

# Non-perturbative renormalization with improved staggered fermions.

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## Abstract

This is a class B proposal, asking for time on the clusters to calculate matching (“Z”) factors using non-perturbative renormalization (NPR) for the quark mass, bilinear and four-fermion operators, using valence asqtad and HYP-smearred staggered quarks on a subset of the coarse and fine MILC lattices. These matching factors are needed to reduce and control the systematic error in the quark mass obtained by the MILC collaboration using asqtad fermions, and in the calculation of  $B_K$  and other kaon matrix elements using HYP-fermions. For both calculations, matching is, or is likely soon to be, the dominant source of error. We propose to use the standard NPR methodology, adapted to staggered fermions. We use the Chroma package, augmented by the addition of momentum sources. We are asking for time on clusters, and have a slight preference for running at Fermilab (where we have done our test runs).

We are requesting 500,000 6n-equivalent node-hours on the clusters.

# 1 Scientific Background

With the exception of (partially) conserved currents, hadronic matrix elements obtained from lattice QCD require matching factors to relate bare lattice quantities to those in conventional continuum schemes. Such matching is essential for electroweak matrix elements because the effective Hamiltonian (including overall Wilson coefficients) has been determined in continuum schemes. Early calculations used perturbative matching, but this inevitably introduces truncation errors. For example, the oft-used one-loop matching leads to errors of  $O(\alpha_s^2) \approx 10\%$ . This is small enough for some applications, but not for precision tests of the standard model (SM).

One way to increase precision is to use two-loop perturbation theory. This has been successfully carried out for the matching factor for light-quark masses with asqtad fermions [1]. For example, it has been used by the MILC collaboration to obtain [2]

$$m_s = 88(0)(3)(4)(0)\text{MeV}, \quad (1)$$

where the errors are statistical, lattice-systematic, matching and electromagnetic, respectively. Thus, even with a two-loop calculation, the dominant error is matching. Furthermore, this error is an educated guess, based on assuming that the truncation error is  $\pm 2\alpha_s^3$ .

Clearly it would be preferable, for a fundamental parameter such as the quark mass, to have a more precise and more controlled determination of the matching factor. This is possible using the method of non-perturbative renormalization (NPR) [3]. Here one trades uncontrolled truncation errors for controlled statistical errors by normalizing gauge-fixed quark and gluon correlation functions at large Euclidean momenta in the same way that one does in perturbation theory (in the regularization independent [RI] scheme).<sup>1</sup> This method has been widely applied with considerable success, most notably with Wilson-like [5] and domain-wall fermions (DWF) [6]. Statistical errors at the sub-percent level are possible, and the chiral extrapolation is straightforward (and is not plagued by non-analytic terms). The dominant systematic is due to the need to use momenta satisfying

$$\Lambda^{\text{QCD}} \ll |p| \ll 1/a, \quad (2)$$

i.e. large enough to be in the perturbative regime, yet small enough for lattice artifacts to be small. It seems that, in practice, such a window can be found with  $1 < |p|a < 2$ , with the final errors being at the percent level. A notable recent application is to the calculation of  $B_K$  using DWF [6]. Here a precision test of the SM requires percent level accuracy in the matching factors, and this has been attained.

In this proposal, we request resources to apply NPR to improved staggered fermions. We have two major motivations, and correspondingly two sub-projects:

- To calculate the matching factor for the quark mass,  $Z_m$ , with asqtad fermions, so as to improve the precision of the determination of the light quark masses from the existing determination of the bare quark masses.<sup>2</sup>

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<sup>1</sup>The only uncontrolled error is that due to Gribov copies. Various studies have found the variation in matching factors from copy to copy to be very small, as expected since they are determined using large momenta. We assume here that this leads to a sub-dominant error. This error can be avoided using Schrödinger functional methods [4], but these are more involved than standard NPR, and we do not propose to use them here.

<sup>2</sup>We understand from conference reports that the MILC collaboration is also implementing NPR for this purpose, although we do not know the methodological details. We think that two independent calculations of this important quantity are warranted.

