Gauge field generation with Exponentiated Clover Fermions

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Introduction

Lattice QCD (LQCD) calculations rely on **Monte Carlo methods** and **importance sampling** to approximate the highly dimensional path integrals and compute observables. In this approach, the most relevant gauge field configurations are sampled from a distribution determined by underlying physics. The resulting ensemble of gauge fields enables the computation of various observables. Consequently, the **generation of gauge field configurations** is a fundamental aspect of Lattice QCD calculations.

A widely used fermion action is the **Clover Fermions**, extends **Wilson Fermions** with the term:

$$S_{clov} = M_0 + c_{SW}\frac{i}{4}\bar{\psi}\sigma_{\mu\nu}F_{\mu\nu}\psi$$

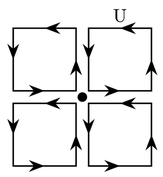

Figure 1. Around a lattice site, oriented plaquettes of gauge links U form the Clover leaf term $F_{\mu\nu}$.

and has features such as:

- O(a) improvement
- Cost effective
- Positive and negative eigenvalues that are equally distributed limits this approach[2]

The last feature significantly affects simulations with small quark masses and large lattices.

Replacing the clover term with an exponential version[3]: $S_{exp-clov} = M_0 exp(c_{SW}\frac{i}{4}\bar{\psi}\sigma_{\mu\nu}F_{\mu\nu}\psi)$ leads **Exponentiated Clover Fermions** which offer:

- O(a) improvement
- Invertible Dirac operator with values bounded from below

Methodology

To efficiently generate gauge fields ensembles, we employed the **Chroma** software suite [1]. This code, together with libraries such as **QUDA** and **QDP-JIT**, provide state-of-art tools for Lattice QCD calculations. In **Chroma**, we have implemented **Exponentiated Clover Fermions** supporting solvers using:

- Unpreconditioning
- Even-Odd preconditioning
- Even-Odd preconditioned for QUDA multigrid

Using existing Clover Fermions on Chroma as a reference, correctness and performance studies were performed with the following:

- **Molecular Dynamics** using the **Leapfrog integrator**
- **Gauge field generation** with the **Hybrid Monte Carlo** algorithm (HMC)

The test used the following setup:

- **Action**:
  - Lüscher–Weisz Gauge Action
  - 2+1 dynamical quarks with even-odd preconditioning
- **Lattice, clover and quark parameters**:

Volume	β	$m_u = m_d = m_s$	c_{SW}	conf. start
$16^3 \times 32$	3.36	-0.3407494145199066	2.038765	Disordered

Results & Discussion

Molecular dynamics tests:

In Molecular Dynamics trajectories, energy and its changes are very susceptible to deviations from correct values, and thus they can reveal implementation errors. We performed tests with step sizes 16,32,64 and 128 and found:

- For both Clover and Exponentiated Clover, energies and energy changes are similar.
- In a trajectory, energy changes (dH) decreases by a factor of ~4 when doubling number of steps. The following table show our results:

Method	$dH[16]/[32]$	$dH[32]/[64]$	$dH[64]/[128]$
Clover	3.9997	4.0619	4.2818
Exp-Clover	3.9993	4.0582	4.2648

Gauge field generation with HMC tests:

182 gauge configurations were generated and we collected information for:

- Wilson plaquettes:

The plot on figure 2 shows a similar behavior for both Clover and exponentiated Clover Fermions with lower values for the latter. This is consistent with simulations performed in [2].

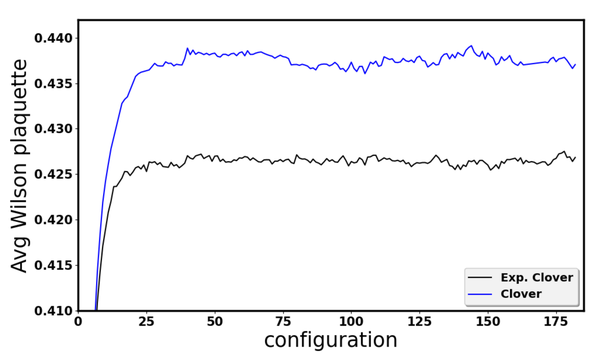

Figure 2. Wilson plaquette

- Computational cost:

Two factors impacting an ensemble generation computational cost are the Molecular dynamics time and the acceptance probability. Exponentiated clover fermions showed:

- Higher acceptance probabilities as
- Approximately 15% computational time increase in a Molecular Dynamics trajectory

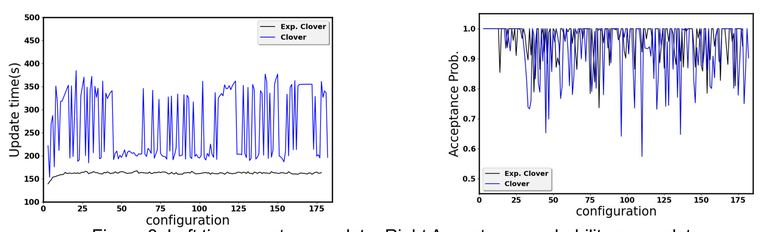

Figure 3. Left time spent per update. Right Acceptance probability per update.

Summary

We have implemented **Exponentiated Clover fermions** in Chroma and preliminary tests verify its correctness and showed:

- **Molecular dynamics trajectories** with both Exponentiated and Clover fermions are consistent.
- **Wilson Plaquette behavior** agrees with previous work.
- **Faster new gauge field generation** for Exponentiated Clover fermions due to higher acceptance probability. To further assess these findings, **additional testing is necessary**.

References
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2- **A. S. Francis, et. al**, PoS **LATTICE2021** (2022) 118, [arXiv:2201.03874 [hep-lat]]. doi:10.22323/1.396.0118
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