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# Dynamical simulations with HYP-link Wilson fermions

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We present results from simulations of two dynamical flavors of improved Wilson fermions with nHYP smeared gauge links. We demonstrate that the simulation is stable at a pseudo-scalar mass of 360MeV, a 2.1fm box and a lattice spacing of 0.13fm.

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## 1. Introduction

Ever since the introduction of the original APE smearing in 1987[1], many applications have shown the beneficial effects of constructing the lattice Dirac operator from smeared links. The hypothesis behind employing smeared links is that short range fluctuations of the gauge field, the so-called dislocations, are responsible for some of the poor scaling behavior and large cost of fermion simulations. For different lattice discretizations of the Dirac operator, the improvement due to smearing comes in different disguises. In Wilson fermions dislocations cause the exceptionally small eigenvalues of the Dirac operator, in staggered fermions the large taste breaking. Domain Wall fermions acquire their residual explicit chiral symmetry breaking through dislocations and they are responsible for the high numerical cost of constructing the overlap operator.

An alternative approach to reduce these effects is the use of special gauge actions, e.g. the Iwasaki action or DBW2, which suppress the occurrence of dislocations. However, it has turned out that these gauge actions themselves induce quite large scaling violations. Smearing the links, however, reduces the effect of the dislocations on the fermions only. They remain part of the gauge dynamics and one can choose a gauge action which does not introduce poor scaling behavior from the gluonic sector. Increased auto-correlation times in molecular dynamics based algorithms have been observed when using improved gauge actions as well. Below, we will show that we do not observe signs of this in our simulations.

Regardless of whether one accepts the explanation of these effects, in many quenched studies it was demonstrated that smearing helps to improve scaling in the situations listed above. It is therefore natural to use it in dynamical simulations too.

The goal of this conference contribution is to convince the reader that simulations of improved Wilson fermions constructed from the recently suggested nHYP links[2] are stable even at a coarse lattice spacing. The additional cost of the smearing is small and more than compensated by the improved conditioning number of the fermion matrix. Exploratory studies of non-perturbative improvement of this action using Schrödinger functional techniques have also been presented at this conference [3].

## 2. Smearing procedure

Most dynamical algorithms are based on molecular dynamics and therefore one needs to differentiate the action with respect to the gauge fields. If one uses smeared links, the derivative of the smeared link with respect to the thin link is needed. This turns out to be a problem for the projection which is part of the definition of the APE smearing,

$$V_{n,\mu} = \mathrm{Proj}_{\mathrm{SU}(3)} \left[ (1+\alpha)U_{n,\mu} + \frac{\alpha}{6} \sum_{\pm\nu\neq\mu} U_{n,\nu;\mu} U_{n+\hat{\nu},\mu;\nu} U^{\dagger}_{n+\hat{\mu},\nu;\mu} \right] , \tag{2.1}$$

with $n$ labeling the site and the result of the projection $B = \mathrm{Proj}_{\mathrm{SU}(3)} A$ is defined as the matrix $B \in \mathrm{SU}(3)$ which maximizes $\mathrm{tr}[A^{\dagger}B + B^{\dagger}A]$. The stout smearing of Morningstar and Peardon [4] is a fully differentiable alternative. However, we found it to be considerably less effective in reducing the effect of the dislocations.



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It also turns out that typically one level of smearing is not enough and one needs to iterate the procedure. However, iterating it too many times leads to Dirac operators with a large footprint. In quenched studies, a particular smearing recipe has proved to be efficient but not over-doing it: HYP smearing[5]. It consists of three levels of projected APE smearing, however, the smearing is restricted such that the smeared link only receives contributions from its hypercube. In Ref. [2] we introduced n-HYP smearing which differs from the original HYP smearing only in that the projection is not to SU(3) but to U(3)

