Lattice QCD with Dynamical up, down and strange Quarks with Earth Simulator

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The Standard Model is a unified gauge field theory of elementary particles consisting of QCD describing strong interactions and Weinberg-Salam theory describing electroweak interactions. Precision verification of the Standard Model is one of the fundamental goals of particle physics in order to establish our understanding of Nature at the fundamental level of basic constituents of matter.

This project attempts to carry out realistic simulation of lattice QCD in which vacuum polarization effects of all three light quarks, i.e., up, down and strange, are included, thereby establishing QCD as the fundamental theory of strong interactions. It also aims to extract predictions for novel phenomena such as quark gluon plasma and for determination of the CKM quark mixing matrix crucial for understanding of CP violation.

This year we completed porting of our code to Earth Simulator, and carried out the first stage of simulations using $20 \times 20 \times 20 \times 40$ lattice at a lattice spacing of a = 0.1 fm. Meson mass data analyzed in terms of polynomials of quark masses show that the discrepancy of hadron mass spectrum calculated by lattice QCD and the experimental ones observed in the quenched approximation almost disappears with three light dynamical quarks. Values of light quark masses calculated from the hadron mass spectrum are reported. Our plan for the next stage of the simulation is sketched.

Keywords: particle physics, Standard Model, quark, hadron, lattice QCD, Monte Carlo simulation, CP non-conservation, quark gluon plasma

1. Physics Goals and Simulations

The Standard Model of elementary particles is a unified field theory consisting of QCD describing strong interactions and Weinberg-Salam theory describing electroweak interactions. Verifying the Standard Model is one of the fundamental goals of particle physics in order to establish our understanding of Nature at the fundamental level of basic constituents of matter. This requires formulating the Standard Model on the four-dimensional space-time lattice, and solving it using large-scale simulations. Research groups in Japan have made significant contributions in this field. Complete simulations without approximation, however, have not been made so far, because they require large amount of computations on one hand, and because algorithms which

can treat odd number of quarks were not developed. Researchers of our group have recently developed an exact algorithm for odd numbers of quarks which enables exact simulations [1]. This project aims to take advantage of this progress and combine it with the computational power of the Earth Simulator to achieve a major step forward in clarifying the fundamental issues of particle physics. These issues include:

- Determination of quark masses and the QCD coupling constant, which are fundamental constants of nature like the electron mass and charge.
- Clarification of the physical property of quark gluon plasma which is believed to have existed in the early stage of the Universe after the Big Bang.
- Determination of hadronic weak matrix elements to constrain the Cabibbo-Kobayashi-Maskawa quark mixing matrix and the Standard Model understanding of CP violation.

This year, we have completed porting and optimization of our lattice QCD codes to the Earth Simulator, and carried out simulations at a lattice spacing a = 0.1fm using a lattice of a size $20 \times 20 \times 20 \times 40$. Here we report results of this year's study.

2. Porting and optimization of the PHMC code for Lattice QCD

2.1. Strategy of porting and optimization

The three-flavor full QCD simulation attempted in the present project is based on the polynomial hybrid Monte Carlo (PHMC) algorithm [1]. Our PHMC code was originally developed at KEK for Hitachi SR8000 and sustains 40% of peak speed. On Earth Simulator, however, the performance turned out to be of order 10%. To explore an effective coding style, we take the basic MULT subroutine for Wilson-Dirac matrix-vector multiplication, and measure the performance for seven types of coding on a single arithmetic processor (AP). Results range from 10 to 73% for a $6 \times 6 \times 6 \times 48$ lattice.

The highest performance is achieved by a code written originally for a vector-parallel machine, Fujitsu VPP500. In this code, sites on the z-t plane are numbered by a one-dimensional array and divided by four to realize a large vector length without list vectors. Other codes with smaller vector lengths (e.g. that for Hitachi SR8000 in which only t direction is vectorized) show lower performance of at most 30%. Hence we rewrite the entire code with the coding style used for VPP500. We subdivide the whole lattice on the x-y plane and assign each region to a processing node (PN) and parallelize with MPI. In one PN, loop indices in the x and y directions and an even/odd flag for four vector loops mentioned above are combined into a one-dimensional index and divided by eight. This enables the compiler to execute an automatic parallelization (micro-tasking) of all appropriate do-loops.

2.2. Vector Processing on single arithmetic processor

The vector processing performance of the code on a single AP is an important fundamental. Our program includes redundant arithmetic calculations at edges in the z direction to realize a long vector length. Therefore we distinguish the performance reported by the system analyzer "ftrace" and that calculatedtheoretically for an effective part excluding the redundant operations. For the latter, total flops equals 1296flopsx#sites. The redundant part costs 2–4% of peak performance.

