Three flavor dynamical QCD project by CP-PACS/JLQCD

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The CP-PACS and JLQCD Collaborations have been making systematic studies of lattice QCD carrying out both chiral and continuum extrapolations. The importance of dynamical quark effects has been clarified by a comparison of quenched QCD and two flavor full QCD simulations. In two flavor simulations, the dynamical effects of $u$ and $d$ quarks are taken into account, but the third quark $s$ is still treated in a quenched approximation. As the final step towards a fully realistic lattice simulation of QCD, two collaborations started a joint project of three flavor QCD, concentrating all big computers available. Based on a series of preparatory studies of exact simulation algorithm and non-perturbative improvement coefficient, a large scale simulation of three flavor QCD has been started. I present the results of light hadron spectrum and light quark masses from the first production runs.

1. INTRODUCTION

A direct calculation of hadronic properties from QCD is a fundamental objective in particle physics. Strong correlations among quarks make a reliable analytic calculation difficult even for basic properties of hadrons such as the mass spectrum and decay constants. So far numerical simulation based on the lattice formulation of QCD is the only reliable way toward this goal.

A systematic study of lattice QCD carrying out both the chiral and continuum extrapolations requires a huge amount of computations, however. The CP-PACS and JLQCD Collaborations have been performing a series of large scale simulations of QCD adopting the fastest computers available. The CP-PACS Collaboration have been mainly using the CP-PACS computer, a dedicated parallel computer with the peak performance of 614 GFLOPS. The CP-PACS was designed and developed in 1996 at the Center for Computational Physics, University of Tsukuba [1]. The main engine for the JLQCD Collaboration is the supercomputers at the High Energy Accelerator Research Organization (KEK). The central computer since 2000 is the Hitachi SR-8000/F1 with 100 nodes achieving the peak speed of 1.2 TFLOPS [2].

As the first step, the CP-PACS Collaboration carried out an extensive study of QCD in the quenched approximation, in which the effects of dynamical quark pair creations and annihilations are suppressed [3]. Performing the first well-controlled chiral and continuum extrapolations on lattices with the spatial extent of about 3 fm, the limitation of the quenched approximation was clearly proven: the light hadron mass spectrum deviates from the experiment by $O(10\%)$.

The next natural step is to incorporate the effects of dynamical $u, d$ quarks (two flavor full QCD). The results of systematic studies by the CP-PACS and JLQCD Collaborations [4] show that the discrepancies in the hadron mass spectrum observed in the quenched study are largely reduced by the dynamical $u, d$ quarks. This demonstrates the importance of dynamical quarks.
In two flavor simulations, however, the third s quark is treated in a quenched approximation yet. On the other hand, we do expect that contribution of dynamical s quark is not small because its mass is of the same order of magnitude as a typical energy scale of gluon dynamics: \( m_s \lesssim \Lambda_{QCD} \). Therefore, introduction of the dynamical s quark in the simulation is the last major step left towards a fully realistic simulation of QCD.

The CP-PACS and JLQCD Collaborations have started a systematic study of three flavor full QCD. The first target is to perform a precise measurement of the light hadron spectrum and light quark masses.

Because the required computer power is enormous, we have decided to concentrate all big computers available to us for this joint project. In Table 1 I list the major computers we are devoting to this project. Fractions of the peak performance which we may fully use for lattice QCD simulations are given for each computer. Summing up these numbers, we may use about 2.5 TFLOPS to simulate three flavor QCD.

In this paper, I present the outline and status of the project. The first step was to develop and test an exact algorithm for three-flavor QCD simulations. From a comparison of various variants of exact algorithms as described in Sec. 2 we have chosen a polynomial hybrid Monte Carlo (PHMC) algorithm. In Sec. 3 I discuss our test study of three flavor QCD using the PHMC algorithm, which indicates that improvement of lattice action is essential for meaningful simulations. We thus adopt the RG-improved gauge action by Iwasaki and the clover-improved Wilson quark action. To achieve full \( O(a) \)-improvement, we then determined the non-perturbative value of the clover coefficient \( c_{SW} \). Based on these preparative studies, we have now started a large scale simulation of three flavor QCD. Results of the first production runs are presented in Sec. 4. Tentative conclusions are given in Sec. 5.