- To calculate matching factors for the operators needed to determine  $B_K$  and related kaon matrix elements using HYP-smear [7] improved staggered fermions. The calculation of the bare matrix elements of these operators are underway using USQCD resources (see proposal by Lee, Jung and Sharpe), but accurate matching factors are needed to provide precision results. As has been repeatedly stressed in USQCD proposals and white papers, a precision result for  $B_K$  allows a strong test of the SM and places significant constraints on new physics.

Both calculations will be done on both the coarse and fine MILC lattices (which is where the bulk of the corresponding masses and matrix elements are, or will be, available). These calculations are relatively computationally inexpensive, as can be seen from the estimates below. In particular, we think that we can attain the desired accuracy with a class B proposal. Extension to the superfine lattices would be straightforward in principle but would require more substantial resources.

To our knowledge, there has been only one previous application of NPR to staggered fermions [8]. This used unimproved (quenched) staggered fermions, and calculated matching factors for the quark mass. It was successful despite the large discretization errors. Although we propose to use somewhat different methodology, we use Ref. [8] as a guide for the determination of the needed resources.

Compared to unimproved staggered fermions, we expect that the discretization errors will be reduced for both asqtad and HYP-smear staggered fermions. Thus we expect the NPR method to be easier to apply (and are correspondingly encouraged that it could be applied without improvement despite the larger discretization errors).

Two side benefits of our proposed calculations are that we can study the size of taste-breaking effects with new quantities (e.g. how do the matching factors depend on taste?), and that we can make extensive comparisons with one-loop perturbation theory, for which many perturbative results exist (e.g. Ref. [12] for bilinears). The latter comparison will give a better sense of the generic truncation errors for quantities where NPR results are not available.

## 2 Methodology

The general NPR method is well established and we do not have space to repeat it here. We will note only some special features associated with the application to staggered fermions. These features are common to both asqtad and HYP-smear variants.

The essence of NPR is to match short distance, gauge-fixed correlators to their continuum perturbative forms. With staggered fermions this matching is non-trivial because the taste and spin degrees of freedom are spread over a  $2^4$  hypercube. In momentum space, this corresponds to breaking up the lattice Brillouin zone ( $-\pi \leq p_\mu a < \pi$ ) into  $2^4$  pieces,

$$p_\mu = p'_\mu + B_\mu \frac{\pi}{a}, \quad (3)$$

where  $B_\mu$  is a hypercube vector (composed of 0's and 1's).  $p'_\mu$  is the physical momentum, which lies in the reduced range  $-\pi/2 \leq p'_\mu a < \pi/2$ . The 16 different values of  $p$  associated with a single physical  $p'$  correspond to the spin-taste degrees of freedom. This formulation in momentum space, which was developed by Ref. [13] and elaborated by Ref. [14], naturally

incorporates the lattice symmetries, in contrast to the position-space hypercube formulation.<sup>3</sup> This is shown by the free propagator, which takes the form (setting  $a = 1$ ):

$$S^{-1}[p' + \pi A, -(q' + \pi B)] = \bar{\delta}(q' - p') \left[ m \overline{(1 \otimes 1)}_{AB} - i \sum_{\mu} \sin(q'_{\mu}) \overline{(\gamma_{\mu} \otimes 1)}_{AB} \right], \quad (4)$$

where the overbarred spin-taste matrices are unitarily equivalent to the usual forms. In other words, apart from the discretization error  $q'_{\mu} \rightarrow \sin q'_{\mu}$ , the propagator is just that for four degenerate fermions with a full  $SU(4)$  taste symmetry. We think that the spin-taste structure of the propagator holds at all orders in perturbation theory, although each term will have a (hypercubic invariant) dependence on the momentum.

