Study of the Standard Model of Elementary Particles on the Lattice with the Earth Simulator

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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. Complete simulations without approximation, however, have not been done 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. This project aims to combine it with the computational power of the Earth Simulator to achieve large progress in clarifying the fundamental issues of particle physics such as asymmetry of matter and antimatter (CP violation) and quark-gluon plasma. This year we have ported our code for lattice QCD simulations to the Earth Simulator and have attempted to optimize the code in order to fully utilize the computational power of the Earth Simulator. At present our code has a vector operation ratio of 99.5% and the parallelization ratio of 99.46%, and sustains 36% of peak when executed for a 24 x 24 x 24 x 48 lattice on 8 nodes. We wish to pursue further optimization including overlap of calculation and communication to raise the performance over 50%. We report the current status of the optimization and comment on our plan for FY2003.

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 done 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. 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.

We wish to carry out simulations of lattice QCD with three dynamical quarks (up, down and strange) using 24 x 24 x 24 x 48 and 32 x 32 x 32 x 64 lattices. Our simulations are carried out using the polynomial Hybrid Monte Carlo method for treating an odd (three) number of dynamical quarks. Our code, vectorized and parallelized, had been run on a variety of computers. This year, we have ported the code to the Earth Simulator, verified the validity, and have attempted to optimize the code. The present standing of these efforts are described below.

2. Porting of the PHMC code for Lattice QCD

Our PHMC (Polynomial Hybrid Monte Carlo) program was originally developed at KEK for Hitachi SR8000. We first executed the program on the Earth Simulator (ES) and found that the results did not agree with that at KEK. The origin was traced to a compiler bug in treating complex number arithmetic, after fixing which correct results were obtained on the ES.

The performance of the original code on the ES was of order 10%, while that for SR8000 reached as much as 40%. The low performance is due to small vector lengths of our code. For SR8000, we mapped the three spatial directions onto the proccesor array, and vectorized the time direction in each processing node. In this case, the vector loop length is half of the lattice size in the temporal direction, which is about 32. While this way of vectorization was suitable for SR8000, a different vectorization with longer loops is required on the ES. We concluded that the PHMC code had to be rewritten for the ES.

3. Optimization of the PHMC code

3.1. Test for coding style

We have much experience on porting the core part of the PHMC program, called a subroutine MULT, to computers with various architectures. In order to find an effective coding style for the ES, the performance of seven types of MULT code was measured on a single CPU of the ES. The results varied from 10% to 73%. The highest performance was achieved by a code in which two of the four-fold do loops (corresponding to four directions of the lattice) are one-dimensionalized and then divided by four to realize a large vector length without list vectors. We have decided to adopt this way of vectorizing the code.

We plan to make calculations for a 24 x 24 x 24 x N_t lattice using a 8 x 12 CPU array (*i.e.*, 12 nodes). We have measured the single CPU performance of the code, adapting the lattice size to the actual run, *i.e.* for 3 x 2 x 24 x N_t/CPU. Figure 1 shows the performance measured by *ftrace* and calculated theoretically. The difference between them arises from the fact that the one-dimensionalization results in a small amount of redundant calculations which are not

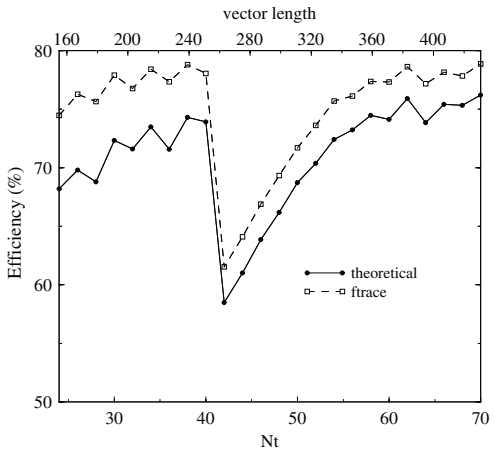

Fig. 1 Performance of subroutine MULT for 3 x 2 x 24 x N_t lattice on 1 CPU.

