For the USQCD Exascale Computing Project

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.

Contents

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. Gradient Flow smearing: 40 Runge-Kutta steps for a total of 2 time units using `WILSON_FLOW` task.
7. Measure topological charge after 2 gradient flow time units using `QTOP_NAIVE` task.
8. Measure the 1x1 Wilson loops both at gradient flow time 0 and 2 (smeared) using `PLAQUETTE`
9. Code: All above tasks are implemented in CHROMA [1]

- Trajectory length used: 1.414 (in CHROMA conventions)
- Integrator: LCM_4MN5FV. This is a 4th order minimum norm symplectic integrator. The parameters for this integrator are those described in [2] (integrator 19 in Table 2).
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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 [3], and follow closely the analysis performed in [4]. A summary of autocorrelation times are listed in Table 1

Table 1. Autocorrelation times with 10,000 Trajectories

Observable	Value	Integrated Autocorrelation
1x1 Wilson loop	0.6116998(3)	3.26(3)
Smeared 1x1 Wilson loop (flow time 2.0)	0.9989961(15)	66(19)
Topological Charge	1.0(1.0)	320(140)

2.1 Computational requirements

This application has been tested on a 16 node cluster with dual 12-core 2.4GHz Haswell CPU per node and QDR infiniband network. Including all measurements the application needs 18 seconds per trajectory, resulting 5K hours to complete 1M trajectories.

References

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