2. EXACT ALGORITHM

With the Wilson-type (staggered-type) lattice quarks, the exact HMC algorithm exists only for the cases of even (four times integer) number of flavors. Because an exact algorithm for odd number of flavors was not known before, inexact R-algorithm has been adopted in previous studies of three flavor QCD. To avoid possible unexpected systematic errors, however, it is highly desirable to adopt an exact algorithm for large scale simulations.

Recently, several exact algorithms for odd flavors have been proposed: the multi-boson algorithm \(^7\) and the polynomial hybrid Monte Carlo (PHMC) algorithm \(^8\), both based on polynomial approximation for the quark matrix and for its determinant. We adopt the PHMC algorithm extending it to clover-improved Wilson quarks. We made a systematic test of several variants of the PHMC algorithm \(^9\). We found that, with appropriate improvements, the PHMC algorithm is equally efficient as the HMC algorithm for the case of two-flavor QCD.
Table 1
Computers for the three flavor QCD project by CP-PACS/JLQCD Collaborations. Performance of our PHMC code was measured in an actual production runs of three-flavor QCD on $20^3 \times 40$ lattices.

| machine     | location            | #nodes | peak speed [GFLOPS] | fraction for LQCD [GFLOPS] | performance of PHMC code |
|-------------|---------------------|--------|---------------------|---------------------------|--------------------------|
| CP-PACS [1] | CCP, U.Tsukuba      | 2048   | 614                 | ~614                      | 20%                      |
| SR-8000/G1  | CCP, U.Tsukuba      | 12     | 173                 | ~173                      | 44%                      |
| SR-8000/F1  | KEK                 | 100    | 1200                | ~768                      | 35%                      |
| VPP-5000 [2] | SICP, U.Tsukuba    | 80     | 768                 | ~230                      | 44%                      |
| Earth Simulator [7] | ES Center       | 640    | 40960               | ~640                      | 31%                      |

From this study, we decide to adopt the PHMC algorithm for the s quark and the HMC algorithm for degenerate u, d quarks. Note that, because the s quark is heavy, the problem of negative determinant at very small quark masses is automatically avoided. Together with additional improvements, we find that the overall CPU time to simulate one trajectory of three flavor QCD is only about 1.5 times more than that for two flavor QCD using our previous HMC code at the same u, d quark masses. We conclude that the PHMC algorithm is sufficiently efficient to carry out a systematic simulation of three flavor QCD with the present power of computers.

We have implemented the code to the computers listed in Table 1. Optimizing the vectorization and parallelization algorithms depending on the characteristics of each machine, we achieved the performance of 20–44% in actual production runs [12], as compiled in the last column of Table 1.

3. CHOICE OF THE LATTICE ACTION

Improvement of the lattice action is effective to suppress lattice artifacts on coarse lattices [13] and has played an essential role in our study of two flavor QCD to reduce necessary computer resources. Because the requirement of computer power is even more oppressive in the three flavor project due to larger number of parameters, improvement will be important for a systematic simulation of three flavor QCD.

3.1. A test study

Using the exact PHMC algorithm, we made a series of test studies at $a^{-1} \simeq 1.5$–2 GeV on $8^3 \times 16$ and $12^3 \times 32$ lattices [14]. For gluons, we test the standard one-plaquette action, the RG-improved action by Iwasaki [15], and the meanfield-improved Symanzik gauge action. For quarks, we adopt the clover-improved Wilson quark action with meanfield-improved clover-coefficient $c_{SW}$.

With the plaquette gauge action, we have encountered a severe lattice artifact at $a^{-1} \lesssim 2$ GeV: the plaquette expectation values shown in Fig. 1(a) indicate unexpected first-order transitions at $\beta = 4.95$ and 5.0. Our study of the lattice size dependence suggest that this is a bulk transition. On the other hand, results with improved gauge actions show no signs of hysteresis, as shown in Fig. 1(b) for the RG-improved action. We suspect that the lattice artifact in the case of plaquette action is due to an effective adjoint coupling from the clover term [14].

In any case, because it is difficult to simulate several points beyond $a^{-1} \sim 2$ GeV, our findings imply that improvement of the gauge action is indispensable to perform a continuum extrapolation. We adopt the RG-improved gauge action for gluons.

