PROCEEDINGS OF SCIENCE

Implementing Hybrid Monte Carlo with stout-smeared chirally improved Dirac operators*

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We discuss our implementation of dynamical Ginsparg-Wilson type fermions using a stout-smeared chirally improved Dirac operator. Such operators have been studied extensively in quenched calculations within the Bern-Graz-Regensburg (BGR) collaboration. Here we discuss the development and testing of the Hybrid Monte Carlo algorithm with this Dirac operator. We study the chiral properties of this operator in a dynamical setup, comparing, e.g., the spectra of the operator for the dynamical and quenched cases. We then discuss quantitative features of the algorithm like autocorrelation and performance.

XXIIIrd International Symposium on Lattice Field Theory
25-30 July 2005
Trinity College, Dublin, Ireland

*for the Bern-Graz-Regensburg (BGR) collaboration

†Supported by Fonds zur Förderung der wissenschaftlichen Forschung in Österreich, project M870-N08 (Lise Meitner Fellowship)

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§Supported by Fonds zur Förderung der wissenschaftlichen Forschung in Österreich, project P16310-N08

PoS(LAT2005)124

1. Chirally improved fermions

Chirally improved (CI) fermions [1] are Ginsparg-Wilson type fermions. The most general ansatz for a lattice Dirac operator reads

$$D_{x,y} = \sum_{i=1}^{16} \alpha^i_{x,y}(U)\Gamma_i \,, \tag{1.1}$$

where Γ_i $\{i = 1 \ldots 16\}$ are the 16 elements of the Clifford algebra and $\alpha^i_{x,y}(U)$ are sums of path ordered products of links U. Inserting D into the Ginsparg-Wilson relation and solving the resulting algebraic equations yields the chirally improved Dirac operator D_{CI}. In principle this can be an exact solution, but that would require an infinite number of terms. In practice the number of terms is finite and the operator is a truncated series solution to the Ginsparg-Wilson relation, respecting the lattice symmetries, invariance under charge conjugation as well as γ_5-hermiticity, but connecting sites only over a certain distance.

For our implementation we use coefficients up to a path length of four [1, 2]. Some of these terms used are sketched in Fig. 1. An operator like this, which is ultra-local, can never fulfill the

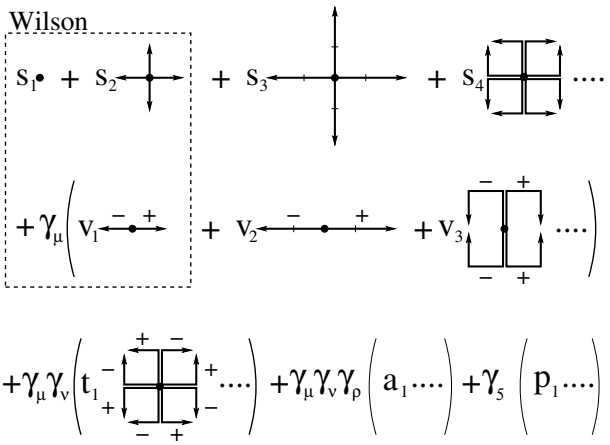

Figure 1: The ansatz for the chirally improved Dirac operator

relation exactly, which of the currently known actions only the overlap action does.

CI fermions have been extensively tested in quenched calculations (see, e.g., Ref. [3]). In these tests it was found that smearing the gauge fields improves the properties of CI fermions significantly and as a consequence on smeared gauge configurations one can go to smaller quark masses without running into the problem with exceptional configurations. On HYP smeared quenched configurations pion masses down to 220 MeV could be reached on lattices of size $16^3 \times 32$ and about 250 MeV on $12^3 \times 24$ lattices. We expect this to improve in dynamical simulations.

2. Dynamical chirally improved fermions

2.1 First attempts

First attempts to use CI fermions in dynamical simulations were presented in [4]. As mentioned, smearing of the gauge fields is helpful for going to small quark masses. In all corresponding

$L^3 \times T$	am	β_{LW}	*res*	Δt	steps	acc.	HMC time	CPU Hours/ HMC Time	a[fm]
$8^3 \times 16$	0.05	5.4	10^{-10}	0.015	50	$\sim$93%	700	0.6 h (16 O)	0.114(3)
$8^3 \times 16$	0.05	5.3	10^{-10}	0.015	50	$\sim$91%	700	0.6 h (16 O)	0.135(3)
$8^3 \times 16$	0.08	5.4	10^{-10}	0.015	50	$\sim$93%	700	0.5 h (16 O)	0.138(3)
$12^3 \times 24$	0.05	5.3	10^{-8}	0.01	100	$\sim$87%	200	4 h (8 H)	0.129(3)

Table 1: Parameters, statistics and some results from our dynamical simulations.

quenched simulations up to now HYP smearing was used. This, however, is not differentiable and therefore does not allow for implementation in a Hybrid Monte Carlo (HMC) updating algorithm. In Ref. [4] we therefore tried to use a partial-global updating scheme and we could collect first experiences on rather small lattices (up to 8^4).