$$\begin{aligned} V_{n,\mu} &= \mathrm{Proj}_{U(3)}[(1-\alpha_1)U_{n,\mu} + \frac{\alpha_1}{6}\sum_{\pm\nu\neq\mu}\tilde{V}_{n,\nu;\mu}\tilde{V}_{n+\hat{\nu},\mu;\nu}\tilde{V}^\dagger_{n+\hat{\mu},\nu;\mu}]\,, \\ \tilde{V}_{n,\mu;\nu} &= \mathrm{Proj}_{U(3)}[(1-\alpha_2)U_{n,\mu} + \frac{\alpha_2}{4}\sum_{\pm\rho\neq\nu,\mu}\bar{V}_{n,\rho;\nu\,\mu}\bar{V}_{n+\hat{\rho},\mu;\rho\,\nu}\bar{V}^\dagger_{n+\hat{\mu},\rho;\nu\,\mu}]\,, \\ \bar{V}_{n,\mu;\nu\,\rho} &= \mathrm{Proj}_{U(3)}[(1-\alpha_3)U_{n,\mu} + \frac{\alpha_3}{2}\sum_{\pm\eta\neq\rho,\nu,\mu}U_{n,\eta}U_{n+\hat{\eta},\mu}U^\dagger_{n+\hat{\mu},\eta}]\,, \end{aligned} \tag{2.2}$$

where $V_{n,\mu}$ is the link from which the Dirac operator is to be constructed. The projection is defined by

$$\mathrm{Proj}_{U(3)}A = A\frac{1}{\sqrt{A^\dagger A}} \tag{2.3}$$

which is differentiable where $A$ is non-singular.

The details of how the derivative is computed are described in Ref. [2]. The technique is very similar to the one use for stout smearing and results in similar computational cost. In principle, the discontinuity where the matrix $A$ is singular could cause problems in the simulation, however, in practice this turns out not to be the case in the simulations presented below. Apart from the simulations described in these proceedings, n-HYP smearing has also been used in overlap simulations [6, 7, 8].

## 3. The simulation

In order to test the performance of the smeared link, we started simulations of two degenerate flavors of improved Wilson fermions on $16^3\times 32$ lattices. We use tadpole improved Lüscher–Weisz gauge action. The clover coefficient is set to its tree level value $c_{SW}=1$. All links of this operator are constructed from n-HYP links, where the coefficients are set to the standard HYP values, $\alpha_1=0.75$, $\alpha_2=0.6$ and $\alpha_3=0.3$.

We generated lattices at two values of the sea quark mass. Both runs give a Sommer parameter $r_0/a=3.8$ which, using $r_0=0.5$fm, translates to a lattice spacing of $a\approx 0.13$fm. One ensemble, labeled heavy in the following—with $\beta=7.2$, $\kappa=0.1272$—has a pseudo-scalar mass of about 520MeV . A lighter run with $\beta=7.1$, $\kappa=0.1280$ renders $m_{\mathrm{PS}}\approx 360$MeV. We use multiple time scale Hybrid Monte Carlo[9] with Hasenbusch's mass preconditioning[10]. We typically ran at 90% acceptance rate at moderate step size and unit length trajectories.

We note in passing, that the overhead in the computation associated with the nHYP smearing—construction of the smeared links and the additional differentiation—is modest. For the light $16^3\times 32$ run 13% of the wall clock time is spent on this part whereas we spend two third of the time on the inversions and 18% on the gauge force. We believe that the cost of the nHYP smearing is more

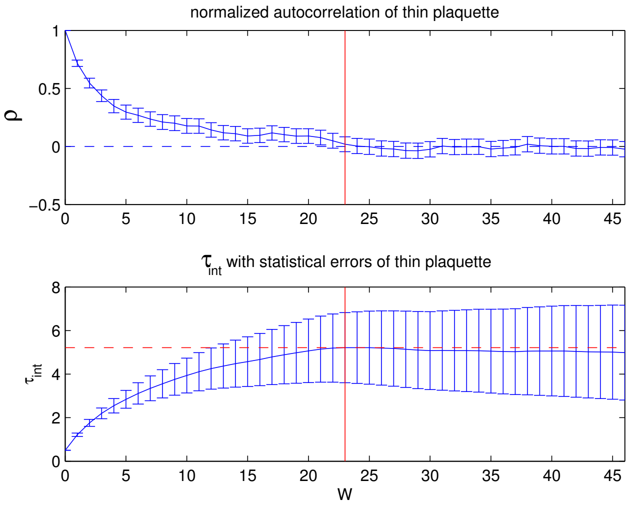


**Figure 1:** Auto-correlation analysis of the plaquette for the light run on the $16^3 \times 32$, $\beta = 7.1$, $\kappa = 0.1280$ lattice.

than off-set by the improvement of the condition number of the fermion matrix and the reduced cost of the inversions.