3.2. Non-perturbative $C_{SW}$

For quarks, we adopt clover-improved Wilson quark action. To completely remove $O(\alpha)$ errors, we need non-perturbative values of the clover coefficient $c_{SW}$, which have not been estimated for three flavor QCD. In [16,17], we have determined the non-perturbative $c_{SW}$ both for the plaquette and RG-improved gauge actions. We use the Schrödinger functional method [15]. For the RG gauge action we adopt the boundary condition...
towards the continuum limit, we are carrying out simulation of three flavor QCD. As the first point in finite volume \[19\]. See \[17\] for details.

In order to remove the finite volume effect, we estimate the non-perturbative \(c_{SW}\) at a fixed physical lattice size \(L^*\). Then the finite volume effect vanishes as \(a/L^*\) in the continuum limit. Correction of the data to \(L^*\) from the results obtained at the simulation point \(L\) is done using one-loop formulae calculated with the SF setup in finite volume \[19\]. See \[17\] for details.

Our final results for \(c_{SW}\) at \(L^* = 6a_{\beta=6}/g_0^2=1.9\) are summarized in Fig. 2 by triangles. We note that the results smoothly converge to the one-loop result for \(L/a = \infty\) (dashed line) in the continuum limit \(g_0 = 0\).

4. THREE FLAVOR QCD

Based on the preparative studies discussed in previous sections, we have started a systematic simulation of three flavor QCD. As the first point towards the continuum limit, we are carrying out jobs at \(a^{-1}\approx 2\text{ GeV} \ (a \approx 0.1\text{ fm})\). We have finished the production runs on a \(16^3 \times 32\) lattice \((L a \approx 1.6\text{ fm})\), and are now carrying out simulations on a \(20^3 \times 40\) lattice \((L a \approx 2.0\text{ fm})\). In this section, I present the results of the first production runs on the \(16^3 \times 32\) lattice \[20\].

4.1. Simulation parameters

With the RG-improved gauge action and clover-improved Wilson quark action, we made simulations at \(\beta = 1.9\) on a \(16^3 \times 32\) lattice \[20\]. The non-perturbative value of \(c_{SW}\) at this \(\beta\) is \(1.715 \ [17]\). We studied six values of the \(u, d\) quark mass in the range \(K_{ud} = 0.1358-0.1370\) corresponding to \(m_{PS,LL}/m_{V,LL} \approx 0.64-0.77\), where \(L\) means the light \(u, d\) sea quark. For the \(s\) quark mass, we studied two points \(K_s = 0.1364\) and 0.1358 corresponding to \(m_{PS,SS}/m_{V,SS} \approx 0.72\) and 0.77, where \(S\) is for the sea \(s\) quark. These values are close to the physical \(s\) quark point \(m_{ps}/m_{ps} \approx 0.68\) from the chiral perturbation theory. The simulation points are summarized in Fig. 3.

We simulated 3000 trajectories at each \((K_{ud}, K_s)\) and accumulated the configurations every 10 trajectories. The HMC step size and the order of polynomial in the PHMC algorithm were adjusted to achieve the acceptance rate of more than 85\% in HMC steps and more than 90\% in PHMC steps. So far, we have measured hadronic observables only when each valence quark is one

![Figure 2](image1.png)

**Figure 2.** Non-perturbative value of \(c_{SW}\) in three-flavor QCD with RG-improved gauge action \[17\]. Open and filled triangles show \(c_{SW}\) at a fixed physical lattice size \(L^*\), obtained by correcting the raw results shown by open circles. Dotted line shows the one-loop result for \(L/a = \infty\). See \[17\] for details.

![Figure 3](image2.png)

**Figure 3.** Simulation points on \(16^3 \times 32\) lattice at \(\beta = 1.9\). Our estimation for the physical point is given by the star. The line shows the chiral limit defined by \(m_{PS,LL} = 0\).
of the sea quarks, L or S. Errors are estimated by a jack-knife method with bins of 50 trajectories.

### 4.2. Meson spectrum

Because the spatial lattice size of $L a \sim 1.6$ fm is not quite large, we concentrate on mesons in this report. We tested point and exponentially smeared sources. Because we obtained the clearest plateaus for effective masses when both quark sources are smeared, we show the results with doubly smeared sources in the following.

