Report of the Review Committee for the KEK Large Scale Simulation Program

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About the Review Committee

In order to support large scale simulations in high energy accelerator science and related fields (mainly theoretical particle and nuclear physics) in Japan, the High Energy Accelerator Research Organization (KEK) is conducting the "Large Scale Simulation Program." Under this program, KEK installs world best supercomputers and calls for proposals of projects to be performed using them. The proposals are reviewed by the Program Advisory Committee, which makes decisions on approval and computer time allocation. During the period of 2003-2008, 118 projects have been accepted in total, and numerous results have been reported by the research groups. To review these achievements and identify possible problems, and in order to gain insight into possible future directions for KEK to proceed, the Director General of KEK requested the Committee to review the Large Scale Simulation Program for the period of 2003-2008.

The charge to the Committee covers the following items:

- To review the research activities performed under the program
- To review the organization of the program
- To review the facility improvement plans for short-, mid-, and long-terms

The members of the Committee are

Hisao Hayakawa	Yukawa Institute for Theoretical Physics, Kyoto University
Piet Hut	Program in Interdisciplinary Studies, Institute for Advanced Study
Satoshi Itoh	Corporate Research Development Center, TOSHIBA Corporation
Hikaru Kawai	Graduate School of Science, Kyoto University
Masao Ninomiya (chair)	Okayama Institute for Quantum Physics
Hiroshi Toki	Research Center for Nuclear Physics, Osaka University
Peter Weisz	Theory Division, Max Planck Institute for Physics
Hitoshi Yamamoto	Graduate School of Science, Tohoku University

The Committee met on December 4 and 5, 2008 at KEK. On Dec.4, 2008, we heard from project leaders about their scientific achievements. We were also informed about the program organization from the supporting staff.

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1 Purpose of the Large Scale Simulation Program

KEK (High Energy Accelerator Research Organization) is a research institute which carries out accelerator-related scientific studies. The major tasks of KEK are particle physics, nuclear physics, and related subjects. For this purpose, KEK has maintained and operated accelerators and detectors for high energy physics experiments. KEK has also maintained the computational facilities required for high energy physics research. The supercomputer system is an integral part of this system.

The usage of the supercomputer system is governed by the Large Scale Simulation Program. It calls for research proposals in particle and nuclear physics and related areas to be performed with the supercomputer of KEK. Applications can be submitted by researchers of all universities as well as those of governmental research organizations in Japan, or by those scientists that the Director-General of KEK considers appropriate.

It is the opinion of Review Committee (Committee for short below) that computational research is continuing to be increasingly more important in particle and nuclear physics research, and certainly is an integral part of the KEK research program. It is widely accepted that simulations of Quantum Chromodynamics (QCD) reveal the nature of the strong interaction. This is a deep statement; indeed it is remarkable that mankind now has a very solid candidate for the fundamental theory of the strong interactions that can be written in an extremely simple mathematical form. In spite of its simplicity at the Lagrangian level, its dynamics is highly non-linear so that one cannot solve the theory without employing numerical computations. The simulation of QCD will precisely show the mechanism of mass production and of confinement of quarks and gluons in Nature through its dynamics. Moreover it will also provide indispensable information for particle physics phenomenology, such as the B physics program to extract physical quantities from experimental results obtained at the current KEKB experiment and in the future SuperKEKB project.

We consider it striking that the simulation of QCD can now be used to calculate the nuclear force more than 70 years after the pioneering work by Hideki Yukawa in 1935. That information may then be used in the studies of nuclear structures. In this way, the simulations are filling a gap between particle and nuclear physics.

The Committee also emphasizes the importance of universality in physics. Indeed, Kenneth Wilson, who is an initiator of lattice QCD, was awarded the Nobel prize for the study of second order phase transitions. The Committee is impressed by the number of research projects that may share common interests with non-equilibrium statistical mechanics. The Committee thus strongly encourages more collaboration with researchers in other fields.

