B-meson decay constants, B^0-$\overline{B^0}$-mixing and the $B^*B\pi$ coupling with domain-wall light quarks and relativistic heavy quarks

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Time Requested: The equivalent of 8.2 million jpsi core-hours on the Fermilab clusters plus 34.1 Tbytes of tape storage (the equivalent of $\sim$ 92000 jpsi core-hours) and 0.02 Tbytes of disk storage (the equivalent of $\sim$ 540 jpsi node-hours) at Fermilab.

Abstract

We propose to continue our determination of the B-meson leptonic decay constants, B^0–$\overline{B^0}$ mixing matrix elements and their ratio, $\xi \equiv f_{B_s}\sqrt{\hat{B}_{B_s}}/f_{B_d}\sqrt{\hat{B}_{B_d}}$, on the 2+1 flavor dynamical domain-wall configurations generated by the LHP, RBC, and UKQCD Collaborations using the relativistic heavy quark action in order to achieve high precision results. We also propose to compute the $B^*B\pi$ coupling because it is an important input to the chiral extrapolation of B-meson quantities and it has a significant computational overlap with our current project. A precise determination of ξ will allow a strong constraint on the apex of the CKM unitarity triangle, and is one of the key goals in flavor physics of the U.S. lattice QCD community, as stated in the 2007 white paper. Our calculation will provide a valuable independent crosscheck of the results of the HPQCD and Fermilab/MILC Collaborations, both of which rely upon the 2+1 flavor Asqtad-improved staggered lattices generated by the MILC Collaboration. We request the equivalent of 8.2 million jpsi core-hours on the Fermilab clusters plus 34.1 Tbytes of tape storage (the equivalent of $\sim$ 92000 jpsi core-hours) and 0.02 Tbytes of disk storage (the equivalent of $\sim$ 540 jpsi core-hours) for this project.

Scientific Motivation

Recent experimental measurements of the mass-differences of the neutral B-meson mass eigenstates Δm_d and Δm_s to $\sim 1\%$ accuracy [1] now allow the possibility of precisely determining the ratio of the CKM matrix elements $|V_{td}|/|V_{ts}|$. The uncertainty in this ratio, however, is limited by the knowledge of the nonperturbative factor $\xi \equiv f_{B_s}\sqrt{\hat{B}_{B_s}}/f_{B_d}\sqrt{\hat{B}_{B_d}}$, which parameterizes the hadronic contribution to B^0–$\overline{B^0}$ mixing [2]. It is likely that new physics would give rise to new quark-flavor changing interactions and additional CP-violating phases; these would manifest themselves as apparent inconsistencies among different measurements of quantities which should be identical within the standard CKM picture. Thus a precise determination of the ratio ξ will help to constrain physics beyond the Standard Model. In fact, there are already possible indications of new physics in B_d-mixing at the $\sim$2.7-σ level, as pointed out in Ref. [3]. Because the importance of ξ to new physics searches is well known to the lattice community, this quantity was highlighted as one of three "key matrix elements" in the USQCD Collaboration's 2007 white paper "Fundamental parameters from future lattice calculations" [4].

Recently, Lunghi and Soni proposed a new approach to constrain the unitarity triangle by using ϵ_K, BR($B \to \tau\nu_\tau$), ΔM_{B_s} and ξ [5]. This method has the advantage that it bypasses the need to use the $B \to \pi l \nu$ semileptonic form factor and $|V_{ub}|$ which still has large uncertainties. Following this approach, however, necessitates increased precision also for the leptonic decay constant f_{B_d} and the individual quantity $f_{B_s}\sqrt{\hat{B}_{B_s}}$.