We test two codes. In the original one, contributions from 8 directions are calculated in one large do-loop and are summed up later. In the revised code, which intends to overlay arithmetic operations and communications in future, the large loop is divided into two loops for z,t and x,y directions. The array structure is also different. The revised code runs about 15% slower. We suspect that this is partly caused by a slow startup of do-loops.

In general, the vector performance of the revised MULT code reaches 55–65% for all three cases. However, it drops by about 10% when the vector length just exceeds a multiple of the size of vector registers, 256.

2.3. Micro-Tasking Parallelization

The cost of automatic parallelization is another important point, because SMP of vector processors is a distinctive feature of PN. The micro-tasking parallelization costs 3 to 4% which is not so high, while memory copy to implement boundary conditions is relatively heavy, being 4% for 1 AP and 7% for 8 AP's.

2.4. MPI Communications

In our code one PN issues an MPI_irsend for a gathered data and an adjacent PN issues an MPI_irecv and then scatters the received data. This enables us to construct long messages. The message size ranges from 0.34MB to 1.64MB, and the throughput ranges from 1.62GB/sec to 5.56GB/sec. These numbers are consistent with the MPI performance reported by the ES Center. The communication performance drops by 20% due to buffer copy for gather/scatter, hence the throughput for the longest message drops to 4.35GB/sec.

2.5. Breakdown of Overheads

In order to show how various overheads affect the overall efficiency, we show in Fig.1 the MULT performance starting from 1 AP up to 72 AP's (9 PN's). The lattice volume per AP is fixed to $4 \times 2 \times 32 \times 62$, which corresponds to a $32 \times 32 \times 32 \times 62$ lattice on a 4×4 PN array. The performance of

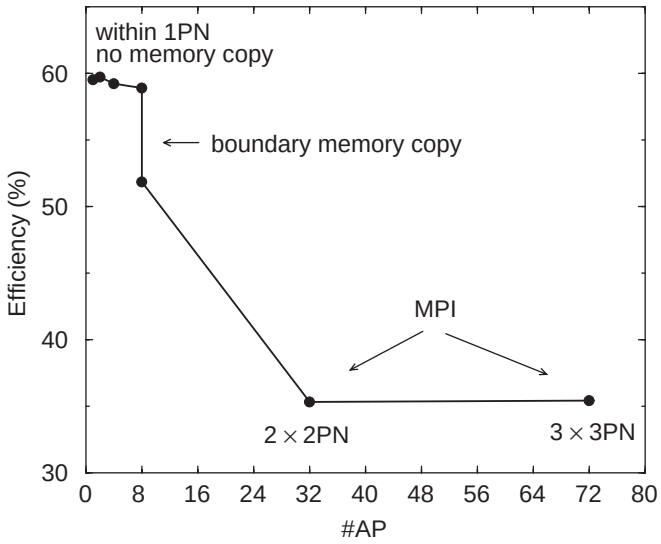

Fig. 1 Efficiency of MULT versus #AP.

61.6% for 1 AP finally drops to 35.4% for 72 AP's. The main cause of the drop is (1) a slow speed of MPI communications which are not overlaid with arithmetic operations, and (2) the cost of memory copy in one PN. Together these two factors cost 40% relative to the total execution time. The fraction becomes higher when volume/node becomes smaller; for a 20x20x20x40 lattice on a 5x2 PN array, 60% of execution time is spent for communications and memory copy.

2.6. Performance of the PHMC Program

Table 1 shows the profile of the entire PHMC program as provided by the ES profiler. The arithmetic calculations and boundary copy/communications in MULT are the two heaviest routines. The multiplication of the inverse clover term (MLCI) and BiCGStab (BiCG) are the third and fourth heaviest, which are relatively light. Therefore, for the next round of simulations on a larger lattice, we plan to overlay arithmetic operations and communications in the MULT routine.

As Table 1 shows the PHMC program runs on the ES with an efficiency of 25–40% for our four target lattice sizes. This efficiency is comparable to that on other machines, 35% on SR8000/F1 at KEK with 32 nodes, 44% on VPP5000 at Tsukuba with 8 nodes, and 20% on CP-PACS with 500 nodes.

3. Physics simulation and results

Using the PHMC code, we have initiated simulations of the light hadron spectrum and the quark mass with three-flavor full QCD. We adopt the renormalization-group improved gauge action and the O (a)-improved Wilson quark action with the non-perturbatively improved clover coefficient obtained in [2]. Simulations are carried out at $\beta = 1.9$ at the scale 1/a~2GeV on a $20 \times 20 \times 20 \times 40$ lattice. Five values of the degenerate up and down quark mass, corresponding to the pion to rho meson mass ratio of 0.8–0.6 are employed for extrapolation to the physical point $m_\pi / m_\rho = 0.18$. Two values are taken for the strange quark mass, chosen close to the physical point so that a short extrapolation or interpolation is sufficient to reach the physical value. We have accumulated about 7000 HMC trajectories at each simulation parameter. Gluon configurations are stored at every 10 trajectories for off-line measurement of physical observables.