Results for the mass of vector mesons consisting of two light sea quarks are shown in Fig. 4 as a function of $1 / K - 1 / K_c$, where $K_c$ is defined by $m_{PS,LL}(K_{ud} = K_s = K_c) = 0$. Results for other mesons are similar. Because the quark mass dependence is quite smooth, we adopt the following polynomial ansätze

$$m_{PS}^2 = B m_{q,sea} + (C + D m_{q,sea})(m_{q,val1} + m_{q,val2})$$

(1)

$$m_V = A' + B' m_{q,sea} + (C' + D' m_{q,sea})(m_{q,val1} + m_{q,val2})$$

(2)

or

$$m_V = A'' + B'' \mu_{sea} + (C' + D' \mu_{sea})(m_{PS,11}^2 + m_{PS,22}^2)$$

(3)

where $m_{q,sea} = 2m_{ud} + m_s$ with $m_q = (1/K_c - 1/K_s)/2$ and $\mu_{sea} = 2m_{PS,LL}^2 + m_{PS,SS}^2$. We test both combinations of $[1] + [2]$ and $[1] + [3]$. Both ansätze fit the data well. We quote the weighted average of two combinations as the central value of the masses, while the difference between two combinations is treated as a systematic error from the chiral fit. To identify the lattice spacing $a$ and the physical point $(K_{ud}^{phys}, K_s^{phys})$, we use either $(M_\pi, M_\rho, M_K)$ ($K$-input) or $(M_\pi, M_\rho, M_\phi)$ ($\phi$-input).

Result for $M_\rho$ from the $K$-input is shown in Fig. 5. The clear discrepancy between experiment (star) and quenched results (open symbols) is largely removed in two flavor QCD (shaded symbols) in the continuum limit. Our new three flavor value is shown by the filled symbol at $a \simeq 0.1$ fm. Quenched (open symbols) and two flavor QCD results (shaded symbols) are also shown.
Figure 6. Relative discrepancy of meson masses in three flavor QCD at $a^{-1} \simeq 2$ GeV [20]. Results of quenched QCD in the continuum limit are also shown by open symbols.

$K$- and $\phi$-inputs lead to consistent values already at finite $a$. Accordingly, we obtain $a^{-1} = 2.05(4)$ GeV from the $K$-input and $2.05(5)$ GeV from the $\phi$-input.

For a precise prediction, we need to extrapolate the results to the continuum limit. However, we may hope that the scaling violation is indeed small for our choice of non-perturbatively $O(a)$-improved action, such that the consistency with experiment is kept in the continuum limit. This should be tested in future.

4.3. Quark mass

Because quarks are confined, their masses are not direct observables of the theory. Therefore, there exist several alternative definitions for the quark mass. Two popular definitions are the axial-vector Ward identity (AWI) quark mass

$$m_q = Z_q \left( \frac{\Delta_4 A_4 P}{2 \langle PP \rangle} \right)$$

(4)

and the vector Ward identity (VWI) quark mass

$$m_q = Z_q' \left( \frac{1}{K - 1/K_c} \right),$$

(5)

where $A_4$ is the fourth component of the axial-vector current, $P$ is the pseudo-scalar density, and $Z$’s are renormalization factors. Different definitions lead to different values for $m_q$ on finite lattices. This was a big source of error in early calculations of $m_q$. In our previous studies of quenched and two flavor full QCD, however, we have shown that they converge to universal values in the continuum limit [34].

In three flavor QCD, we found that, although the differences between $K$- and $\phi$-inputs are absent, the AWI and VWI quark masses disagree at $a^{-1} \simeq 2$ GeV. We also noted that the choice of “$K_c$” in (5) introduces a sizable ambiguity in the values of VWI quark mass: From Fig. 3 we obtain even negative value of $m_{ud}$ when we adopt $K_c$ defined by $m_{PS,LL}(K_{ud} = K_s = K_c) = 0$. Such ambiguities will be removed in the continuum limit.

At the present stage having data only at a value of $a^{-1}$, we would like to concentrate on the AWI quark mass which does not suffer from the ambiguity of $K_c$ and, in the case of two flavor QCD,
shows a smaller scaling violation than VWI quark masses 31. To convert to the quark mass in the MS scheme, we match the renormalized mass with the lattice data at $\mu = a^{-1}$ using a meanfield-improved one-loop $Z$ factor 21, and let it run to $\mu = 2 \text{ GeV}$ using the 4-loop beta function.