The first step of our proposed calculation is to determine  $S^{-1}$  on Landau-gauge fixed lattices. Following Ref. [8], and many other works, we use momentum sources (i.e.  $\exp(ip_{\mu}n_{\mu})$  on the entire lattice) rather than point sources. The resultant volume averaging greatly reduces the noise, although this comes at the cost of having to calculate a new propagator for each momentum (rather than Fourier transforming the free end of a point-source propagator). Since we are interested in precision, and since we can build upon previous work to choose optimal momenta, we think that the advantages outweigh the disadvantages. Furthermore, we need to contract propagators with hypercube operators, which involve quark and antiquark fields at different positions on a  $2^4$  hypercube. Thus we would need 16 point sources were we to use them, and we would lose the volume averaging at the operator insertion.

$S^{-1}$  is a  $16 \times 16$  matrix, and thus requires 16 inversions for each physical momentum. We package these together in our analysis program, and Fourier transform on the free end, producing the desired matrix.<sup>4</sup> We then decompose this matrix into the spin-taste basis. Only the parts proportional to the matrices  $(1 \otimes 1)$  and  $(\gamma_{\mu} \otimes 1)$  should be non-zero—checking this tests the enforcement of lattice symmetries on our finite sample. Removing the (periodic) delta-function with the definition  $S^{-1}[p'] \equiv S^{-1}[p', -p']/V$ , the wave-function renormalization is given in the “RI’ scheme” by (with  $a = 1$ )

$$Z'_q(p') = -i \frac{1}{12N_T} \sum_{\mu} \frac{p'_{\mu}}{p'^2} \text{Tr} \left[ \overline{(\gamma_{\mu} \otimes 1)} S^{-1}[p'] \right]. \quad (5)$$

where  $N_T = 4$  is the number of tastes.  $Z'_q(p')$  is needed for subsequent parts of the calculation, and can also be compared, after chiral extrapolation, to perturbative results. We plan to experiment with different “latticity” choices of  $p'_{\mu}$  to see if this reduces kinematic discretization errors [6]. We can convert from the RI’ scheme to the more conventional RI scheme (i.e. from  $Z'_q$  to  $Z_q$ ) using perturbation theory, and this is assumed below.

The mass renormalization factor  $Z_m$  may then be determined using

$$\frac{1}{12N_T} \text{Tr} \left[ \overline{(1 \otimes 1)} S^{-1}[p'] \right] = Z_q(p') \left[ Z_m(p')m + C_1 \frac{\langle \bar{q}q \rangle}{p'^2} + \dots \right]. \quad (6)$$

More precisely, we must extrapolate  $Z_m$  to the chiral limit in order to make this a mass-independent renormalization constant. The second term in eq. (6), which can be derived using

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<sup>3</sup>We note that Ref. [8] did not use simple momentum space fields, but rather Fourier transformed the position-space hypercube fields. This leads to additional taste-breaking terms in the free propagator. We think that the present method is preferable.

<sup>4</sup>We also check that the physical momentum is conserved, after averaging over configurations.

the operator-product expansion [9], is an example of the non-perturbative effects that are always present at some level even in short distance correlation functions. It must be removed by fitting, and makes this a sub-optimal method for determining  $Z_m$ .

A better method for calculating  $Z_m$  is to calculate the matching factor for the scalar, taste singlet bilinear,  $Z_s$ , and use  $Z_m = Z_s^{-1}$ , which follows from the approximate axial symmetry of staggered fermions. More generally, we want to calculate the insertion of staggered bilinear operators  $\mathcal{O}$  having arbitrary spin-taste. We spare the reviewers a recap of the details, but only note that these operators are spread out over a  $2^4$  hypercube, and generically involve gauge links. For the scalar of most interest, however, the operator is ultra-local and does not involve gauge links. By contracting together two momentum-source propagators (one appropriately conjugated) we can construct a vertex function  $\Lambda^\mathcal{O}[p', -p']$ . In general the momenta can be different (and this has been used to good effect in DWF studies [6] to avoid exceptional momenta), but, for simplicity in this presentation we assume that the incoming and outgoing momenta are the same. In practice, we plan to investigate both equal and unequal possibilities.