The largest systematic uncertainty in most lattice calculations of B-meson quantities is the chiral and continuum extrapolation. This error can be reduced with an improved determination of the $B^*B\pi$ coupling. The $B^*B\pi$ coupling is defined from the matrix element of the light quark axial vector current between B and B^* states. Fixing it determines the leading interaction in the chiral Lagrangian for heavy-light B-mesons. The coupling of this interaction appears in chiral perturbation theory expressions for the ratio of B^0–$\overline{B^0}$ mixing matrix elements and for the form factors of semileptonic $B \to \pi$ and $B \to D^{(*)}$ decays where it fixes the strength of the B^* pole contribution. Phenomenologically $g_{B^*B\pi}$ is only poorly known and the literature exhibits a wide spread of values [6, 7, 8, 9, 10, 11, 12]. For example in our recent publication [13] computing B^0–$\overline{B^0}$ mixing in the static limit, we assumed a 40% uncertainty in $g_{B^*B\pi}$ to account for the spread in the literature.

Both the HPQCD and Fermilab/MILC Collaborations are also computing the B^0–$\overline{B^0}$ mixing matrix elements. The HPQCD Collaboration has recently published a determination of ξ to 2.6% precision [14], and the Fermilab Lattice and MILC Collaborations expect to have a result with similar errors soon [15, 16]. Both of these computations, however, rely on the 2+1 flavor Asqtad-improved staggered ensembles generated by the MILC Collaboration. Therefore, for such a phenomenologically-important quantity as ξ, it is valuable to have an independent crosscheck using a different light quark formulation. Previous calculations of $g_{B^*B\pi}$ on the lattice have used static b-quarks [6, 17, 18, 19], propagating heavy quarks around the charm mass [8, 20] or interpolations between static and propagating results [18]. In these calculations a comparison between quenched and $N_f = 2$ dynamical flavors suggests a small effect and discretization errors are generally small, except for [19]; the biggest systematic uncertainty arises from the chiral extrapolation. Currently, the work by Ohki, Matsufuru and Onogi provides the result with most comprehensive error budget, $g_{B^*B\pi} = 0.516(5)(33)(28)(28)$, where the errors in order of listing are: statistical, chiral extrapolation, perturbative renormalization and discretization [19]. This calculation is carried out with $N_f = 2$ dynamical flavors and uses the static limit for the b-quarks. However, a computation using $2 + 1$ flavors of dynamical light quarks and heavy quarks directly at the mass of the b-quark has

Table 1: Available RBC/UKQCD 24^3 and 32^3 ensembles. The pion masses on the coarser 24^3 lattices are given in Ref. [25], while the pion masses on the finer 32^3 lattices are preliminary estimates. Most ensembles were recorded every five trajectories, but the $am_l/am_s = 0.006/0.030$ ensemble was recorded every 4 trajectories.

a(fm)	L	m_l	m_s	m_π(MeV)	approx. # configs.
≈ 0.08	32	0.004	0.030	307	600
≈ 0.08	32	0.006	0.030	366	900
≈ 0.08	32	0.008	0.030	418	600
≈ 0.11	24	0.005	0.040	331	1600
≈ 0.11	24	0.010	0.040	419	1700
≈ 0.11	24	0.020	0.040	558	700
≈ 0.11	24	0.030	0.040	672	600

not been performed. We are therefore submitting a Type A proposal to extend our calculation of the B^0-$\overline{B^0}$ mixing matrix elements $f_{B_s}\sqrt{\hat{B}_{B_s}}$, $f_{B_d}\sqrt{\hat{B}_{B_d}}$, and ξ, which we started last year, and additionally compute the coupling $g_{B^*B\pi}$ using dynamical domain wall fermions and relativistic b-quarks.

Our calculation uses the 2+1 flavor dynamical domain wall ensembles generated by the LHP, RBC, and UKQCD Collaborations with lattice spacings of $a \approx 0.11$ fm and $a \approx 0.08$ fm. For the determination of ξ we compute several partially-quenched light domain-wall valence quark propagators on each ensemble. This allows us to extrapolate to the physical light quark masses and the continuum in a controlled manner using chiral perturbation theory (χPT), which is particularly simple for the case of domain-wall fermions. For the determination of the coupling $g_{B^*B\pi}$ we plan to perform the computation only at the unitary points. The leading light-quark discretization effects in our calculation are expected to be of $\mathcal{O}(a^2p^2)$. We use the relativistic heavy quark (RHQ) action developed by Christ, Li, and Lin for the heavy b-quarks [21, 22]. The RHQ method extends the Fermilab approach [23] by tuning all of the parameters of the clover action nonperturbatively [24]. The RHQ action is accurate to $\mathcal{O}(a^2p^2)$, but to all orders in $(am_b)^n$; thus it allows the computation of heavy-light spectrum quantities with discretization errors of the same order as in light-light quantities.

