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 physics and related fields in Japan, the High Energy Accelerator Research Organization (KEK) started the "Large Scale Simulation Program" in April 1996.Under the program, KEK calls for proposals of projects to be performed employing the supercomputer at KEK. The proposals are reviewed by the Program Advisory Committee, which decides approval and computer time allocation. Since 1996, 77 projects have been accepted in total, and many results have been reported by the research groups. To review these achievements and identify possible problems, and to gain insight into possible future directions of the program, the Director General of KEK asked the Committee to review the Large Scale Simulation Program for the period starting in April 1996 and ending in March 2002.

The charge to the Committee covers the following items:

- To review the scientific research activities performed under the program.
- To review the effectiveness of the program.
- To review whether the computing resources and support available for the program were appropriate.

For each of the items, recommendations for future directions are also appreciated.

The members of the Committee are

Paul B. Mackenzie	*Fermi National Accelerator Laboratory, USA*
Toshihide Maskawa	*Yukawa Institute for Theoretical Physics Kyoto University*
Denis Perret-Gallix	*French National Center for Scientific Research (CNRS), France*
Ichiro Sanda (Chairman)	*Nagoya University*
Toshikazu Takada	*Fundamental Research Laboratories NEC Corporation*
Akira Ukawa	*Center for Computational Physics University of Tsukuba*
Koichi Yazaki	*Tokyo Woman's Christian University*

The Committee met on December 12 and 13, 2002 at the Computing Research Center at KEK.

1. Purpose of the Large Scale Simulation Program

KEK (High Energy Accelerator Research Organization) is a research institution for carrying out accelerator-related scientific studies. The major task of KEK is particle and nuclear physics research. For this purpose, KEK has maintained and operated accelerators and detectors for high energy physics experiments. KEK has also maintained the computational capacity required for particle and nuclear 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 collaborative research proposals in high energy physics and related areas using the supercomputer of KEK. Applications can be made by researchers at all universities as well as those of governmental research organizations in Japan, or by those that the Director-General of KEK considers appropriate.

It is the opinion of the Review Committee (Committee for short below) that computational research is an indispensable component of particle physics research and an integral part of the KEK research program in a number of ways. The simulation of the Standard Model, and in particular of the QCD non-perturbative sector, is an indispensable major part of the entire B physics program to extract meaningful physical quantities from experimental results at the B Factory. Computational research is also crucial in nuclear physics and in related fields such as astrophysics and others.

The Committee 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 develop the required computing environment, the entire physics community appreciates the KEK effort.

2. Scientific achievements

Modern large scale computing has enabled unprecedented advances in many areas of physics. The KEK Large Scale Simulation Program has enabled significant advances in several of these areas. The Committee heard from seven groups currently working under the program. The great diversity in the physics enabled by large scale supercomputing is well represented by these groups. For example, computers have enabled the well established techniques of perturbative quantum field theory to be pushed to new heights. The scminami group has developed a method for the automatic computer generation of Feynman amplitudes that is widely used at LEP and in particle searches for future colliders. Very different calculational techniques have been used to make advances in nuclear physics. The scnucl/scsokaku group has used the KEK supercomputer to understand areas relevant to strangeness nuclear physics and possible heavy ion experiments at J-PARC.

In nonperturbative quantum field theory especially, large scale numerical simulations

have made possible the solution of previously intractable strongly coupled theories. In addition to being a significant intellectual achievement, this has an urgent practical importance to the experimental programs of KEK and the world. Tens of billions of yen are being spent at KEK and around the world on B physics experiments that cannot be completely analyzed theoretically without calculations from QCD, a strongly coupled field theory that cannot be solved without large scale simulation. These experiments are required, for example, to determine the elements of the Cabibbo-Kobayashi-Maskawa matrix. These fundamental parameters of the Standard Model are essential clues to further understanding of beyond the standard model physics, and are central targets of current particle physics experiments. The Large Scale Simulation Program has enabled the scqcd group to be world leaders in these calculations. Even larger computations are still required to complete calculations required by experiments at KEK and around the world, so there is a need for continued leadership in this field.