The major drawback of such algorithms is that the computer time increases as V^2. We therefore decided to proceed with implementing the HMC method, which is, however, technically significantly more complicated for actions like ours, that have many interaction terms.

2.2 Hybrid Monte Carlo

In quenched calculations it was found that the tadpole improved Lüscher-Weisz gauge action had certain advantages over the Wilson gauge action in the sense that the configurations produced with this action were smoother than the ones produced by the Wilson gauge action. We therefore used the same gauge action in our studies.

Smearing is an essential quality improving ingredient in our Dirac operator. The recent introduction of the differentiable "stout"-smearing [5] opened the possibility to implement HMC for smeared fermionic actions like ours.

In principle HMC is directly applicable for D_{CI}; problems like the discontinuities one has to deal with in HMC for the overlap action do not occur for our action – it is not an exact GW action, which is an advantage in this regard. It can be expected that HMC for CI retains the very favorable $V^{5/4}$ scaling properties which it shows for staggered and Wilson fermions.

The problems of implementation were mostly technical. Much of the work went into developing automated methods to write down the fermionic force for all 2428 different terms of our operator. Otherwise the HMC code we used so far is rather conservative. We use a standard pseudo-fermion action with two mass degenerate fermion flavors $S_f = |D^{-1}\xi|^2$. The integration scheme is leap-frog integration, as the solver for $D^\dagger D$ (needed for the molecular dynamics evolution) the standard conjugate gradient algorithm, and as the solver of D alone (needed in the accept/reject step) the BiCGStab was used.

It is well known that the performance of the inverter may be significantly improved by providing a good guess for the solution. Using an optimal linear combination of the twelve previous solutions caused the number of conjugate gradient iterations, required for the inversion of the D_{CI} during the molecular dynamics evolution inside a trajectory, to fall by a factor between two and three (chronological inverter by minimal residual extrapolation).

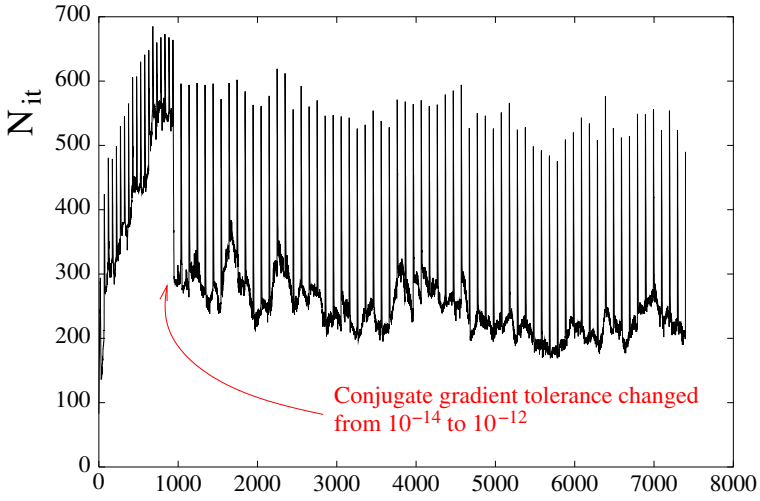

Figure 2: Number of conjugate gradient iterations for each molecular-dynamics step ($12^3 \times 24$ lattice; a=0.135 fm; $am = 0.05$). We use the information from 12 previous solutions as starting guess for new solution. The peaks correspond to the number of iterations required in the accept/reject step.

Here we concentrate on the algorithmic aspects of our work; in another contribution to these proceedings we give first results of the physical aspects [6].

2.3 Parameters and statistics

First tests of our code were done on $8^3 \times 16$ lattices. As we already know from the quenched tests this lattice size does not allow for small bare quark masses, we chose $am = 0.05$ and $am = 0.08$. Runs with $12^3 \times 24$ lattices are in progress; there we approach much smaller masses am down to 0.02.

In Table 1 we present some parameters and results of our simulations. The conjugate gradient residual for the molecular dynamics evolutions is denoted as *res*, initially, when we started our small lattice runs, we chose a very small value (10^{-10}). We then gradually increased it in accordance with the folklore of other dynamical simulations (with other actions) and are currently using $res = 10^{-7}$ during the HMC trajectory but still 10^{-10} in the accept/reject step.

The lattice spacing a was determined [6] using the Sommer scale in order to have a first estimate. Eventually we will use the hadron masses to set the scale.

The runs were done on a cluster of Sun Fire V20z each with two Opteron 248 processors at 2.2 GhZ (at the Karl-Franzens-Universität, Graz) and on the Hitachi SR8000 at LRZ Munich. In the table (16 O) denotes 16 of the Opteron processors (8 nodes) in parallel, (8 H) denotes 8 SR8000 nodes. Just to get an idea about timing, we note that for the $12^3 \times 24$ lattice at $am = 0.05$ one trajectory takes ~ 4 hours on 8 nodes of the Hitachi.