3.1. Meson masses

We focus on the meson spectrum since our lattice size of La~2fm is not sufficiently large for baryons [3].

Figure 2 shows the J parameter defined by

$$J = m_{V,LS} \frac{m_{V,LS} - m_{V,LL}}{m^2_{PS,LS} - m^2_{PS,LL}}$$

which measures the magnitude of hyperfine splitting between pseudo scalar and vector mesons containing a strange quark. The three flavor results from the present simulation (circles) are compared with the previous results in two-flavor[4] and quenched QCD [5] (triangles). We see that J in three-flavor QCD stays at values systematically higher than in quenched and two-flavor QCD, and is consistent with experiment.

Our lattice size La~2fm is smaller than that used in quenched or two-flavor QCD. Because finite-size effects generally lower the J parameter [3], we conclude that the consistency of J between three-flavor QCD and experiment is not an artifact of finite-size effects.

We carry out chiral extrapolations for up and down quark mass using polynomial forms up to quadratic order in quark masses. Two functional forms are tested, type I being linear

Table 1 Profile (%), performance (GFlops) per 1AP and total efficiency (%) of the PHMC program.

size	$20 \times 20 \times 20 \times 40$	$24 \times 24 \times 24 \times 48$	$32 \times 32 \times 32 \times 64$	$32 \times 32 \times 32 \times 62$
node	5×2	3×4	4×4	4×4
Profile (%)				
copy	36.9	28.6	21.4	24.6
MULT	24.8	29.4	34.8	34.1
MLCI	13.4	18.3	20.1	17.8
BiCG	9.8	9.2	8.8	8.9
Performance/AP (Gflops)	2.01	2.29	2.87	3.18
efficiency (%)	24.9	28.6	35.9	39.8

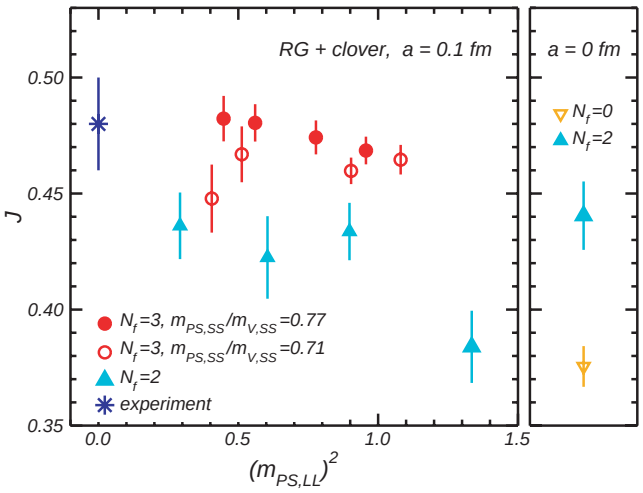

Fig. 2 The J parameter in two- and three-flavor QCD at lattice spacing a = 0.1 fm (left panel) and in two-flavor and quenched QCD in the continuum limit (right panel).

in sea quark masses and type II also containing quadratic terms. In this article we report results from type I fits. We fix the lattice spacing and the physical up and down quark mass with experimental pion mass and rho meson mass. The strange quark mass is fixed with either the K meson mass m_K (K-input) or phi meson mass m_ϕ (phi-input).

In Fig. 3, deviations from experiment are plotted for K, K* and phi meson masses at lattice spacing 1/a~2GeV obtained with type I chiral fits. A progressively better agreement with experiment as one starts from the quenched approximation (no dynamical quarks; Nf = 0) and moves beyond two-flavor (Nf = 2) to three-flavor dynamical QCD (Nf = 3; present calculation) is indicated, as anticipated from the agreement of the J with experiment. The consistency of the three-flavor value with experiment observed at a finite lattice spacing makes us hope that scaling violation is small and the consistency with experiment holds in the continuum limit as well. This should be verified in a future study. Uncertainty due to fitting forms should also be investigated.