2.1 Study of lattice QCD with large scale numerical simulation (scqcd group)

With the VPP-500 computer, this group has computed, B_K , m_π , d , f_π , proton decay matrix elements, f_B , B_B , and $\alpha_{\pi\pi}$using the quenched approximation. These calculations involved controlling the chiral behavior. For B_K this required solving the operator mixing problem, using chiral Ward identities. Their result on B_K has been used as a standard value by the Particle Data Group, which indicates that the number is widely used by the high energy physics community. The Committee notes that the B physics computations are essential to the completion of the analysis of the Belle experiments.

As the SR8000 computer became available in 2000, they started unquenched calculations including dynamical up and down quarks. Their results on f_B , B_B ,the SU(3) symmetry breaking ratio $(f_{B_s}\sqrt{B_{B_s}})/(f_B\sqrt{B_B})$ are leading the worldwide competition, and show that the quenched approximation introduces significant error of about 10%. They have stated that all above computations should be repeated with a dynamical strange quark. It is noted that 90% all the available time from the Supercomputer System has been used by this collaboration. The Committee congratulates the group for achieving these world leading results.

The Committee recognizes that these results are of vital importance, not only to the experimental program of KEK, but also to the world wide high energy physics community. Full unquenched results of the same quality (which need more computing power) are required for the completion of this calculational program. There is therefore a substantial opportunity for continued accomplishment of essential results, if sufficient computing resources are available. The Committee also heard that there will be strong competition from US and European groups within a year.
It strongly urges KEK to take all necessary steps for the collaboration to stay at the top.

2.2 Monte Carlo study of the color confinement mechanism and monopoles in QCD (scknzw group)

This group attempts to prove the conjecture made by t'Hooft that monopole condensation in QCD is crucial in understanding the confinement mechanism. They have observed, using dynamical fermions, (1) Abelian and (2) monopole dominance. Among other results of interest is a pictorial description of the color flux distribution between the quark and anti-quark in a meson.

The results of this group represent considerable progress in conceptual understanding of the confinement mechanism. The group, however, has not achieved its goal of deriving useful effective theory which can be used to understand hadron dynamics at low energy. It is noted that appreciable time allocated for the collaboration has not been used.

2.3 Automatic Feynman amplitude computation and application to HEP (scminami group)

The group has developed an automatic generator of helicity amplitudes (GRACE) for 1 or 2-body $\longrightarrow$ n-body scattering at tree level in the standard model and the minimal supersymmetric standard model. It is, actually, a generator of "event generators". This package has been extensively used at LEP. A new package is in final testing for one-loop diagrams (n=2 and some n=3). Higher loop corrections are being studied. In most cases the limitation comes from computer system performance (CPU, memory and disk size). Quadruple precision is essential for these calculations. This package will be widely used in hunting for SUSY particles at the LHC and future linear colliders.

As the effort along this direction is essential for understanding experimental data from high energy physics detectors, several groups around the globe are now developing similar packages. In order to keep the leading position, it is important that this original effort continue to be supported by the appropriate computing system. The Committee congratulates the group for achieving world leading results for many important reactions.

2.4 QCD at finite temperature and density (sctaro group)

This group studies hadron masses at finite temperature and density with anisotropic lattices. Extrapolation to the chiral limit has been examined. Pole and screening masses as functions of T have been obtained for pseudoscalar, vector, scalar, and axial-vector masses. First attempts to study hadron masses at finite density have been made and the chiral order parameter $\langle\bar{\psi}\psi\rangle$ has been calculated for finite chemical potentials. It is noted that appreciable time recently allocated for the group has not been fully used. The program is relevant to *p-A* (and possible *A-A')* experiments at J-PARC.