To obtain the matching factor for the operator, we first amputate in the standard way

$$\Gamma^\mathcal{O}[p'] = S[p']^{-1} \Lambda^\mathcal{O}[p', -p'] S[p']^{-1}, \quad (7)$$

where we stress that all quantities in this equation are  $16 \times 16$  matrices. In general, one must also include operator mixing, but this is not the case for most bilinears, and we do not include it here so as to avoid cluttering the notation. We now obtain the matching factor  $Z_\mathcal{O}$  by projecting:

$$\frac{Z_q(p')}{Z_\mathcal{O}(p')} = \frac{1}{12N_T} \text{Tr} \left\{ \overline{(\gamma_\mathcal{O})}^\dagger \Gamma^\mathcal{O}[p'] \right\}, \quad (8)$$

where  $\gamma_\mathcal{O}$  is the appropriate spin-taste matrix. To obtain the final result one must extrapolate to the chiral limit, multiply by the appropriate perturbative renormalization factor to obtain a nominally scale independent quantity, ensure that non-perturbative contributions are suitably small by studying the  $p'$  dependence, and attempt to extrapolate away discretization errors proportional to  $(ap')^2$ . These steps are non-trivial, but have been carried out successfully in previous NPR calculations.

The same method applies to four-fermion operators, except that one has, of course, four external legs, and that all cases involve operator mixing.

Our resulting matching factors will not, strictly speaking, be mass independent, as we cannot extrapolate the strange sea-quark mass to zero (it being fixed in the MILC configurations to close to its physical value). We will estimate the resulting systematic along the lines followed in Ref. [6], and expect this to be small. We can also study this numerically by using the coarse MILC lattices with different values for the strange mass.

Finally, we note that, since we use the MILC asqtad configurations, we must assume that the use of a rooted fermion determinant leads to the correct continuum limit. This is plausible, based on the extensive numerical results and theoretical work summarized in Refs. [10, 11].

### 3 Code details

We have chosen to carry out our calculations using the Chroma software package because of its portability, flexibility, and accessibility. The Chroma system is portable so that code written

and tested on our native scalar computers can be run on parallel workstations with minimal modification. Chroma uses an xml input system to specify its calculations, which leads to a great amount of flexibility in running jobs. There is no need to recompile code for every modification, and a complex series of manipulations can be specified from a single input file. Chroma is accessible to us in the sense that many useful algorithms can be run “out of the box.” This allows us to focus code development on the specific needs of our project. In particular, we use the built in Landau gauge fixing, HYP-smearing and asqtad inversion options.

Because we want to invert directly on momentum sources (as discussed above) we have written routines to construct such sources for staggered propagators, and integrated them into the “factories” of Chroma so that they can be used in the standard way. We have written routines to Fourier transform these propagators and output them in an xml format convenient for analysis with Mathematica. Our analysis will be done locally.

At this stage our code is fully developed and tested for the calculation of the momentum-source propagators for asqtad fermions, from which we can directly extract the quark renormalization  $Z_q(p)$  and the mass renormalization  $Z_m(p)$ . These tests have been done on finite temperature  $12^3 \times 4$  lattices available from the “Gauge Connection” (chosen not for physical relevance but for computational expediency given our limited local resources). Using 40 lattices (with parameters  $\beta = 5.25$ ,  $ma = 0.008$ ,  $N_f = 2$ , which puts the lattices on the confined size of the transition, with  $a \approx 0.25$  fm) we have confirmed that momentum sources dramatically reduce the errors compared to point sources, with the final errors in  $Z_q$  for  $ap \approx 1$  being 0.1% or less.

We have successfully run our code on the Fermilab clusters using MILC lattices, with CPU time from a Class C development allocation. These runs give us the timing information used to make our estimates below.

