○ Establishment of the Research System for Computational Science

An optimal software and execution environment will be developed to enable life science and computational life science researchers to efficiently utilize the HPCI environment centered on K computer. For this purpose, close and continuing collaboration will be established with research and development groups. In addition, the wide-spread use and dissemination of information, the promotion of increased understanding, and the development of research and educational personnel with respect to the HPCI, which are all closely connected with the research and development groups, will be sought, based on collaboration with organizations in other strategic fields, the Advanced Institute for Computational Science (AICS), and the High Performance Computing Infrastructure Consortium.

I High Performance Computing Development Group (Head: Makoto Taiji, RIKEN)

I-1 Efficient management of computational resources

I-1-1 Implementation plan

To provide researchers in Strategic Field 1 with the environment needed to generate epoch-making results through maximum use of the HPCI, the improvements and operation of computing environments (software and execution environment, etc.) which commenced in FY 2011 will be continued in FY 2012. Additionally, computing environments compatible with the HPCI environment will be developed and put into operation, so that life science researchers (including those in the health care and pharmaceutical industries, etc.) with little experience in using high performance computers will be able to function more efficiently in the HPCI environment.

I-1-2 Implementation details and results

1) Efficient management of computational resources

1-1) Trial-use periods V and VI

Based on a survey of prospective application software and its current state of development, software better optimized for use on K computer (HI-Muscle and AMBER) was chosen and designated for use during trial-use periods V and VI.

1-2) Consumption plan for the efficient use of computational resources and redistribution of resources after K computer was made available for joint use

A target computational resource consumption level was determined, based on the operating policy on joint use of K computer and on the current development situation of application software for each research theme in Strategic Field 1, to encourage efficient consumption of allotted resources by participants. Although the general K computer operating policy assumes 100% operation and utilization rates in allocating its computational resources, the actual utilization rate had been between 60 and 70%. Reflecting this figure, the actual usable computational resources were estimated to be roughly 60% of the allotted resources. Based on this assumption, the target

consumption level for the FY 2012 use period (from September 28, 2012, to March 31, 2013) was set at 10% of the allotted resources per month.

As computational resources allocated to strategic fields cannot be carried over to the following fiscal year, and thus must be used within the allocated fiscal year, heavy use of K computer near the end of the fiscal year was expected. To bring forward the timing of its use, the "Computational resource consumption plan" (Figure 1) was drawn up. In light of the developmental state of the respective applications for each theme, the red arrows in the figure indicate the period when each application was scheduled to be in full operation. Users of applications in advanced stages of development were especially encouraged to fully consume the respective allotted resources before year's end.