2.5 Spectral analysis of nucleon excited states in lattice QCD using the maximum entropy method (scmelqcd group)

This group studies nucleon excited states by extracting spectral functions from nucleon operator correlators using the maximum entropy method they proposed previously. A parity projection has been made to identify the $N'1440$) and N^* (1535) in the spectral functions. Finite volume effects have been found to be important for light quark masses and the long-standing puzzle of the level ordering between the two excited states has been resolved in the infinite volume limit.

The program started recently and is not time consuming. It is important in hadron spectroscopy which is one of the subjects of J-PARC.

2.6 Nuclear structure and heavy ion reaction studies with microscopic computational approaches (scnucl/scsokaku group)

Three subjects are being pursued by this group: (1) the structure of hypernuclei, (2) the structure of stable/unstable nuclei, and (3) heavy ion collisions at intermediate energy. For subject (1), they use the Gaussian basis to study light hypernuclei and extract information on *Y-N* and *Y-Y* interactions. Λ-Σ coupling has been found to be essential for a unified description of the light hypernuclei. Subjects (2) and (3) use anti-symmetrized molecular dynamics as a microscopic approach to nuclear many-body systems. The exotic structure of neutron rich nuclei and the observed features of multi-fragmentation in heavy-ion collisions have been nicely explained. It is noted that appreciable time has been allocated and mostly used, implying that program tuning has been well taken care of. The subjects are frontier topics in nuclear physics and are closely related to strangeness nuclear physics and possible heavy ion experiments at J-PARC.

2.7 Numerical astrophysics (scastro)

This group consists of two subgroups: a supernova subgroup and a numerical relativity subgroup. The supernova (SN) subgroup has developed SN simulation codes (sophisticated 1-dimensional and simplified 2- and 3-dimensional codes), obtained *r*-process heavy element abundances in qualitative agreement with the observed ones, and reanalyzed the neutrino events from SN1987a considering the possibility of neutrino oscillation. The numerical relativity subgroup has studied coalescing binary neutron stars and resulting gravitational radiation. Four-dimensional Einstein equations and general relativistic hydrodynamical equations have been numerically solved.

Ample time has been allocated but has not been fully used. Better tuning for the supercomputer may be necessary. The program is important not only in astrophysics but also in particle and

nuclear physics and is relevant to neutrino physics at J-PARC.

3 Computational resources and user environment

The supercomputer hardware was well chosen to be the most cost-effective possible at the time of its selection. It is well-suited to the main application of the computer, the large scale simulation of lattice QCD. The hardware has been used very effectively for its main purposes. It has been the most powerful computer used for lattice QCD for the last several years.

At the time of its installation in 2000, it was the ninth most powerful computer in the entire world according to the Top500 List of Supercomputers. Its position has dropped to number 53 in 2002, and will continue to drop rapidly in the coming years. An upgrade will become urgent if KEK is to maintain its top position in lattice gauge theory and other major large scale simulation programs. The six year rental period of the present contract is too long to ensure a system that stays at the forefront of the competition. It would be preferable for future rental contracts to be shorter.

Supporting hardware infrastructure is important for optimal use of the supercomputer. The planned upgrade of networking to remote sites to gigabit ethernet will improve the ability of remote users to use the supercomputer and to collaborate effectively. Increased disk storage is desirable as disks become increasingly cheap. Support for computing for which the supercomputer is not optimal may be desirable. Inexpensive PC farms may provide an effective solution for some of the computing tasks of users of the supercomputer. The effectiveness of various types of hardware for different types of computing tasks should be considered carefully in future plans for upgrading the system.

Sufficient support staff to help optimize the use of the supercomputer is essential to its effective use. It is particularly important that recently vacated staff position for lattice QCD be filled in a timely way. Workshops on the use of the supercomputer may facilitate the work of outside users.

4 On the reviewing system

The Large Scale Simulation Program Advisory Committee has been in charge of reviewing and selecting the proposals to be run on the supercomputer facility. As stated in section 2, the Committee has been satisfied by the quality of the research conducted using the supercomputer facility. Therefore it concludes that the reviewing and program selection process has been performed smoothly.