Our results are summarized in Fig. 7. Previous results from quenched and two flavor full QCD, extrapolated to the continuum limit, are also shown for comparison 33,34. We see that quark masses decrease when we increase the number of dynamical quark flavors. In three flavor QCD, we obtain $m_{ud}^{\overline{\text{MS}}} = 2.89(6) \text{ MeV}$ and $m_s^{\overline{\text{MS}}} = 75.6(3.4) \text{ MeV}$ at $a^{-1} \approx 2 \text{ GeV}$, where the central values are from the $K$-input and the errors include systematic errors estimated by the difference between the $K$- and $\phi$-inputs. With the effects of dynamical $s$ quark, both $m_{ud}$ and $m_s$ are decreased by about 15% from the previous two flavor values. The ratio $m_s/m_{ud} = 26.2(1.0)$ is consistent with the one-loop estimate of chiral perturbation theory 24.4(1.5) 22.

5. TENTATIVE CONCLUSIONS AND OUTLOOK

We have presented the status of the joint project of three flavor QCD simulation by the CP-PACS and JLQCD Collaborations. We employ exact HMC algorithm for light $u, d$ quarks and exact PHMC algorithm for $s$ quark. To reduce the lattice artifacts, we adopt the RG-improved gauge action and non-perturbatively $O(a)$-improved clover quark action. As the first step toward a systematic study of the fully realistic QCD on the lattice, we made simulations at $a^{-1} \approx 2 \text{ GeV}$ on $16^3 \times 32$ lattices. These simulations show that, with the effects of dynamical $s$ quark, light meson mass spectrum agrees well with experiment already at $a^{-1} \approx 2 \text{ GeV}$. We also found that the quark masses $m_{ud}$ and $m_s$ are lower than the two flavor values by about 15%. We are currently performing simulations at the same simulation points on $20^3 \times 40$ lattices to study finite lattice volume effects. Although a continuum extrapolation is not made yet, these results are quite encouraging to further carry out large scale simulations of three flavor QCD.

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REFERENCES

1. For the details of the CP-PACS computer, Y. Iwasaki, Nucl. Phys. B (Proc. Suppl.) 60A (1998) 246. See also http://www.ccp.tsukuba.ac.jp/.
2. http://scwww.kek.jp/
3. CP-PACS Collaboration: S. Aoki et al., Phys. Rev. Lett., 84 (2000) 238; Phys. Rev. D 67 (2003) 034503.
4. CP-PACS Collaboration: A. Ali Khan et al., Phys. Rev. Lett., 85 (2000) 4674; Phys. Rev. D 65 (2002) 054505.
5. JLQCD Collaboration: S. Aoki et al., Phys. Rev. D 68 (2003) 054502.
6. http://www.cc.tsukuba.ac.jp/mimosa/
7. http://www.es.jamstec.go.jp/esc/eng/
8. C. Alexandrou et al., Phys. Rev. D60 (1999) 034504.
9. T. Takaishi and Ph. de Forcrand, Int. J. Mod. Phys. C13(02)343.
10. Ph. de Forcrand and T. Takaishi, Nucl. Phys. B(Proc. Suppl.) 53 (1997) 968; R. Frezzotti and K. Jansen, Phys. Lett. B402 (1997) 328.
11. JLQCD Collaboration: S. Aoki et al., Phys. Rev. D 65 (2002) 094507.
12. S. Aoki et al, hep-lat/0310015.
13. CP-PACS Collaboration: S. Aoki et al., Phys. Rev. D60 (1999) 114508.
14. JLQCD Collaboration: S. Aoki et al., Nucl. Phys. B (Proc. Suppl.) 106 (2002) 263.
15. Y. Iwasaki, Nucl. Phys. B258 (1985) 141; Univ. of Tsukuba report UTHEP-118 (1983), unpublished.
16. CP-PACS and JLQCD Collaborations: K.-I.
Ishikawa et al., Nucl. Phys. B (Proc. Suppl.) 119 (2003) 433.

17. CP-PACS and JLQCD Collaborations: K.-I. Ishikawa et al., [hep-lat/0309141]

18. M. Lüscher et al., Nucl. Phys. B491 (1997) 323; K. Jansen and R. Sommer, *ibid*. B530 (1998) 185; B543 (2002) 517.

19. S. Aoki, R. Frezzotti and P. Weisz, Nucl. Phys. B540 (1998) 501.

20. CP-PACS and JLQCD Collaborations: T. Kaneko et al., [hep-lat/0309137]

21. S. Aoki et al., Phys. Rev. D58 (1998) 074505.

22. H. Leutwyler, Phys. Lett. B378 (1996) 313.