Cost of QCD simulations with $n_f = 2$ dynamical Wilson fermions

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Cost estimates for simulations of full QCD with $n_f = 2$ Wilson fermions by hybrid Monte Carlo are presented. The extrapolations are based on the average number of iterations, $N_{\text{it}}$, of the iterative solver within the fermionic part of the HMC molecular dynamics, which is closely related to the minimal eigenvalue of $M^\dag M$. The cost formula is determined as a product of the scaling functions of iterative solver and integrated autocorrelation time of $1/N_{\text{it}}$ as function of the inverse lattice pseudoscalar mass. Timings by SESAM/TχL allow to fix the pre-factor.

It is demonstrated that a 2-flavor dynamical determination of light hadron masses with a statistical precision comparable to the corresponding quenched results from CP-PACS is the appropriate task for a 100 Tflops system.

1. INTRODUCTION

Realistic QCD simulations with dynamical fermions require to operate beyond the $\rho$ decay threshold and closer to the continuum limit. High energy physics can profit from lattice QCD as soon as systematical and statistical errors are comparable to or smaller as experimental ones [1].

In order to make best usage of the next generation QCD machines concerning these physical goals, we should employ the most appropriate lattice actions and simulation algorithms. Hence, cost predictions are needed for different lattice discretizations and algorithms beyond $\frac{m_{\text{PS}}}{m_{\text{V}}} = 0.5$.

As suggested by R. Kenway (Edinburgh), chairman of the Lattice 2001 panel discussion, we determine the costs of the SESAM and TχL experiments to estimate the costs of future hybrid Monte Carlo simulations with two degenerate flavors of standard Wilson fermions.

2. SESAM/TχL SIMULATIONS

SESAM/TχL has generated 10 ensembles of full QCD vacuum configurations with $O(5000)$ HMC trajectories each, at $\beta = 5.6$ and 5.5 in the region $0.57 < \frac{m_{\text{PS}}}{m_{\text{V}}} < 0.85$ with two flavors of Wilson fermions. The lattice sizes are $16^3 \times 32$ (SESAM) and $24^3 \times 40$ (TχL), corresponding to physical sizes (from $\rho$ mass) of $1.372(36)$ fm (SESAM) and of $1.902(34)$ fm (TχL) after chiral extrapolation. We used the standard hybrid Monte Carlo algorithm [2], boosted by BiCGStab as solver [3], $ll$-SSOR preconditioning [4] and the educated guess procedure (chronological inversion method) [5]. Running primarily on APE100 systems at DESY/Zeuthen, DFG/Bielefeld and INFN/Rome, the total costs of the simulations amount to about 0.06 Tflops-yrs.

In table 1 we give important quantities from SESAM/TχL. We have exploited both $o/e$ and SSOR preconditioned fermion actions [4]. The latter series are used for the cost analysis, as SSOR shows better scaling behavior.

3. SCALING FITS

Figure 1 presents fits to the average number of iterations, $N_{\text{it}}$, of the $ll$-SSOR preconditioned BiCGStab solver, as function of $1/m_{\text{PS}}a$. Note that the $\beta = 5.6$ result scales much better than $\beta = 5.5$. Presumably, smoother gauge fields allow for better $ll$-SSOR preconditioning.

Figure 2 shows fits to the integrated autocorrelation times of the series of $1/N_{\text{it}}$, the inverse number of iterations. $1/N_{\text{it}}$ is related to the minimal eigenvalue of $M^\dag M$. Its autocorrelation time is comparable to that of the topological charge. Again, we observe a strong $\beta$ dependence.
Table 1
Characteristic quantities from SESAM/TχL. The it-SSOR trajectories are indicated by #.

| β  | L/mV | 16^4 × 32 | 24^4 × 40 |
|----|------|-----------|-----------|
| 5.6 | | 0.83 | 0.81 | 0.76 | 0.68 | 0.70 | 0.57 |
| | T_{equi} | 5200 | 5400 | 3220 | 2030 | 2350 | 2600 |
| | τ_{int} | 19(4) | 25(6) | 33(4) | | | |
| 5.5 | L/mV | 0.85 | 0.80 | 0.75 | 0.68 |
| | T_{equi} | 3500 | 4000 | 5000 | 5000 |
| | τ_{int} | 19(2) | 24(3) | 38(2) | 47(3) |

Table 2
Costs of simulations with 2 flavors of Wilson fermions in analogy to the quenched setting of CP-PACS.

| a [fm] | N_flops | | | | | |
|--------|---------|---|---|---|---|---|
| 0.102  | 0.46    | 0.75 | 0.70 | 0.60 | 0.50 | 0.40 |
| | | 0.58 | 18 | 25(8) | 4.3 | 32 | 800 |
| 0.076  | 1.2     | 1.8 | 3.5 | 7.0 | 15 | |
| | | 95(35) | 2.8(1) | 48 | 400 |
| 0.064  | 3.7     | 6.7 | 12 | 23 | 50 | |
| | | 485(150) | 2.8(1) | 64 | 200 |
| 0.050  | 17      | 28 | 60 | 120 | 260 | |
| | | | | | | |

Figure 1. Scaling of iterative solver and integrated autocorrelation time.

4. COST FORMULA

Comparing the sustained CPU time for one HMC trajectory on APE100 with the costs for the iterative solver allows to determine the normalization of the cost function. Multiplication with the autocorrelation time gives the effort to generate one statistically independent configuration at given β as function of 1/a and m_{PS} a. We assume the volume to scale like (L/a)^5 (unlike (L/a)^4.55 of Ref. [1]) and the temporal lattice extent to be twice as large as the spatial extent L.

\[
\beta = 5.6: N_{\text{flops}} = 2.3(7) \cdot 10^7 \cdot \left( \frac{L}{a} \right)^5 \cdot \left( \frac{1}{a m_{PS}} \right)^{2.8(2)} \\
\beta = 5.5: N_{\text{flops}} = 1.6(4) \cdot 10^7 \cdot \left( \frac{L}{a} \right)^5 \cdot \left( \frac{1}{a m_{PS}} \right)^{4.3(2)}
\]

5. EXTRAPOLATIONS

The CP-PACS quenched simulations achieved finite a results for light hadrons with errors < 1% and continuum result with errors between 1 and 3%. Linearly extrapolating (1) in a and \( \frac{m_{PS}}{m_{V}} \), we find the upper bounds to the CPU time (see table 2) needed to carry out an analogous simulation with \( n_f = 2 \) Wilson fermions.

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