional Incite resources at Oakridge provide further motivation for the needed RHMC enhancements to Chroma and Intel tuning for CPS.

While this proposal is being made jointly by LHPC and RBC, clear responsibility for the actual computer runs will devolve to the group whose code is being run. Should our request to run only on QCDOC be granted, then RBC would be responsible for the actual configuration generation. If running on clusters is requested then this will be done by either LHPC using an improved version of Chroma or by RBC using a cluster-optimized version of CPS.

VIII. RESTRICTED PHYSICS TOPICS

As is required for the proposed use of USQCD resources, the configurations that are generated as part of this proposal will be made available to the US community as generated. This will include both those configurations generated using the USQCD computers and those provided as compensation for UKQCD access to these configuration. These configurations can be used without restriction by all members of the USQCD collaboration. We would also plan to make them available to others, outside of the US, on a per request basis, provided that their intended use does not conflict with the plans of those in LHPC, RBC or UKQCD.

Since the propagators which are generated as part of this proposal can be used with very little added work to duplicate the studies which we plan to carry out, we plan that these will be released for US community use in July 2009. However, they will be made available on a per request basis for those who wish to undertake specific projects which do not conflict with our plans.

Within our three collaborations these generated configurations and propagators will be used without restriction.

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APPENDIX A: ESTIMATE OF TIME REQUIREMENTS

This appendix provides a rough summary of the RBC-UKQCD experience with and understanding of the RHMC algorithm as applied to 2+1 flavor DWF simulations. An estimate for the computation cost of generating an independent gauge configuration using the strange quark mass as a single Hasenbusch mass preconditioner[**?**] is given by the formula:

$$\text{Cost} \;=\; \underset{\text{(A)}}{L^4} \;\cdot\; \underset{\text{(B)}}{L_s} \;\cdot\; \underset{\text{(C)}}{L} \;\cdot\; \underset{\text{(D)}}{\tfrac{1}{m_\pi}} \;\cdot\; \Big(\underset{\text{(E)}}{\tfrac{c_1}{m_s}} + \underset{\text{(F)}}{\tfrac{c_2}{m_l}\langle\overline{q}q\rangle}\Big). \tag{A1}$$

Here the linear size of the system (L), the light quark mass (m_l), the strange quark mass (m_s) the pion mass (m_π) and the chiral condensate, ($\langle\overline{q}q\rangle$) are all expressed in lattice units. If the quantities in this expression are put in physical units, one finds:

$$\text{Cost} = \Big(\frac{L}{\text{fm}}\Big)^5 L_s\Big(\frac{\text{MeV}}{m_\pi}\Big)\Big(\frac{\text{fm}}{a}\Big)^7\Big(\frac{\text{MeV}}{m_K}\Big)^2\bigg(C_1 + C_2\Big(\frac{a}{\text{fm}}\Big)^3\Big(\frac{m_K}{m_\pi}\Big)^2\bigg) \tag{A2}$$

The various terms are justified as follows:

(A) The total number of space-time lattice sites which appears multiplicatively when counting most of the operations needed to perform a step in the HMC method.

(B) The extent of the lattice in the fifth dimension.

(C) The weak volume dependence of the step size expected for the leap-frog integrator [10, 11].

(D) Critical slowing down of the algorithm, assumed to have a critical index of 1.

(E) The dependence of the number of conjugate gradient iterations on the strange quark mass. This effects high-frequency modes because of our Hasenbusch preconditioning technique.

(F) The dependence of the number of conjugate gradient iterations on the light quark mass. This term comes from the low-frequency modes. Its coefficient, $\langle \overline{q} q \rangle$, represents the small relative number of modes which contribute to this portion of the fermion force.

We can summarize our $24^3 \times 64$, $1/a = 1.62(5)$ GeV simulation experience by giving values for the constants C_1 and C_2 in Eq. A2. With a light quark mass of $m_l = 0.5 m_s$, we generate about 40 trajectories per day, find that the light quark portion of the RHMC takes 10% of the time and treat every 50 time units as approximately independent. This yields:

$$C_1 = 0.01021, \quad C_2 = 0.3226. \tag{A3}$$

Equation A2 has been used to estimate the computer time required for the various runs discussed in this proposal.