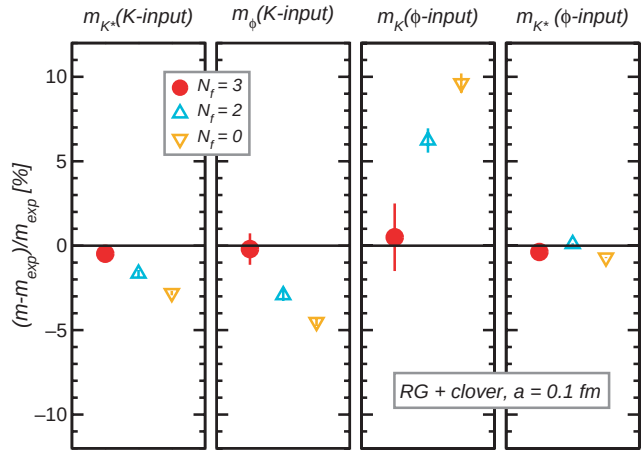

Fig. 3 Deviation of meson spectrum from experiment for quenched (Nf = 0), two-(Nf = 2) and three-flavor (Nf = 3) full QCD.

3.3. Quark masses

The physical quark masses, m_{ud} for degenerate up and down quark and m_s for strange quark, are calculated through the axial-vector Ward identity (AWI):

$$m_q = \lim_{t\to\infty} \frac{\langle \partial_4 A_4(t) P(0)\rangle}{\langle P(t) P(0)\rangle}$$

The matching to the $\overline{MS}$ scheme is carried out at the scale $\mu = 1/a$ using the one-loop Z factor with the tadpole improvement. The renormalized mass is evolved to μ = 2GeV using the 4-loop β function.

Figure 4 compares m_{ud} and m_s in three-flavor QCD with our previous results in two-flavor and quenched QCD [4, 5]. The up and down quark mass m_{ud} decreases about 10–15% compared to two-flavor case, while the strange quark mass is similar. Assuming scaling violation to be small, our preliminary value for light quark masses in three-flavor QCD are given by

$$m_{ud}(\overline{MS}, 2GeV) = 3.10(7)\ MeV$$
$$m_s(\overline{MS}, 2GeV) = 82.1(7.1)\ MeV$$

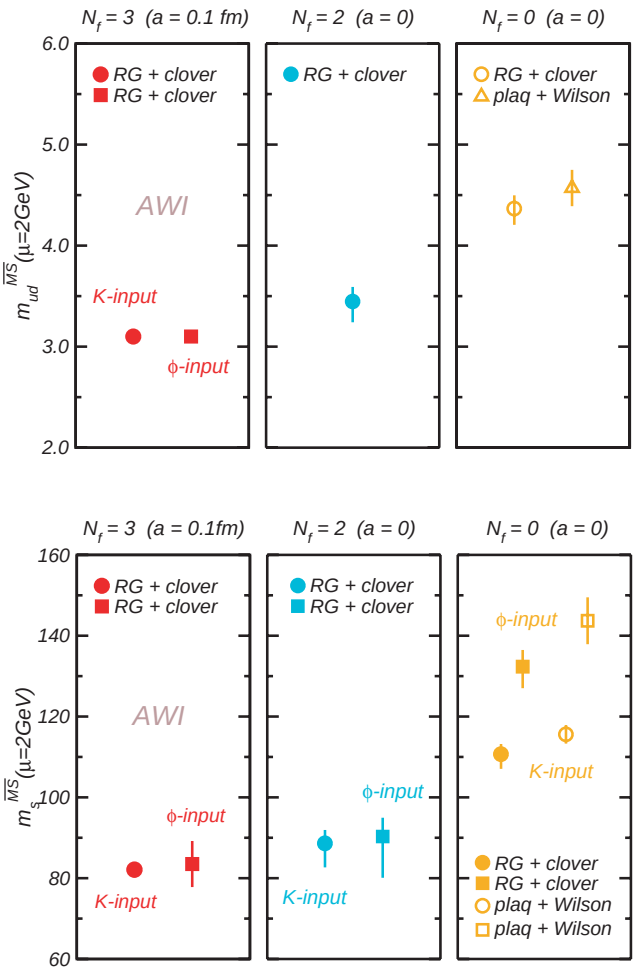

Fig. 4 Comparison of m_{ud} (top figure) and m_s (bottom figure) between full and quenched QCD. The left, middle and right panels in each figure show results in three- and two-flavor and quenched QCD, respectively.

4. Plan for Fiscal 2004

This year we have successfully completed the planned simulation at the lattice spacing a~0.1fm. In order to make a continuum extrapolation, we need data at two more points with different lattice spacings. Since the action we employ is designed such that scaling violation is $O(a^2)$, we plan to carry out simulations at $a = \sqrt{1/2} \times 0.1 fm$ on a $28 \times 28 \times 28 \times 56$ lattice and at $a = \sqrt{3/2} \times 0.1 fm$ on a $16 \times 16 \times 16 \times 32$ lattice. We have improved and tuned our code for the former simulation including overlapping of calculations and communications, and have started preliminary runs for the purpose of choosing parameter values. While generating a full set of configurations will take more than a year even on Earth Simulator, we hope to report first results from the new runs by the end of fiscal 2004.

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