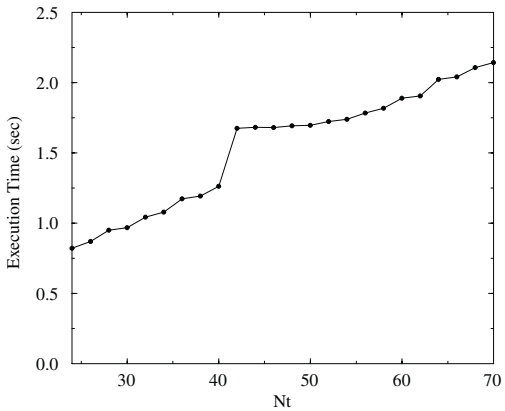

Fig.2 Execution time of subroutine MULT (1000 times) for 3 x 2 x 24 x N_t lattice on 1 CPU.

included in the theoretical estimate. The performance is plotted versus N_t and the vector length. The drop at N_t= 42 appears to be connected to a startup latency of the ES which has a vector register length of 256. This does not impede our calculations since for our target of N_t= 48−64 the efficiency is 69%−77% (ftrace) and 66%−73% (theoretical).

Figure 2 shows execution time vs. N_t. The execution time is almost independent of N_t for N_t= 42−54. In general, larger N_t is better for QCD calculations if execution time is reasonable. Thus we may adopt N_t= 54 for actual calculations.

From these tests, we have decided to rewrite the entire PHMC program with the same style.

3.2. Tuning of the core subroutine MULT

We took the strategy of adopting the *automatic parallelization* for 8 CPU in each node and use of MPI for inter-node parallelization. Before rewriting the PHMC program, we have coded the subroutine MULT compatible with this strategy. The automatic parallelization and the MPI parallelization are successfully applied to this routine.

The performance of a single node for 8 x 6 x 24 x 64 lattice (corresponding to 24 x 24 x 24 x 64 lattice on 3 x 4 = 12 nodes) was 40GFlops, or 62% efficiency. The performance is a little smaller than that mentioned in sec.3.1. The difference comes mainly from the difference of the do-loop structure. In the original code, contributions from the four directions are calculated within one large loop. Because we plan to overlap the calculation time with MPI communication time, we have to divide the large loop to three or four loops. The change of the do-loop structure results in O (10%) drop of efficiency. The cost for auto-parallelization is small and remains within 2% or so.

We have encountered a serious problem with the inter-node MPI communication. The present MPI library provided by the ES Center does not enable us to overlay the communication time on the arithmetic operation time. The MPI communication cost is not small for the MULT subroutine, and hence also for the PHMC program. For example, the total performance of MULT for a 16 x 12 x 24 x 64 lattice executed on 2 x 2 nodes drops to 25GFlops/node or 39% efficiency compared to the 62% efficiency achieved for single node as quoted above. We have asked the ES Center to develop a communication library allowing us the overlay. We understand that such a library will be available soon.

3.3. Rewriting the PHMC program

We have rewritten all of our PHMC program, which has about 36000 lines, following the strategy described in sec. 3.2. The rewriting was carried out at the Center for Computational Physics (CCP)(university of Tsukuba) and KEK. The code including MPI communications was first tested at CCP and then verified at the ES center.

3.4. Vectorization of the PHMC code

At present, the PHMC program does not compile if the highest compiler optimization option is specified. One of the reasons is an apparent compiler bug, which has already been reported to the ES Center support team.

Another reason is failure of automatic vectorization. We therefore tried to vectorize do-loops using compiler directives and rewriting the code itself when necessary. We have succeeded to vectorize all theoretically possible do-loops. Some of the original do-loops had to be subdivided into small fractions and therefore arithmetic operations are not dense enough for some loops. We think that there still remains room to improve vector performance of the program.

3.5. Automatic parallelization

The current version of the program is coded in a way that for all possible and necessary loops, the length of the outermost loop is a multiple of 8, and hence the loops can in principle be automatically parallelized across 8CPU's of each node. Using compiler directives, almost all of subroutines (including MULT) are parallelized.