In 2008 the Nobel Prize in physics celebrated three Japanese particle physicists, which reemphasized the importance of pure science. For the future of pure science, that has to treat increasingly more complex problems, the Committee believes that computational methods will become more important and even essential. The activities under the KEK simulation program are exactly in this direction and should be promoted. The Committee certainly understands that the computational resources necessary to carry out leading edge research in these fields are very high. Since it is extremely difficult for individual research groups to obtain and maintain this size of computing resources, the entire particle and nuclear physics community appreciates the KEK efforts of providing the world leading supercomputers.

For the Large Scale Simulation Program to acquire continuous support from broader communities, the Committee cannot ignore the role of outreach and publicity of the Program. Many scientific works have been published in leading scientific journals and are also partly summarized in the KEK annual report. However since this Program is categorized in a basic science, it is important to deliver the relevant messages to non-experts in an easy-to-understand manner. In this connection we consider it very important to regularly report the research achievements to the mass media including newspapers. In order to plan and manage the strategy of publicity on scientific achievement, the Committee recommends that KEK enhances the impact of its public relations office by incorporating a staff member who would play a role of science communicator. Its coverage should naturally include the scientific outputs from the Large Scale Simulation Program.

Finally in order to efficiently use the scientific knowledge and technical experiences obtained through this Program, it should be discussed how various software modules developed in this Program could be made open to be freely used by other research groups.

2 Scientific achievements

Although theoretical physics has developed very rapidly in the last century, many important problems are left to be solved. Many of them are highly non-linear, and the role played by computational physics becomes increasingly more important. The simulation of QCD is a typical example. In spite of the simple form of the fundamental equation, its solution cannot be obtained without employing large scale numerical simulations. The research fields covered by the KEK Large Scale Simulation Program are not limited to lattice QCD, but include broad scientific programs related to accelerator science, such as superstring theory, nuclear physics, and accelerator design. During the review committee meeting, the Committee heard from six groups currently working under the program.

2.1 Lattice QCD

QCD is our candidate theory of the strong interactions. Although it is only an effective theory in Nature because of the existence of the other interactions (weak, electromagnetic and gravitational) it is generally thought that (unlike e.g. QED) it can mathematically exist on its own and describe hadronic physics at all energies. As stated above it would indeed be remarkable if the theory of strong interactions was encapsulated in the simple QCD Lagrangian describing the interaction of quarks and gluons.

The high energy behavior of some hadronic processes can be computed in QCD using renormalized perturbation theory because of the property of asymptotic freedom. The agreement between theory and experiment for these processes (e.g. the evolution of structure functions in deep inelastic scattering, jet production etc.) is very good, typically of the order of $< 10\%$ in all cases investigated. But this alone does not establish QCD as the theory of strong interactions. To accomplish this requires the study of low energy phenomena including the stable particle spectrum, resonances, and scattering amplitudes. This in turn requires non-perturbative methods and the only systematic method known to date is to regulate the theory on a space-time lattice and to compute the theory using numerical simulations. Because of the huge number of degrees of freedom, the necessity to control systematic effects introduced by the approximations, and the vast amount of CPU time to produce independent field configurations and use them to measure observables, supercomputer power is essential.

Another path of research is to already accept QCD as the fundamental theory (for which there is indeed already good evidence), and to make predictions for non-perturbative quantities such as form factors of hadronic currents and matrix elements of other composite operators encountered in the weak interactions which are an essential input for computing parameters in the Standard Model such as the Kobayashi-Maskawa matrix elements.

There are various lattice groups at KEK working on projects of lattice QCD. The main goal of the leading group (scqcd) is to supply the matrix elements referred to above. Indeed as described in the last report their computation of B_B made a big impact and was used by many groups. But nearly all important topics are covered by the KEK lattice projects including investigations of the confinement mechanism, resonance and scattering phenomena, physics at finite temperature and density (relevant to heavy ion experiments), investigations of the effective nuclear forces and the neutron electric dipole moment. It is indeed a colorful program. The KEK groups have made significant contributions in all these fields. Certainly the availability of the supercomputer power was essential to produce the quality of their results, but some of the success is also due to innovative ideas (which are perhaps inspired by the potential computing power), new types of measurements (some of which will be mentioned below) and improvements in data analysis (e.g. the maximal entropy method of the scmelqcd group).