As a first study we made runs on small lattices checking equilibration, lattice spacing and the the ρ and π meson correlators.

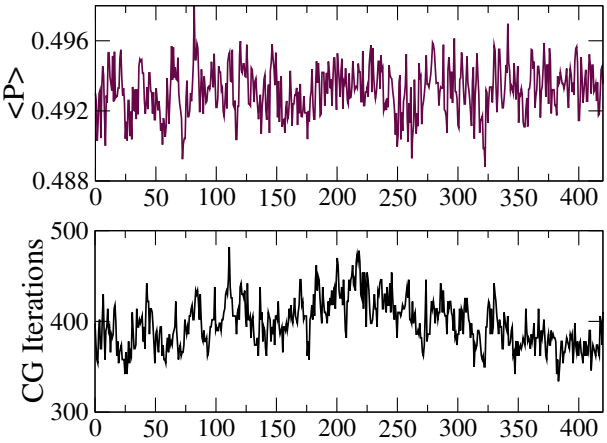

Figure 3: History of the plaquette (upper part) and the number of CG iterations (lower part) in the accept/reject step (2nd run in Table 1).

3. Results

In Fig. 2 we plot the number of conjugate gradient iterations against molecular dynamics time. After 1000 inversions we decided to reduce the conjugate gradient tolerance was from 10^{-14} to 10^{-12}. The drop in the number of iterations is quite evident from this plot.

To demonstrate autocorrelation we show in Fig. 3 the histories of the plaquette and the number of BiCGStab iterations in our accept/reject step. Visual inspection indicates a time scale of roughly 25 and a possible second time scale $\mathscr{O}(200)$.

We computed the integrated autocorrelation time from the number of BiCGStab iterations required for the accept/reject step. This is widely believed to be the longest autocorrelation present and in our case this is about 36 trajectories. In contrast the autocorrelation time for the plaquette, which is the most local quantity and therefore is expected to have the shortest autocorrelation time is less than 2 trajectories. Obviously the runs are yet to short for a precise determination of the autocorrelation times.

The D_{CI} – due to the truncation – obeys the GW Relation only approximately. In the quenched calculations it has exhibited, however, very good chiral properties. We may now check, whether this feature survives or even improves in the simulation with dynamical fermions. As a simple check we plot in Fig. 4 the low lying spectrum of D_{CI} along with the Ginsparg-Wilson circle for three typical gauge configurations and compare with a spectrum from a quenched simulation with similar lattice parameters. As can be seen from the figure, the spectrum follows the Ginsparg-Wilson circle remarkably well at least for the low-lying modes, that have been determined, and that are important towards the continuum limit. This assures us to a certain extent that the good chiral properties observed in the quenched studies are indeed also present in the dynamical case. We conclude that the chiral properties of D_{CI} on dynamical configurations are roughly the same as on quenched configurations of the same lattice spacing.

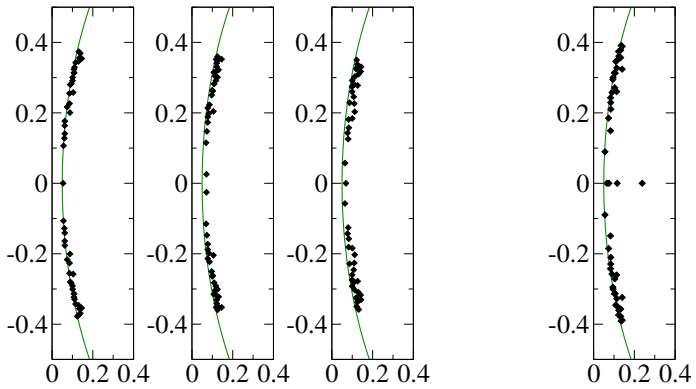

Figure 4: L.h.s: Three spectra of D_{CI} ($am = 0.05$) on dynamical configurations of $8^3 \times 16$, $a = 0.14$ fm. R.h.s: Sample D_{CI} ($am = 0.05$) spectrum on a quenched configuration with similar parameters, i.e., lattice size $8^3 \times 16$, $a = 0.15$ fm.

4. Summary and outlook

We presented recent results of our work in progress on implementing Ginsparg-Wilson type fermions in a full dynamical QCD simulation. Dynamical chirally improved fermions with stout-smeared links can be implemented using an HMC algorithm with all its well-known favorable properties, like $V^{5/4}$ scaling. The Dirac operator retains its good chiral properties which allowed – in quenched simulations – to reach pion masses down to 250 MeV on moderately sized lattice of $12^4 \times 24$. We expect to be able to reach such values also in the dynamical fermion case. We hope to obtain pion masses of about 300 MeV in our recently started runs and hope to be able to go below that in the future. More results on our simulations, i.e., meson masses and topological charge, can be found in [6].

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