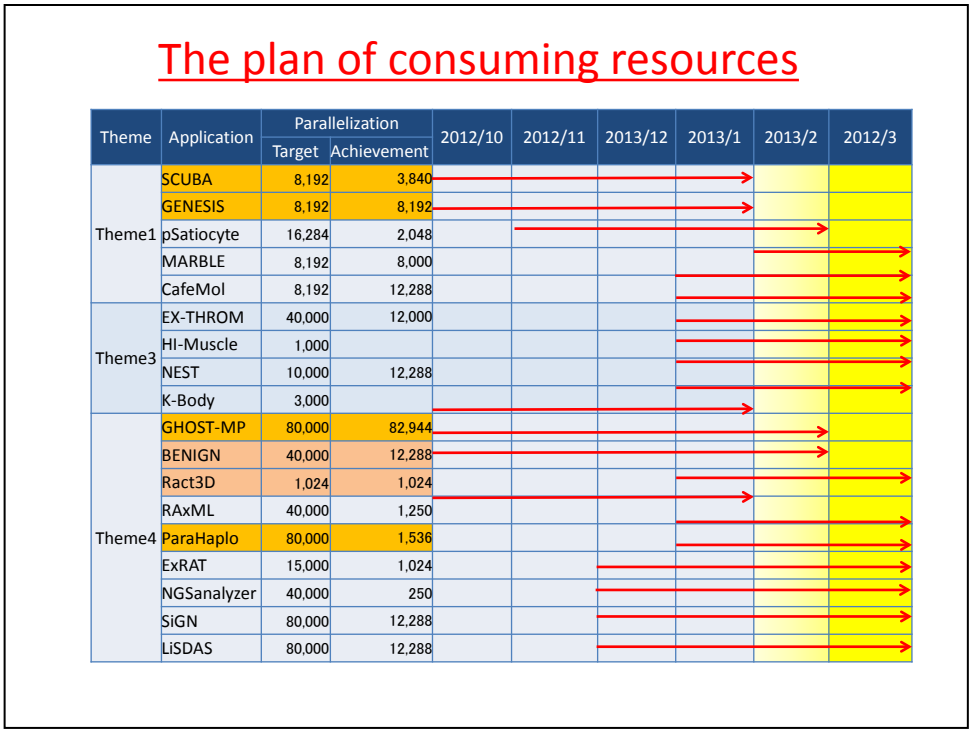

Figure 1: Computational resource consumption plan

As there were variations in the consumption of computational resources among the themes as of December 2012, computational resources were reallocated within Strategic Field 1. In addition, as one theme had already consumed its allotted resources by February 2013, a reallocation of resources within Strategic Field 1 was also performed as an exceptional measure.

In sum, as a result of the computational resource consumption target set for each month, as well as the encouragement to bring forward the use of K computer for applications in advanced stages of development, and the reallocation of resources within the field, approximately 70% of the computational resources allocated to Strategic Field 1 were consumed by the end of March 2013. This result exceeded the original target of 60% consumption, reflecting the effective use of the allotted computational resources. The resource consumption results for each theme are shown in Figure 2 ("Computational resource consumption as of the end of March 2013").

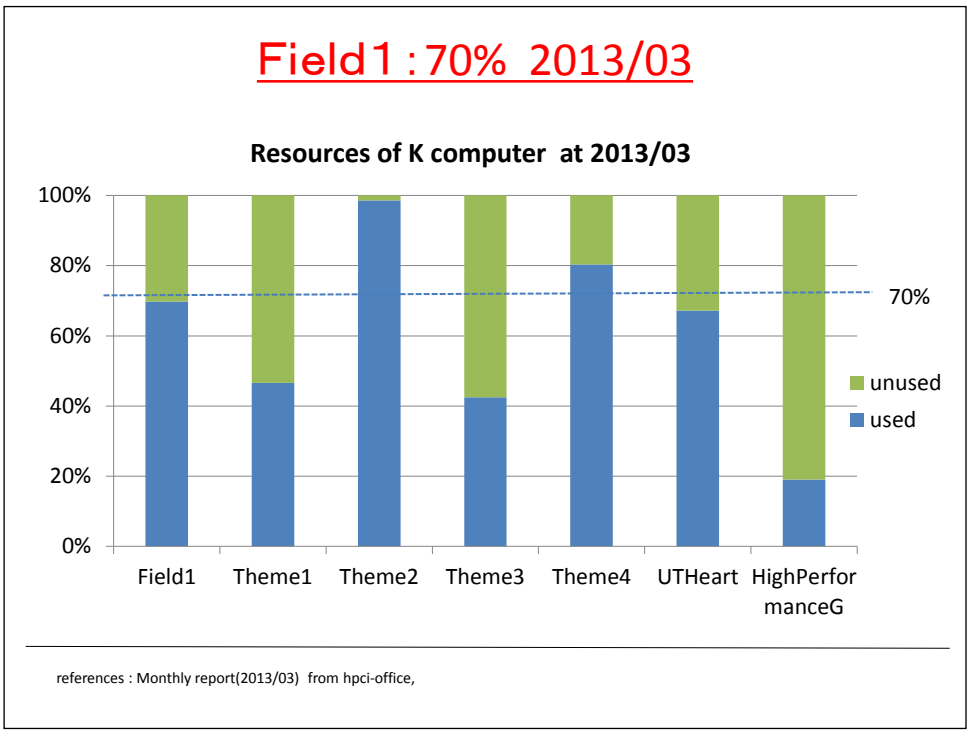

Figure 2: Computational resource consumption as of the end of March 2013

2) Management of the computing environment to optimize use of the HPCI environment within Strategic Field 1

The computing environments (software and execution environments) developed in FY 2011 were maintained in FY 2012. Specifically, the storage system for saving large data used in genomic analysis, and the computer system for high performance software development, were maintained.

I-2　HPCI user research support

I-2-1　Implementation plan

Lectures, seminars, and other opportunities regarding parallel programming will be organized with the cooperation of organizations in other strategic fields, cooperative institutions, the AICS, etc., to educate personnel (developers and users) capable of utilizing the HPCI environment.

I-2-2　Implementation details and results

1)　K computer user research support

1-1)　Structure of the research support

To provide research support, with the advice of the AICS Processor Research Team and the Research and Development of Next-Generation Integrated Simulation Software of Living Matter (Grand Challenge Application Project), the High Performance Computing Development Group designed the structure shown in Figure 3 (“Organization of the High Performance Computing Development Group”), encouraging the development of high performance computing applications pursued by each research theme.