The lattice groups at KEK belong to the leading groups in the world. They have many influential well cited publications and have made numerous presentations at seminars and at international conferences. Indeed at this year's major lattice QCD meeting one of the members S. Hashimoto, gave a plenary talk on the KEK program and in 2007 H. Matsufuru was invited to do the same.

At the meeting the committee heard reports from three lattice groups: scqcd, scnfqcd and scmelqcd. During the last years the first two groups have achieved some research highlights which have received wide recognition and which deeply impressed the Committee. Before describing these achievements in more detail the committee would like to recommend that, despite (and because of) the enormous progress during the past years, KEK should continue to strongly support the fundamental research in this important field.

scqcd scqcd was in the last term the biggest user of the supercomputer resources at KEK. One of their major successes during the past year is to clearly establish that QCD exhibits the phenomena of spontaneous chiral symmetry breaking, which explains the small mass of the pion and is the basis of chiral perturbation theory as an effective low energy description. The reason for their success was their use of a very special lattice fermion regularization, which goes under the name of Ginsparg-Wilson (GW) or Neuberger fermions, that maintains an exact chiral symmetry. It is the only realistic lattice formulation which has this property; other formulations explicitly break the chiral symmetry, and with them it is in general difficult to disentangle the effects from explicit and spontaneous symmetry breakings. The KEK group was the first group to make serious dynamical simulations with the GW fermions. At present the luxury of such an elegant formulation must be paid for by a higher (at present a factor of ~ 30) cost in CPU time compared to other formulations. Hence the special need for computer power.

During the last years the group has measured many physical quantities including electromagnetic pion form factors and current correlation functions (as measured e.g. in electron-positron scattering). They have obtained various parameters associated with chiral symmetry breaking including meson decay constants and verifying various relations obtained using chiral symmetry Ward identities (summarized in chiral perturbation theory). They have obtained the chiral condensate using various measurements which are all consistent with one another. One particular original innovation which we would like to emphasize is their realization that topological properties of the infinite volume system can be extracted from studies of finite volume effects in sectors of fixed topology.

The group has an ambitious plan for the future including studies of larger lattices and approaching the continuum limit, developing algorithms, including the most recent algorithmic developments in the codes, improving actions and measuring matrix elements relevant to B-physics in particular.

The standard of research by this group has been excellent and the Committee congratulates them on their achievements.

scnfqcd The goal of the scnfqcd group is to obtain nucleon-nucleon potentials used in quantum mechanical contexts from first principles. In 2007 the group made a huge step towards this goal and showed that an effective potential defined through a well-defined Bethe-Salpeter amplitude in QCD showed all the important characteristics of common phenomenological potentials. At large distances the potential coincides with a Yukawa potential, at intermediate distances the potential has an attractive well and at short distances the potential has a repulsive core. This would constitute the first explanation of the repulsive core from first-principle calculations of quark-gluon dynamics. The paper was recognized in Nature as one of the research highlights in 2007. Although the computation was done using configurations obtained in quenched simulations it is extremely CPU intensive because of the complicated structure of the observables.

Results on the potential in the tensor channel have also been obtained, which agree with some phenomenological studies. Also the extension of the work to further study hyperon potentials will be very exciting.

The approach looks very promising indeed. But a lot of work must be done to substantiate the main claims. In this connection, the energy dependence of the potentials was already investigated. Perhaps more important, is the investigation of the nature of the core due to the particular local operators employed, and the general theoretical connection between Bethe-Salpeter amplitudes and effective potentials.

The Committee hopes that KEK, realizing its importance, will further support the endeavors of this group.