With the additional resources requested in this proposal, we expect to determine the ratio ξ to a precision comparable to those of HPQCD and Fermilab/MILC. For the coupling $g_{B^*B\pi}$ we should be able to do at least as well as existing calculations but using $2+1$ flavors for the light quarks and heavy quarks at the value of the b-quark mass.

Computation Method

We list the available 2+1 flavor dynamical domain wall ensembles generated by the RBC, UKQCD, and LHP collaborations in Table 1 and refer to these by their spatial volumes in lattice units; the coarser "24^3" ensembles have $a \approx 0.11$ fm and the finer "32^3" ensembles have $a \approx 0.08$ fm. The domain-wall valence quark propagators are generated on these configurations using the same values of the domain-wall height ($M_5 = 1.8$) and the fifth-dimensional extent ($L_s = 16$) as in the

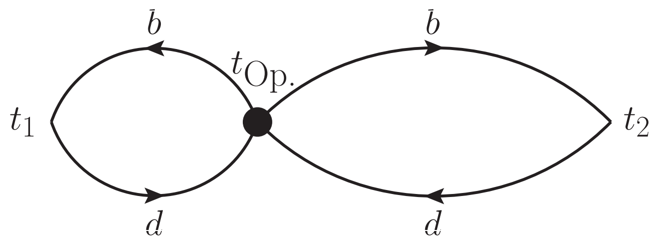

Figure 1: Three-point lattice correlation function for B^0-$\overline{B^0}$ mixing.

sea sector. This allows us to use the determinations of the light and strange valence quark masses and the residual quark mass from RBC/UKQCD's analysis of the light-pseudoscalar meson masses and decay constants [25]. For the computation of B^0-$\overline{B^0}$ mixing matrix elements, we generate both unitary and partially quenched data points, whereby the additional correlated data are expected to give us better control over the extrapolation to the physical light quark masses. For the computation of $g_{B^*B\pi}$ we can reuse the light quark propagators and plan to run the computation only on unitary data points. In order to best take advantage of the larger number of configurations available on the coarser 24^3 ensembles, 24^3 and 32^2 data will be fitted together and simultaneously extrapolated to the physical light quark masses and the continuum using partially-quenched heavy-meson χPT [26] supplemented by analytic terms $\propto a^2$ to parameterize light-quark discretization effects.

For the b-quarks we use the relativistic heavy quark action [21, 22]. The appropriate parameters have already been determined for the 24^3 lattices in Ref. [24] and the tuning of the parameters on the 32^3 lattices is currently underway. We expect to have the parameters available soon. By tuning the value of the hopping-parameter κ such that the kinetic meson mass M_2 is equal to the physical spin-averaged B-meson mass and tuning the value of the clover coefficient c_{SW} so that we reproduce the correct hyperfine splitting $m_{B_s^*} - m_{B_s}$, we match the lattice action onto the continuum action through $\mathcal{O}(pa)$, leaving errors of $\mathcal{O}(p^2a^2)$. Because the RHQ action treats the heavy-quark mass to all-orders in m_ba, the coefficient of the $\mathcal{O}(p^2a^2)$ heavy-quark discretization errors is a function of m_ba. Fortunately, however, El-Khadra, Kronfeld, and Mackenzie, showed that the function of m_ba is always bounded to be of $\mathcal{O}(1)$ or less [23].