### 3.1 Auto-correlation

In order to make sure that using smeared links does not lead to increased auto-correlation times, we compute $\tau_{\rm int}$ for the plaquette and the plaquette constructed from smeared links which is less UV dominated. We use the methods of Ref. [11]. For the light ensemble, we find $\tau_{\rm int} = 5.2(1.4)$ and $10(4)$ respectively, see Fig. 1. The heavy runs with $m_{\rm PS} \approx 520$MeV have $\tau_{\rm int} = 6(2)$ and $9(3)$, which are surprisingly similar (if one ignores the large errors). However, the parameters of the algorithm have been tuned more carefully for the light run which might explain the absence of critical slowing down.

In particular in simulations with the DBW2 gauge action, the auto-correlation time of the topological charge frequently are hundreds of trajectories. We test for this on a smaller lattice, $12^3 \times 24$, $L \approx 1.4$fm and $m_{\rm PS} \approx 450$MeV. We measure the topological charge as defined by the index of the overlap operator after every fifth trajectory. The result is shown in Fig. 2. We find no detectable sign for increased auto-correlation.

We take these two findings as evidence that the intuitive expectation that the smeared links do not have any negative effects on the auto-correlation time is indeed confirmed.

### 3.2 Stability

In order to get reliable results from a simulation one needs to be sure that it is stable. How to check for stability is matter of some debate. We have tried to look for signs of meta-stabilities as put forward by Refs. [12] and [13] and the distribution of the lowest eigenvalue of the Hermitian Dirac operator advocated in Refs. [14] and [15].

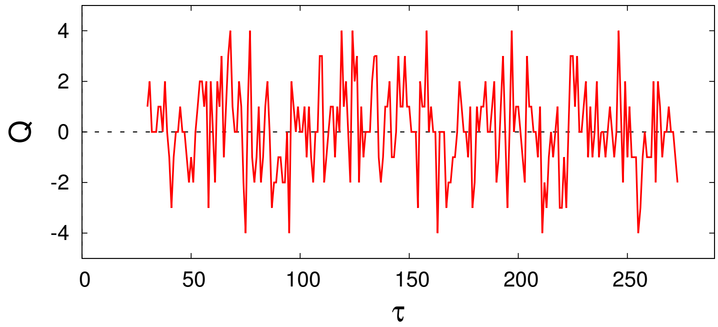


**Figure 2:** Monte-Carlo history of the topological charge. Each unit on the x-axis corresponds to five trajectories of unit length by which the measurements are separated.

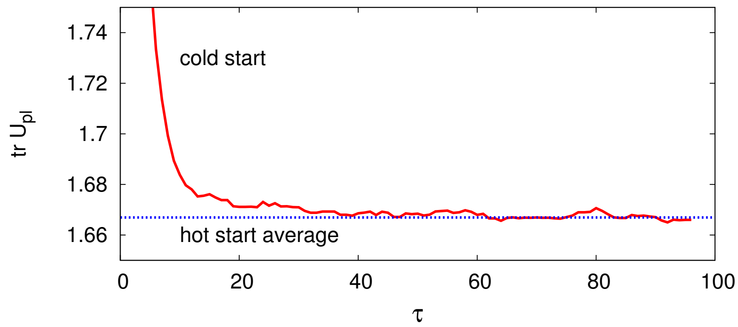


**Figure 3:** Monte-Carlo time history of the plaquette from a cold start. The horizontal line denotes the average from the hot-start. There is no sign for instabilities from a first-order phase transition

First to the meta-stabilities: the method is to compare observables (typically the plaquette) as a function of Monte–Carlo time from a stream which is started from a hot configuration with a stream which starts from a unit, cold configuration. The result for the light run is shown in Fig. 3. We observe that the cold start reaches the average of the plaquette from the hot start after about 50 trajectories and there is no sign for intermediate meta-stabilities.

Since this is reassuring, we can now turn to the distribution of the lowest magnitude eigenvalue of the Hermitian Dirac operator $Q = \gamma_5 D$. Ref. [14] uses this distribution as the main indicator for the stability of a simulation. Due to the singularity in the force where $Q$ has a zero eigenvalue, instabilities occur once these surfaces are crossed too often during the generation of the ensemble. A situation where the distribution of the lowest eigenvalue is far away from zero (where far is defined in units of the width of the distribution) is interpreted as stable.