Three ongoing code development projects are needed to do all the calculations outlined above. The first is to implement the contraction of two propagators with a staggered bilinear operator of arbitrary spin-taste. For a general operator this involves the inclusion of gauge links. However, for asqtad fermions, we are most interested in the local scalar operator, and this does not require gauge links, so we will implement this (and the related pseudoscalar insertion) first. This is very straightforward using the Chroma tools. We expect both parts of this project to be completed well before July 2008.

The second project is the implementation of inversions with unimproved staggered fermions in Chroma, since this is what is needed for HYP-smearred staggered fermions. We expect that generating these inversions will require stripping down some previously written code and reintegrating it into the libraries. Since we will first be calculating using asqtad fermions, this project is less urgent, but we aim to have this completed early in the 2008-9 allocation cycle.

The third project is the development of code to contract four propagators together with staggered four-fermion operators of arbitrary spin and taste and involving HYP-links. This is required to calculate matching factors for kaon mixing matrix elements. We hope to have this completed by the end of summer 2008, in time for use with the HYP-smearred propagators.<sup>5</sup>

We stress that, despite not having all the contraction code finished at this time, we are ready to do production calculations of asqtad propagators immediately, using tested code, since we can store the resultant propagators for subsequent analysis. In other words, we are not dependent

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<sup>5</sup>It is also of interest to do the matching calculations for asqtad fermions, since that would allow a non-perturbative renormalization of the  $B_K$  results from Ref. [16].

on having all the contraction code completed by the beginning of the allocation period. This flexibility is important also because we can calculate additional quantities that we identify to be of interest at a later stage.

## 4 Proposed calculations

The set of calculations we propose are essentially the same for both valence asqtad and HYP-smearred quarks—the only difference being the addition of HYP-smearing, which is computationally negligible. We propose using both coarse and fine lattices (specifically, those of size  $20^3 \times 64$  at  $a \approx 0.125$  fm, and  $28^3 \times 96$  at  $a \approx 0.09$  fm). We plan to use three quark masses per lattice spacing in order to do the chiral extrapolation. In most cases we can match the valence and sea quark masses, rather than use partially quenched results, although we suspect, based on accumulated experience with other quantities, that there will be a very weak dependence on the sea quark mass. We stress that the quark-mass dependence is expected to be analytic (there being no chiral logarithms in this short-distance quantity), and our aim is to use small enough quark masses that we are in the linear regime (which we can test by having three masses). This was the approach chosen in the previous successful NPR calculation using staggered quarks [8].

We have tentatively chosen  $am = 0.01, 0.02$  and  $0.03$  for the valence quark masses on the coarse lattices, and  $am = 0.006, 0.012$  and  $0.02$  on the fine lattices (so that the physical quark masses are about the same).<sup>6</sup> The leading order mass dependence is linear, and comes dominantly from discretization errors proportional to  $am$ . (Mass dependence due to physical effects is quadratic in  $m$  at short distances, although long-distance chiral symmetry breaking effects lead to linear mass dependence as the renormalization scale is reduced.) Thus it may be that using smaller values of  $am$  on the fine lattices is unnecessary. To make our timing estimates, however, we make the more conservative choice of using the same physical masses at both spacings. Our final choice of masses on the fine lattices will be chosen based on ongoing analysis of the data itself.

With regard to the choice of momenta, we need enough points within the window  $\Lambda_{\text{QCD}} \ll p \ll 1/a$  to allow comparison of the  $p^2$  dependence with perturbative expectations. In practice it appears that  $(pa)^2 < 2$  is sufficient for the upper bound, and that residual  $(ap)^2$  errors can be removed by fitting [8, 6]. Here we can take advantage of the small errors in propagators from momentum sources to sketch out the momentum dependence thoroughly on a few lattices, and use this sketch to decide on the appropriate window. To be concrete, we estimate CPU requirements assuming that we ultimately do production runs using 6 different physical momenta (each, we recall, corresponding to 16 different lattice momenta). The precise choice of momenta will be guided by previous work, e.g. the recent detailed study using DWF [6].