We construct the B^0-$\overline{B^0}$ 3-point function as shown in Fig. 1. The location of the effective four-fermion operator, $t_{\text{Op.}}$, is fixed and we vary the locations of the B^0 and $\overline{B^0}$ mesons, t_1 and t_2, over all possible time slices. This requires one point-source light quark propagator and one point-source b-quark propagator originating from $t_{\text{Op.}}$. These propagators can be used for both the B^0 and $\overline{B^0}$ mesons, thereby reducing the computational cost. At the sink we project out the zero-momentum component using a gauge-invariant Gaussian sink. At the moment we are comparing the possibilities of using a smeared sink for only the heavy quark versus for both the heavy and light quarks; we will also tune the Gaussian radius on the 24^3 and 32^3 dynamical ensembles in order to optimize the signal.

The discretization errors in the four-fermion operator are reduced by rotating the b-quark at the source as in Ref. [15]. By computing the rotation parameter d_1 at tree-level in tadpole-improved lattice perturbation theory we improve the operator to $\mathcal{O}(\alpha_s ap)$. We calculate the renormalization factors needed to match the lattice operator onto the continuum using 1-loop tadpole-improved lattice perturbation theory, such that the truncation errors are of $\mathcal{O}(\alpha_s^2)$. At this order, the desired operator only mixes with one other lattice operator through $\mathcal{O}(1/m_b)$ [15]. Fortunately, because the additional operator resides at a single lattice site, we can reuse the point source light- and b-quark propagators to compute the additional 3-point correlation function. Because the quantity

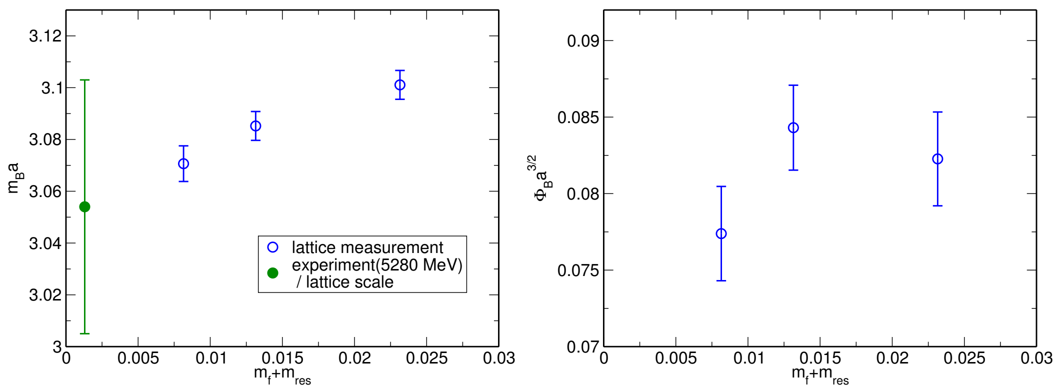

Figure 2: Preliminary results computed on 24^3 lattices. The left plot shows the mass of the B-meson in dependence of the light sea-quark mass $m_f + m_{\rm res}$, computed from the $\langle PP \rangle$ correlator. The right plot shows the unrenormalized decay amplitude Φ_B over $m_f + m_{\rm res}$ computed with $\langle PP \rangle$ and $\langle PA \rangle$ correlators for point sources and point sinks (without rotating the b-quarks). Only statistical errors are shown.

$\xi \equiv f_{B_s}\sqrt{\hat{B}_{B_s}}/f_{B_d}\sqrt{\hat{B}_{B_d}}$ is a ratio, much of the uncertainty due to the truncation of perturbation theory should cancel, even if the truncation errors in the numerator and denominator are more significant. Thus far we have used approximately 30% of our 2009/2010 allocation and will use the rest of the allocation primarily by generating domain-wall light quark propagators on the 32^3 ensembles. Figure 2 shows some preliminary results for 24^3 lattices. Using m_{B_s} as input to tune the RHQ action we find that our determination of m_B agrees with the experimental value as shown in the left plot. The right plot shows the decay amplitude Φ_B computed without rotating the b-quarks and using the $\langle PP \rangle$ and $\langle PA \rangle$ correlators with point sources and point sinks. We find that the statistical errors are $\approx 3\%$. This will be reduced further through the use of smeared sinks for the b-quarks and the additional statistics requested in this proposal.

