Key Performance Indicator for autocorrelation times of low energy observables in Lattice QCD

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ABSTRACT: This is a description of a code for measuring the autocorrelation times of selected low energy observables in Lattice QCD calculations. The test case at hand is pure SU(3) gauge theory using the Wilson gauge action. As the continuum limit is approached in such calculations, the autocorrelation times of observables are know to grow fast rendering these calculations impractical. Here we monitor the autocorrelation times of 1x1 Wilson loops constructed from smeared links via gradient flow. In addition we monitor the autocorrelation time of the topological charge. The application code for these calculations is CHROMA.

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1 Introduction

The continuum limit in lattice QCD calculations is taken by tuning the lattice bare coupling to a critical point where a second order phase transition occurs. In the neighborhood of this second order phase transition point, the Monte Carlo Algorithms used to perform the calculations show critical slowing. In order to access the efficiency of such algorithms a careful study of autocorrelation times of several observables needs to be done. Given that the problem is generic and appears both in calculations with or without dynamical fermions, we use pure SU(3) gauge theory as our benchmark. Pure gauge theory calculations require relatively small amount of computational resources to thoroughly study autocorrelation times. Given that our target application is QCD with dynamical fermions we restrict ourselves to algorithms suitable for dynamical fermions.

2 Benchmark setup

Our benchmark is defined as following:

- 1. Pure SU(3) gauge theory
- 2. Action: Wilson gauge action
- 3. Bare gauge coupling $\beta = 6.179$
- 4. Lattice size 32^4
- 5. Simulation algorithm: Hybrid Monte Carlo
- 6. Code: CHROMA

Steps for running the benchmark:

- 1. Download and compile CHROMA by following instruction on: http://jeffersonlab.github.io/chroma
- 2. Checkout from GitHub the Wilson KPI package:
 - > git clone git@github.com:orginos/Wilson-KPI.git

3. Untar the file wl_32_32_b6p179-kpi.tar.gz and follow the instruction is the README file it contains. In order to run you need to modify the pbs_hmc.sh script to match the requirements of your queueing system. The required input file to start the calculations is included in the package.

Results from running this test case have been published in [1], and follow closely the analysis performed in [2].

References

- [1] A. S. Gambhir and K. Orginos, PoS LATTICE2014, 043 (2015).
- [2] S. Schaefer, R. Sommer, and F. Virotta (ALPHA), Nucl. Phys. **B845**, 93 (2011), 1009.5228.