In Fig. 4 we have plotted the distribution of $|\lambda_0|$, the magnitude of the eigenvalue of $Q$ with the smallest absolute value. It contains the result for the light and the heavy run along with its bare PCAC quark mass. For the heavy ensemble, we find a mean of the distribution $\mu = 49$MeV and a width of $\sigma = 3$MeV, the width is defined as in Ref. [14]. The light run has a median gap of 23MeV and also a width of 3MeV. As argued in Ref. [14] the width is independent of the quark mass. Also both of our runs fulfill $3\sigma < \mu$, the criterion of stability given in that paper. If one assumes that $\sigma$

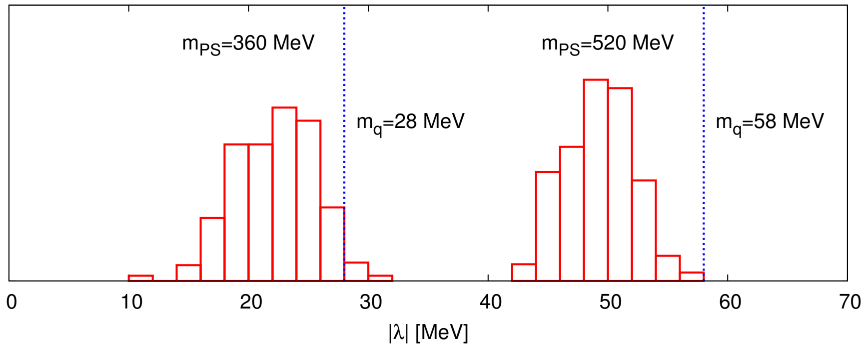


**Figure 4:** Distribution of the modulus of the lowest eigenvalue of the Hermitian Dirac operator $\gamma_5 D$ for the two large volume runs.

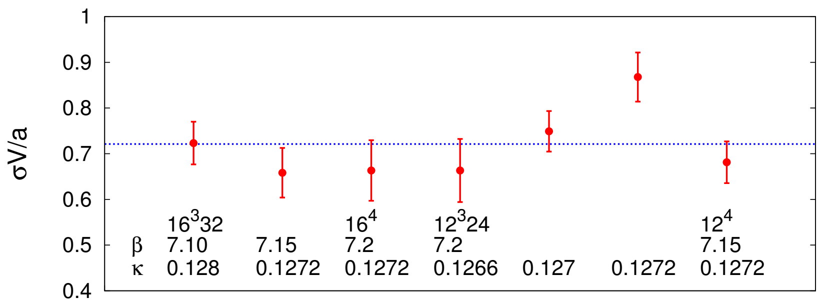


**Figure 5:** Scaling of the width $\sigma$ of the distribution of the lowest eigenvalue of $Q$ for various volumes and lattice spacings.

is independent of the sea quark mass, and also assumes that the lower bound of stability is given by this criterion, one gets that a pion mass of 240MeV is reachable with our setup without running into problems with the stability. As a side remark, we notice that the bare quark mass is quite close to the median of the gap, however, some unknown renormalization constants are needed for a quantitative comparison.

In the same paper[14] it has been argued that the combination $\sigma V/a$ should be a scaling quantity. Our result for a selection of our runs is displayed in Fig. 5. We find a value of about 0.7 whereas the original publication[14] found for thin link unimproved Wilson fermions values around 1. However, since we use the bare width $\sigma$ in this plot, a meaningful comparison is again not possible.

## 4. Summary

At this conference, we presented new results from simulations with nHYP smeared improved Wilson fermions in 2fm boxes at a coarse lattice spacing of about 0.13fm and light pion mass $m_{\rm PS} \approx 360$MeV. We showed that the simulations are stable in this region where ordinary thin link Wilson simulations are at least very difficult. Contrary to special gauge actions (e.g. DBW2) which suppress dislocations, smeared links have no negative impact on auto-correlation times. Given the experience of quenched simulations we also expect an improved scaling behavior. This however, is subject of future studies.

If one assumes the stability bound of Ref. [14] to be correct, we could simulate at pion masses down to 240MeV without running into problems with the stability. This would correspond to a $m_{PS}L \approx 2.4$. From the scaling arguments of the same paper one would conclude that all reasonable parameter values in the p-regime are accessible even at such a coarse lattice spacing.

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