The additional lattice 3-point lattice correlation function needed to compute the $B^* B\pi$ coupling is shown in Fig. 3. The result can be nonperturbatively renormalized since the nonperturbative renormalization factor for the axial-vector current for domain-wall fermions has already been determined. The heavy quarks will be treated using the relativistic heavy-quark action. This setup allows us to reuse the computationally expensive domain-wall light quark propagators for the calculation of $g_{B^* B\pi}$. The new light-quark sequential propagator, however, will require additional somewhat significant resources.

Run Plan and Resource Allocation

The most computationally intensive portion of this project are the domain-wall propagator inversions, for which we use the optimized domain-wall inverter in the Chroma lattice QCD software package [27]. We use our own code, written using the Chroma and QDP++ libraries, to calculate the $\Delta B = 2$ operator. We are checking the matrix element code against that used for the current Fermilab/MILC calculation.

So far in our first year of running, we have generated domain-wall propagators on every 10^{th} trajectory available on the 24^3 ensembles and are currently implementing the contraction, four-quark operators and $\mathcal{O}(pa)$ improvement terms. As soon as we have checked our code, optimized the smearing width to obtain a good signal, and verified that the 24^3 data look sensible, we will

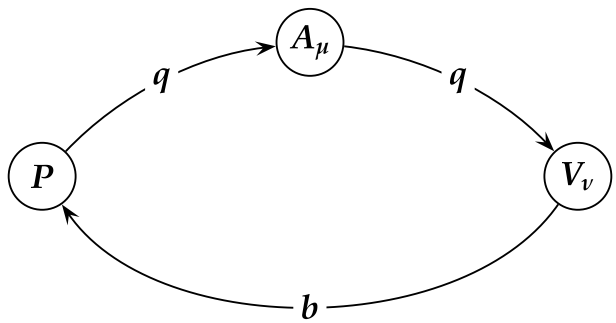

Figure 3: Three-point lattice correlation function for the $g_{B^*B\pi}$ coupling.

Table 2: Proposed domain wall valence and sea quark mass combinations for the calculation of the $B^0 - \overline{B^0}$ matrix elements. The computation of the additional sequential propagator for $g_{B^*B\pi}$ will use the entire set of configurations but be computed only on the unitary points.

a(fm)	L	m_l	m_s	$m_{val.}^{\rm dwf}$	# configs 2009/2010	# configs 2010/2011
≈ 0.08	32	0.004	0.030	0.004, 0.006, 0.008, 0.025, 0.030	300	300
≈ 0.08	32	0.006	0.030	0.004, 0.006, 0.008, 0.025, 0.030	450	450
≈ 0.08	32	0.008	0.030	0.004, 0.006, 0.008, 0.025, 0.030	300	300
≈ 0.11	24	0.005	0.040	0.005, 0.01, 0.02, 0.03, 0.04	800	800
≈ 0.11	24	0.010	0.040	0.005, 0.01, 0.02, 0.03, 0.04	850	850
≈ 0.11	24	0.020	0.040	0.005, 0.01, 0.02, 0.03, 0.04	300	400

proceed with the computation on the 32^2 ensembles. Due to our recently finished work in the static limit [13], the ground for the data analysis and chiral extrapolation is already set, although some adjustments will be needed. Table 2 summarizes our running plan for the allocation period 2009/2010 and 2010/2011. We plan to compute five valence quark masses per ensemble. The lightest three are equal to the light sea quark masses on the three ensembles per lattice spacing, and the heavier two bracket the physical strange quark mass to allow for an interpolation. As we learned form the analysis of static B-meson data, 2-point correlators on configurations separated by 10 trajectories are essentially uncorrelated. In order to further reduce autocorrelations, we move both the temporal and spatial positions of the operator from configuration to configuration.