There are still some subroutines having a similar do-loop structure and memory usage, and yet one automatically parallelized, while the other not parallelized or yielding incorrect results under the same compiler directives of parallelization control options. We have been in consultation with the ES Center support group to resolve these problems.

3.6. Inter-node parallelization

Inter-node communications are coded with MPI library and are tested on the ES. As mentioned in sec. 3.2., we will replace the MPI with a new library which enables us to overlay communications on calculations.

3.7. Performance of the current code

Since automatic parallelization is not completed, we have measured the performance of the current code using MPI for parallelization of 8 CPU within each node. The performance for 24 x 24 x 24 x 48 lattice is 105 GFlops, or 41% efficiency, when executed on 4 nodes (32CPU's), and 183 GFlops or 36% efficiency on 8 nodes (64CPU's). The vector operation ratio is 99.5% and the parallelization ratio is 99.4576%. The parallelization efficiency is larger than 50% if the number of CPU is less than 185 CPU (or 23 nodes).

4. Plan for FY2003

4.1. Tuning of the PHMC code

We wish to pursue optimization of our code for higher efficiency. As of the end of FY2002, we are waiting for answers from the ES Center support team on

1. a communication library which enables overlay on calculations,

2. the coding style most suitable for automatic parallelization.

As soon as the information on these points become available, we shall revise all of the program. We plan to finalize the code tuning before the end of May, achieving 50% performance or more for actual runs.

4.2. Production runs for physics

We shall start the production run for a 24 x 24 x 24 x 48 lattice as soon as possible. The target will be generation of 3000 PHMC trajectories, or 300 gluon configurations. In this fiscal year, we concentrate on the light hadron spectrum and quark masses. Other quantities can be calculated off-line using the gluon configurations which we shall store on tape. When the runs on a 24 x 24 x 24 x 48 has progressed to a reasonable degree, we wish to start runs on a 32 x 32 x 32 x 64 lattice.

5. Comments

We spent all of this fiscal year for porting and optimization of our PHMC code, and encountered a number of problems on the way. We received much help from the ES Center support group to solve them, but some of the problems had to be relegated to NEC. Given that we have to come to the ES Center and do a large amount of work within a limited time, it would help us enormously if in-depth consultation with software experts on the ES compiler and automatic parallelization were made available on site.

地球シミュレータによる素粒子標準模型の研究

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素粒子標準模型とは、強い相互作用を記述する量子色力学（QCD）と、弱電磁相互作用を記述するWeinberg-Salam理論を統合した場の理論である。標準模型の確立は、クォークとレプトンに基づく自然界の素粒子描像を確立する上で、素粒子物理学の最大の課題の一つである。それには、標準模型を四次元時空格子上に定義して、大規模数値シミュレーションにより解く必要がある。従来は、膨大な計算規模と、奇数種類のクォークに対する計算アルゴリズムが未開発であったことの二つの問題から、完全に近似無しのシミュレーションは行うことができなかった。アルゴリズムの問題については、本グループによる最近の成果により、近似のないシミュレーションを行う方法が確立した。本研究課題は、この発展を基礎として地球シミュレータの計算力を適用することにより、真に自然界に対応した素粒子標準模型のシミュレーションを実現し、物質反物質の非対称性（CPの破れ）やクォーク・グルオン・プラズマの解明など、我々の自然認識の根幹に関わる素粒子物理学の懸案の解決に大幅な進展を期するものである。平成14年度は、基本プログラムであるPHMCプログラム（約36000行）の移植と最適化を行った。現時点で、問題規模24×24×24×48格子を8ノードで実行した場合、ベクトル化率99.5%、並列化率99.46%、実効性能36%を実現している。今後、通信と計算を重ねることにより、実効性能50%以上を目標とした最適化を行う。またそれと並行して、24×24×24×48格子及び32×32×32×64格子における物理計算を進める予定である。

キーワード：素粒子物理学、標準模型、クォーク、ハドロン、格子量子色力学、QCD、モンテカルロシミュレーション、CP非保存、クォーク・グルオン・プラズマ