2.2 Nuclear theory

There are varieties of investigations in nuclear physics that aim at understanding nuclei made of protons and neutrons. We would eventually prefer to use the nucleon-nucleon interaction derived from QCD, the (candidate) fundamental theory of the hadronic interaction, for the consistent description of all the nuclei. Indeed there have been a series of studies to develop theoretical methods to achieve this goal, but they are not yet complete. Thus in the meantime, the majority of theoretical models use effective interactions and try to describe nuclei numerically in order to compare with experimental data.

There was one project on nuclear physics presented at the review committee meeting. Actually there are many other nuclear physics projects which need supercomputers. Presently many research groups are also using the supercomputer at Research Center for Nuclear Physics (RCNP) of Osaka University.

The project presented here (scamd group) is on the anti-symmetric molecular dynamics (AMD) calculation of nuclear structure and nuclear reactions. The AMD formulation is based on a wave packet description of nucleons and anti-symmetrization of many-particle wave packets usually taken as Gaussian functions with positions and momenta as variational parameters. The advantage of the AMD model is that it can describe not only nuclei with a shell-model structure (one-center) but also those with a cluster structure (multi-center) using the variational method without assuming these different nuclear structures from the outset. In the time dependent formalism, the group solved the many-body Schrödinger equation for the description of reaction dynamics and succeeded to reproduce the mass distribution of the multi-particle fragmentation. At the same time, they have investigated the liquid-gas phase transition and showed clear signals of the transition in the AMD framework. The fact that they are able to reproduce the multi-particle fragmentation and the liquid-gas phase transition suggests that the AMD model may be used to describe various nuclei with varieties of mass number.

With the powerful supercomputer, they are now able to calculate nuclei with a mass number as high as 40. The ground state was found to be spherical, while in the low excitation spectrum they found a state having a $C_{12} + Si_{28}$ cluster configuration, which shows a rotational band. They are in fact able to reproduce the experimental data of the rotational band built on the cluster state. This is a big achievement of the AMD model for nuclear structure. There are now many such cases demonstrated for various nuclei.

It is the opinion of the Committee that KEK should keep supporting this project in the future. For the further development of the AMD description of nuclei, it would be important to use the nucleon-nucleon interaction and three-body interaction and to work out various clustering phenomena. This project surely needs more computational power.

2.3 String theory

Superstring theory is a prime candidate for the unified theory of all four interactions in the Nature. It naturally contains the gravitational force as well as the other elements in the current Standard Model of elementary particles. The theory can be formulated in 10 space-time dimensions and the four-dimensional space-time in the present universe is expected to emerge as a consequence of the theory. It is in this sense that superstring theory is called *the* theory of everything, *i.e.* matter, forces and even space-time. Although the self-contained formulation of the theory is not known to date, there are several candidates. Since the dynamics of the string is extremely complicated, numerical simulation may play an essential role in deriving any interesting physics predictions from the theory.

At the review committee meeting, the Committee heard a report from the sc-matrix group, which is one of the leading groups pursuing numerical simulations of string theory. In the past year the group attempted to test the AdS/CFT correspondence which is a remarkable aspect of string theory. It implies that, under some circumstances, quantum gauge theory and classical gravity describe the same physics. So far, it has been verified for many explicit examples and is therefore believed to be valid in more general conditions. The group simulated a one-dimensional gauge theory in the strong coupling regime and compared the results with those of the corresponding gravitational theory. The result is encouraging; it confirms the correspondence in this case to an excellent precision.

The Committee was impressed by the ambitious future plan presented by the group to examine the emergence of four-dimensional space-time. It is indeed an extremely interesting question whether it can be derived from string theory by its numerical simulation. The Committee encourages the group to pursue their research program and recommends KEK to support the group by providing more powerful machines.