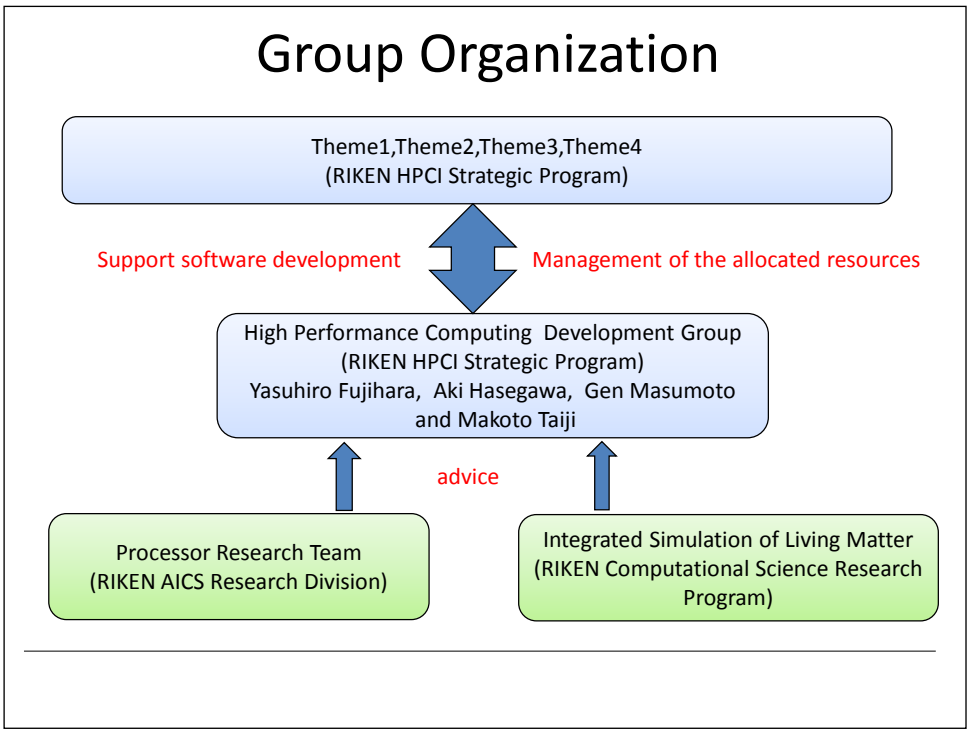

Figure 3: Organization of the High Performance Computing Development Group

In addition, one person was put in charge of each application, to better understand the requirements of the given application and to better offer support.

During K computer trial period V, based on reports from personnel in charge of software applications, applications that were showing progress in adapting to K computer, specifically HI-Muscle and AMBER, were approved as registered applications on K computer. Including those applications that had been registered during trial periods I to IV (MP-CAFEE, GHOST-MP,

GENESIS, SCUBA, EX-Throm, and BENIGN) a total of eight applications have been authorized for use on K computer. A total of 10 users were registered as trial users to promote the use of K computer. During the trial period, the High Performance Computing Development Group was the contact office between AICS and users, circulating announcements, relaying user requests to AICS regarding K computer, etc., and thereby acting as a bridge between AICS and users. After K computer was made widely available, the High Performance Computing Development Group participated in K computer user lectures held on September 27, 2012, and October 10, 2012, to share and disseminate information. It also participated in K computer operation discussion meeting held on March 7, 2013, to convey to the HPCI-OFFICE and AICS the requests of Strategic Field 1, and exchange ideas with these organizations on the future operation of K computer.

1-2) Host of a lecture and discussion meeting

On January 31, 2013, a K computer user lecture aimed primarily at the members of Strategic Field 1 was held. With the title, "How to fine-tune K computer," the lecture provided Fujitsu Limited with a comprehensive overview of tuning K computer, including a description of methods for its use, the performance of collective communication, and fast Fourier transform (FFT) libraries. In a lecture entitled "An introduction to K MapReduce (KMR) – a MapReduce library for K computer," Dr. Motohiko Matsuda of AICS gave a general description of MapReduce and described the developmental state of KMR.

Discussions were also held with developers designing software on K computer for other strategic fields, in order to exchange information.

1-3) Developmental support

High performance computing developmental support was provided for the development of the following applications.

A) pSpatiocyte
B) AMBER
C) MARBLE
D) BENIGN
E) SCUBA
F) GENESIS
G) GHOST-MP, MP-CAFEE, etc.

Acknowledgement

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