We have timed propagator inversions for the domain-wall valence quark masses listed in Table 2 on the 24^3 and 32^3 2+1 flavor domain wall lattices using Chroma on the Fermilab clusters; these are given in Tables 3. We have also timed clover inversions on the 24^3 lattices using the parameters determined in Ref. [24]; these are shown in Table 4. In order to propagate the errors in the nonperturbatively-tuned parameters of the RHQ action through the remainder of the calculation, we will compute the less expensive heavy-quark propagators with seven parameter sets on each ensemble. For the $B^*B\pi$ coupling calculation we will follow this procedure only for the heaviest mass $m_l = 0.02$ on the 24^3 lattices and assume the error on the remaining ensembles to be comparable in order to reduce the number of expensive sequential light-quark propagators. Nevertheless we expect

Table 3: Time to calculate a single domain-wall propagator with $L_5 = 16$ using Chroma on the Fermilab "jpsi" cluster.

a(fm)	L	m_l	nodes (jpsi)	time (hours)	jpsi core-hours
≈ 0.08	32	0.004	32	4.06	1040
≈ 0.08	32	0.006	32	3.07	786
≈ 0.08	32	0.008	32	2.46	630
≈ 0.08	32	0.025	32	0.96	246
≈ 0.08	32	0.03	32	0.84	215
≈ 0.11	24	0.005	16	1.91	244
≈ 0.11	24	0.010	16	1.27	163
≈ 0.11	24	0.020	16	0.79	101
≈ 0.11	24	0.030	16	0.59	76
≈ 0.11	24	0.040	16	0.48	61

Table 4: Time to calculate a single clover propagator using Chroma on the Fermilab "jpsi" cluster. The time for the 32^3 ensembles is an estimate based on scaling the 24^3 time by the ratio of the volumes.

a(fm)	L	nodes (jpsi)	time (hours)	jpsi core-hours
≈ 0.08	32	–	–	8
≈ 0.11	24	1	0.41	4

to determine $g_{B^*B\pi}$ with sufficient precision. Using these timings, the total computing resources required to compute the B^0–$\overline{B^0}$ mixing matrix element using all of the light quark masses listed in Table 2 and to compute $g_{B^*B\pi}$ on the entire set of configurations for the unitary point is given in Table 5. Our total computing request is 8.2 million jpsi core-hours, and includes both the time needed to compute the quark propagators plus an additional 10% for testing code, calculating 2-point and 3-point correlation functions, and analysis.

We would like to continue our running on the Fermilab clusters. Two of the authors (R.V. and O.W.) are now experienced in running on the Fermilab clusters, and the performance of the domain-wall inverter in Chroma on the Fermilab clusters is better than that of the domain-wall inverter in CPS on the QCDOC. The 24^3 propagators may be run efficiently either on kaon or on jpsi, but the 32^3 ensembles are sufficiently large that the propagators should be generated on jpsi. Thus we would like either a 40%-60% split between time on kaon and jpsi, or all of the time on jpsi. The smaller numbers of cores, decreased memory, and decreased scratch disk space make it impractical to compute the domain-wall propagators on pion, although we can use pion to generate the b-quark propagators, which are smaller by a factor of $L_s = 16$. The b-quark propagators, however, make up a small percentage of our allocation.

We would also like to save all of the domain-wall propagators to tape at Fermilab for enough time to allow their use in other projects and by other groups. Table 6 shows the file sizes of the domain-wall quark propagators for the two different lattice volumes, in both GB and jpsi-equivalent core hours assuming that they are stored on tape. A comparison of Table 6 and Tables 3 reveals

Table 5: Computer time needed to determine the B^0-$\overline{B^0}$ mixing matrix element and $g_{B^*B\pi}$ coupling using the sea quark ensembles, valence quark masses, and numbers of configurations listed in Table 2 for the allocation period 2010/2011.