2.4 Simulation study of beam-beam effects in accelerators

In high-intensity colliders such as the current KEK B factory, the beam-beam effect often limits the achievable luminosity. Currently, the only practical method to estimate beam-beam interactions is the so-called strong-strong simulation where each particle in a bunch is traced in the field of the on-coming bunch whose charge distribution changes with time. Even though about 10^5 particles are at present combined into one 'macro particle' in order to save CPU time, the required CPU power necessitates a supercomputer. In colliders with finite beam crossing angles, a technique called crab crossing is employed to maximize the luminosity. Again, the only technique to estimate the beam-beam effect in this scenario and thus the achievable luminosity is the strong-strong simulation. For the beam-beam effect without crab crossing at the current KEK B-factory, there is a reasonable agreement between the measurement and the simulation. As for the crab crossing, however, only a small improvement in luminosity has been observed in reality while an improvement of about a factor of two was expected from the simulation. It is of critical importance to understand the reason for the discrepancy not only for the current KEK B-factory but also for the future super B-factory. Even though this study is of utmost practical importance, very limited manpower is allocated at this time. We hope that more human resource will be made available for this project. Meanwhile, collaborations with researchers working on simulations of galaxy motions might turn out to be fruitful. It should also be pointed out that techniques developed here will also be useful for LHC, J-PARC, and ILC.

3 Recommendations and suggestions for the future plans

3.1 Recommendations for short-term future strategy

The Committee was deeply impressed by the successful research activities performed under the Program. They are even pushing the study of particle and nuclear physics to a new stage, which would not have occurred without the world-leading computing power provided by KEK. A significant part of these successful activities has been done by researchers outside of KEK, which shows the effectiveness of the concept of sharing the resources among the broader community in the country.

For maintaining and further extending these highly successful research activities being performed under the Program, it is essential to keep the world-leading computational power at KEK. In lattice QCD, in particular, the groups based at KEK and University of Tsukuba have occupied a leading position in the global lattice QCD community. KEK should maintain such a strength by continuously supporting them with sufficient computational resources. Since the development of the computer industry is very fast, it is important to upgrade the machine in a timely manner. The Committee heard that the current supercomputer, the BlueGene/L installed in 2006, is no longer in the position of leading the world competition in the field of lattice QCD. The upgrade planned in 2011 will therefore be mandatory to keep and enhance the strength of the Japanese research activities.

It is also the opinion of the Committee that computational physics may extend the field of science. An interesting example was demonstrated by the scnfqcd group at the review committee meeting. They are now able to calculate the nuclear force using lattice QCD, which can then be used for the study of nuclear structure. Through this study, we expect a very interesting collaboration between particle and nuclear physicists. In this sense, the Committee found that the plan of the Joint Institute for Computational Fundamental Science, which was presented by a KEK member, is very timely and interesting. The Committee understood that KEK is going to establish a new joint institute for computational physics together with University of Tsukuba and the National Astronomical Observatory of Japan (NAOJ). This will stimulate particle, nuclear and astrophysics researches, and may open a new frontier in high energy physics. We therefore strongly urge the three institutes to make every efforts to enhance collaborative works among particle, nuclear and astrophysics.

In Japan, there is a big national project of constructing 10 Pflops scale supercomputer ongoing at the RIKEN Kobe. The machine construction will be completed around 2012. This will have a huge impact on all the fields of computational sciences including fundamental physics. Given the leading role played in the past by the lattice QCD community to the development of supercomputers, it is natural for this community to join the project in order to share their experiences. Since the computational sciences largely share the methods, *i.e.* algorithms, tuning methods etc., it will benefit the entire community. In this sense, the Committee recommends KEK, together with other members of the joint institute, to consider more collaborations with other communities in computational sciences through this national project.

In summary, for the short-term future of the Large Scale Simulation Program the Committee strongly recommend that the upgrade of the supercomputer planned in 2011 is done in a timely manner. This is mandatory in order to keep the leadership role in large-scale simulations that KEK has become famous for. The plan of the joint institute will further enhance the role of KEK in this and other fields in computational sciences.