4.1 On the selection of the projects

The Committee finds that some of the applications could have been run on more appropriate

computer architectures like PC clusters. Moreover some of the requested and allocated CPU time budgets have been only partially consumed by the users, although thanks to the bi-annual reviewing system, the free time has been reallocated to other users ending up in a full use of the resources.

The Committee therefore recommends that a broader scope of CPU resources available in the computer center should be opened to the Program Advisory Committee in order to redirect applications to other facilities, if appropriate.

For large CPU time requests, the application should be first tested and validated in order to be approved. Small amounts of test time should be made available on request to users for this purpose.

4.2 On the post evaluation of the projects

The Committee understands that all research results are reviewed by the Large Scale Simulation Program Advisory Committee. It is recommended that the laboratory make this evaluation more rigorous and transparent. The Committee finds the official reports of the fiscal year from 1997 to 2001 inadequate to evaluate the research efforts. Neither the motivation nor the usefulness of the results is very clear. It is recommended that each report should be written in such a way that researcher in other fields can understand it.

It is also noted that there are only three written reports for fiscal Year 2000. This is clearly unacceptable. It is this type of attitude that destroys public confidence towards the computational laboratory, which was earned over many years of hard work.

It is recommended that a critical review by experts in the field be made for each project at the end of its proposed period. The Committee also recommends that a summary of activities that can be understood by the general public be posted on a web page.

5 Organization of the program

5.1 Committee structure

Currently, the operation of the KEK supercomputer system is under the supervision of the Supercomputer System Operation Committee appointed by the head of the Computing Research Center, while the approval of projects and resource allocation in the Large Scale Simulation Program are determined by the Program Advisory Committee.

Since the research program and computer operation are closely related to each other, they should be organized in an unified manner so that the scientific program and the computer operation are consistent with each other. This is especially important when the future direction of the supercomputer research programs is to be decided.

The Committee therefore suggests that establishing a single committee under the Director

General of KEK, whose function covers both the the organization of the Large Scale Simulation Program and the operation of the supercomputer system, will further enhance the scientific effectiveness of the KEK supercomputer facility. The future direction of the supercomputer program is also to be discussed by the new committee.

5.2 A suggestion for a long term strategy

Although the task of the present committee is to review the supercomputer system of the laboratory, it felt it necessary to emphasize the importance of a solid and well structured computing environment for the future endeavors of the particle and nuclear physics community in Japan as well as in Asia.

It, therefore, suggests that KEK evaluate the general needs of community and the role that the KEK computing center could play as a major node in the global network of particle and nuclear physics computing activities.

6 Summary

Particle and nuclear physics research is, nowadays, highly demanding of high precision, massive computation. New projects cannot be carried out successfully without the support of powerful computing systems in an well structured framework. The efficiency and competitiveness of Japanese research is at stake.

Although some improvements have been proposed by the Committee, in general, it is the opinion of the Committee that the Large Scale Simulation Program has provided an excellent framework for achieving the research goals of its community. The program has provided the high performance computing resources that are essential not only to members of KEK, but also to researchers outside of KEK. In this way, the program has encouraged the collaborative effort of communities of physicists to attack many interesting problems. The Committee finds this system to be very effective, and hence should be continued and strongly supported to benefit the entire physics community.

The research quality has been very high in general; in non-perturbative QCD, in particular, they have been leading the world in calculating a number of quantities indispensable for B physics. The Committee strongly urges KEK to continue full support of the supercomputer facility and its collaborative use by researchers through the Large Scale Simulation Program.

The problem of the reviewing system is universal in all research projects supported by the Ministry of Education and Science. The system should be overhauled. The Committee hopes that by pointing out the problem at all possible occasions, a change can be triggered. It also hopes that

the KEK Large Scale Simulation Program will take the first step along this direction.

Finally, the Committee hopes that further discussions will occur to enhance the role and activity of the Computing Research Center in wider areas of computer science in Japan and abroad, including Asian countries.