32^3 $a = 0.08$ fm domain-wall propagators	3.063 $\times 10^6$ jpsi core-hours
24^3 $a = 0.12$ fm domain-wall propagators	1.322 $\times 10^6$ jpsi core-hours
32^3 $a = 0.08$ fm clover propagators	0.076 $\times 10^6$ jpsi core-hours
24^3 $a = 0.12$ fm clover propagators	0.092 $\times 10^6$ jpsi core-hours
32^3 $a = 0.08$ fm sequential domain wall propagators	1.709 $\times 10^6$ jpsi core-hours
24^3 $a = 0.12$ fm sequential domain wall propagators	1.162 $\times 10^6$ jpsi core-hours
2-point and 3-point correlators, code testing and analysis	0.742 $\times 10^6$ jpsi core-hours
Total	8.166 $\times 10^6$ jpsi core-hours

Table 6: File sizes of domain-wall propagators for various spatial volumes. The equivalent cost to store the file on tape uses the conversion 1 Tbyte tape = 2,694 jpsi core-hours.

a(fm)	L	size (GB)	tape storage cost (jpsi core-hours)
≈ 0.08	32	2.25	6.1
≈ 0.11	24	0.95	2.6

that calculating the domain-wall propagator is ~ 30 times more expensive than storing it for the cheapest propagator, and ~ 500 times more expensive for the costliest propagator. Thus it is more efficient to save and reuse the domain-wall propagators than to recalculate them. The total storage space needed to save all of the propagators listed in Table 2 is given in Table 7. Our total tape storage request is 34.1 Tbytes of tape at Fermilab.

Summary

At the end of this project we expect to have a precise determination of the B-meson leptonic decay constant and the B^0-$\overline{B^0}$ mixing matrix elements, along with a very precise determination of their ratio ξ including dynamical light quark effects and relativistic heavy quark effects. This would fulfill one of the key goals in flavor physics of USQCD stated in the 2002 strategic plan and the 2007 white paper "Fundamental parameters from future lattice calculations" [4]. Use of two lattice spacings, multiple quark masses, and heavy meson chiral perturbation theory will give us control over the systematic errors associated with both the chiral and continuum extrapolations. This computation will provide a valuable and independent crosscheck for ξ to the determinations by HPQCD and Fermilab/MILC. Moreover, this measurement, when used in a unitarity-triangle analysis, will place an important constraint on physics beyond the Standard Model. We also expect to determine the $B^*B\pi$ coupling using the relativistic heavy quark action and $N_f = 2 + 1$ dynamical sea quark flavors with a precision at least comparable to or better than existing determinations.

The domain-wall propagators that we will generate can be used for the calculation of other interesting physics quantities, and we encourage other members of the lattice QCD community

Table 7: Mass storage needed to save all of the domain-wall propagators listed in Table 2. The equivalent cost to store the file on tape uses the conversion 1 Tbyte tape = 2,694 jpsi core-hours.

	2009/2010	2010/2011
32^3 $a \approx 0.08$ fm propagators	11.81 TB	11.81 TB
32^3 $a \approx 0.08$ fm sequential propagators	—	4.73 TB
24^3 $a \approx 0.11$ fm propagators	9.23 TB	9.74 TB
24^3 $a \approx 0.11$ fm sequential propagators	—	7.79 TB
Total	21.06 TB = 56756 jpsi core-hours	34.07 TB = 91785 jpsi core-hours

Table 8: Additional disk storage needed to save 2-point and 3-point correlation functions, logfiles, and analysis files in the "/project" area at Fermilab. The equivalent cost to store the file on disk uses the conversion 1 Tbyte disk = 26,940 jpsi core-hours.

	2009/2010	2010/2011
estimated	0.02 TB	0.02 TB
Total	0.02 TB = 539 jpsi core-hours	0.02 TB = 539 jpsi core-hours

to do so. Along with the B^0-$\overline{B^0}$ matrix elements and the $B^*B\pi$ coupling, we will compute the B-meson decay constants f_B and f_{B_s}, as well as their ratio f_B/f_{Bs}. We would also like to retain exclusive rights to calculate the D- and D_s-meson decay constants and the beyond the Standard Model contributions to $B^0-\overline{B^0}$ mixing using these propagators in the future. All of the propagators generated will be stored at Fermilab and will be made available immediately for non-competing analyses. Researchers who wish to use them should contact us to arrange access.

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