3.2 Suggestions for mid- and long-term future

The Committee was asked to evaluate not only the short-term, but also the medium-term and long-term future of the computational efforts of KEK.

For the medium-term, the above collaboration should be encouraged to increase its scope. We suggest the KEK-NAOJ-Tsukuba collaboration to carry out a detailed feasibility study for the possibility of developing a dedicated machine that is best suited for their requirement. One possible direction would be a dedicated machine in the line of the GRAPE efforts lead by Prof. J. Makino at NAOJ; the experiences of the Tsukuba group that developed the CP-PACS and PACS-CS should also be very useful. Given that the directors of KEK, NAOJ and Tsukuba have already signed a contract for the joint research institute, it would be natural to develop a detailed blueprint for the strategy of designing and building their own computational resources. It should integrate the efforts of computer scientists as well as those of computational physicists.

For the long-term future, such a joint center could become a national center for computational science. Given that the new RIKEN Kobe center will be largely focused on applied science simulations, the new center could specialize in pure science simulations. In order to minimize the total cost, the new center should seriously investigate the possibility to develop the above-mentioned dedicated machine. We believe that with a funding around the scale of 100 million dollars, it would be possible to build a leading-class supercomputer. The center would then become the world's leading center in simulations in pure science.

To summarize, the scientific potential for establishing a world-class center is abundantly present in KEK. The expertise of the staff, the quality of the supercomputers used, and especially the splendid track record of published simulations that have led to multiple scientific break-throughs, all argue for KEK to be the perfect place to co-host such a new center for simulations in pure science under collaboration with other distinguished research institutes such as NAOJ and University of Tsukuba. Such a center could attract visitors from all over the world, if it were to succeed in becoming the world's leading center for such simulations.

Last year's Nobel prizes in physics went to Japanese theoretical physicsts for their great work more than thirty years ago. In order to continue this great tradition, now is the time to add the infrastructure for work that will be honored in 2040. Unlike theoretical physics of a generation ago, most current work involves computer simulations. Unless Japan takes a world-leading position in terms of developing hardware and software for such simulations, it will not be able to continue its current preeminence, no matter how high the quality will be of the individual Japanese researchers.

4 Summary

The direction of science to proceed might now be changing drastically. The scientific achievements made by the research groups under the KEK Large Scale Simulation Program clearly indicate that the computational method may lead new scientific discovery. The microscopic dynamics of QCD can now be studied in the theoretically cleanest manner by keeping exact chiral symmetry. The bridge between particle and nuclear physics is being built by the new lattice calculation of the nuclear force; the goal is to understand the structure of nuclei with minimum ad hoc assumptions. The computational methods may even extend our understanding of the universe at the most fundamental level, *i.e.* from non-perturbative studies of the string theory. Another application that is surely essential for KEK is the simulation of accelerators. All these recent research works strongly indicate that numerical simulations are changing the way to scientific discovery.

KEK has been playing a key role in this field of science by providing the leading-edge supercomputers to the Japanese particle and nuclear physics community. This in fact has induced the above mentioned new scientific discoveries, and all the community recognizes and highly appreciates KEK's effort. The Committee therefore strongly recommends that the supercomputer system is upgraded in a timely manner to the scale that the researchers can achieve another series of discoveries. The users of the KEK system certainly have the potential to do it.

The Committee heard about the newly established joint institute among KEK, NAOJ and Tsukuba. This will further enhance the scientific development by promoting collaborative works among researchers in particle, nuclear and astrophysics. It may provide an interesting example that the computational method may lead the whole of future scientific development. For the new institute to be successful, KEK's support on the funding and man-power will be important.

In 2008, three Japanese physicists received the Nobel prize for their work done in pure science, with a paper published more than thirty years ago. Future Nobel prizes in pure science will no doubt be based largely on computer simulations instead. Now is the right time for Japan to prepare for the future, and to give its pure scientists the best chance to compete internationally.