Based on our pilot study, we choose 50 lattices per ensemble. We note that this is comparable to the number used in the quenched staggered study (30-50 configurations of size  $32^4$  [8]) and the recent DWF study (75 configurations of size  $16^3 \times 32$  [6]).

We collect the time estimates for the calculation using asqtad valence fermions in Tables 1, 2 and 3. Timings are based on our test runs on the pion and kaon clusters at FNAL, converted to 6n-equivalents using the factors given in the call for proposals. The total cost for gauge fixing and asqtad inversions is thus 318,000 6n equivalent node hours.

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<sup>6</sup>These values are for the asqtad quarks; values for HYP-smearred quarks will be chosen to correspond to approximately the same physical quark masses.

size	time (6n)	configs	sea masses	total (6n-hrs)
$20^3 \times 64$	9 hrs	50	3	1,350
$28^3 \times 96$	60 hrs	50	3	9,000
				10,350

Table 1: Estimated time required to gauge fix lattices (6n-hrs)

$am$	time (6n)	configs	momenta	total (6n-hrs)
.03	1.2 hrs	50	$6 \times 16$	5,760
.02	1.8 hrs	50	$6 \times 16$	8,640
.01	5 hrs	50	$6 \times 16$	19,200
				38,400

Table 2: Asqtad inversion estimate on  $20^3 \times 64$  lattices (6n-hrs)

The computations for the HYP-smearred inversions are the same, but we expect the simplicity of the action will lead to a speed up of about a factor of two. Assuming this factor, and noting that gauge-fixing need not be repeated (since it precedes HYP-smearing) we estimate that the total cost for HYP-smearred inversions is 154,000 6n equivalent node hours.

A summary of our estimates is given in Table 4. Adding in a contingency for HYP-smearing, Fourier transforms, and the calculation of contractions, we come to our **total request of 500,000 6n equivalent node hours**. Since we have obtained access to the Fermilab clusters, and have become familiar with running on them, our preference would be that any allocation we are granted be on the Fermilab clusters.

## 5 Storage requirements

As noted above, we plan on storing both the gauge-fixed lattices and the propagators from momentum sources. Our estimate of the required storage is given in Table 5. If these are stored on disk, this corresponds to 6300 6n-equivalent node-hours using the official conversion factors.

$am$	time (6n)	configs	momenta	total (6n-hrs)
.02	9 hrs	50	$6 \times 16$	43,200
.01	16 hrs	50	$6 \times 16$	76,800
.006	31 hrs	50	$6 \times 16$	148,800
				268,800

Table 3: Asqtad inversion estimate on  $28^3 \times 96$  lattices (6n-hrs)

calculation	coarse (6n-hrs)	fine (6n-hrs)	total (6n-hrs)
gauge fixing	1350	9000	10,350
ASQTAD inversions	38,400	268,800	307,200
HYP-smearred inversions	19,200	134,400	153,600
			471,150

Table 4: Total time estimate (6n-hrs)

data	total (Gbytes)
gauge-fixed configs	25
Asqtad props	145
HYP-smearred props	145
total	315

Table 5: Total storage estimate (Gbytes).

## 6 Sharing and exclusivity

We are happy to make the lattices and propagators available to the collaboration if there is interest. We ask for exclusivity for the calculations of bilinear or four-fermion operator matching factors outlined above, for a period of 6 months after the propagator calculations have been completed.

## 7 Summary

We are proposing to use NPR to calculate a variety of matching factors for improved staggered fermions, quantities that are essential if the ongoing calculations of quark masses and kaon matrix elements are to reach high precision. Although not all the analysis code is finished, we are ready immediately to begin production of asqtad propagators with momentum sources and to do the first level of analysis on them. We can reuse the saved propagators and gauge-fixed lattices repeatedly as more elaborate contraction codes are completed.

We stress this point because we are, to some extent, slowed down by the yearly cycle of the USQCD allocation procedure. This is particularly a concern for Andrew, who is a graduate student. If our proposal is successful, we would like to inquire if there is any possibility of obtaining some of our allocation before the next allocation cycle begins.

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