

II Planning and Coordination Group (Satoru Tomita, RIKEN)

II-1 Human Resource Development and Education

Our mission is to foster the skills necessary to support research and development in high-performance computing and to raise awareness of career opportunities in computational life sciences among young people. To accomplish these goals, we organized specialized training programs in collaboration with Advanced Industrial Science and Technology (AIST), Computational Biology Research Center (CBRC) and Osaka University, and have developed educational outreach programs for high school students and undergraduate and graduate students.

II-1-1 Advanced Industrial Science and Technology (AIST), Computational Biology Research Center (CBRC), HPCI Educational Program

HPCI Seminar Series (12 sessions: 2012 October 12 - 2013 January 25)

The mission of the CBRC HPCI Educational Program is to promote maximal utilization of computers in life science research and education, and to provide leading-edge information on computing in biology. A twelve-session seminar series was presented by external invited researchers and CBRC researchers and offered as a University of Tokyo credit-earning course, entitled Special Lectures on Computational Biology (2012 Winter Semester: Department of Computational Biology, Graduate School of Frontier Sciences). Total participants numbered 324, including 115 graduate students. The curriculum consisted of introductory general lectures for graduated students followed by extensive discussions of the state-of-the-art in computational biology research and development.

HPCI Workshop

An HPCI workshop entitled “How does High Performance Computer pave the way for life science in the future?” was held at the AIST Tokyo waterfront annex on November 1.

The workshop was focused on multi scaled high performance computing research from the levels of Molecules to Organs. Invited speakers included Professor Shu Takagi (School of Engineering, The University of Tokyo) who spoke about Organs, Dr. Koichi Takahashi (RIKEN Quantitative Biology Center) Cells, Assistant Professor. Yasuyuki

Okawa (Faculty of Medical Sciences, Kyushu University) DNA sequences, and Professor Hiedeaki Fujitani (RCAST, The University of Tokyo) TOPIC. Total participants numbered ~80. This workshop also held as part of BiWO2012: Bioinformatics Week in Odaiba 2012. Furthermore, a satellite seminar was presented by K computer users (Drs. Atsushi Suenaga, Tomoshi Kameda, and Satoshi Yamazaki, before the HPCI workshop.

HPCI Tutorial

One of the most attractive components of the HPCI tutorial is hands-on training with each participant using their own personal computer. Experience has shown this approach to be an effective means of introducing programming to beginners. We provided the following three courses:

- Bioinformatics (4 classes)
- Bioinformatics for Drug Discovery (5 classes)
- HPCI Tutorial Seminar (1 class)

All classes were taught by leading researchers who introduced cutting-edge research examples and new techniques of analysis. Total participants were 97, 37, and 41, respectively.

II-1-2 Osaka University, Graduate School of Engineering Science, Education Program for Predictive Medicine and Drug Discovery on High Performance Computational Infrastructure

Biosimulation Series (12 sessions: 2012 December 1 - 22)

The Biosimulation Series consisted of twelve lectures on mathematical modeling approaches to studying biological phenomena and four hands-on training sessions on computational simulation techniques for undergraduate students. The series was held at the Osaka University Graduate School of Engineering Science as for a two-credit course and was also made available as part of the extension curriculum. In all, 14 students participated (11 graduate students earned university credits, and 1 participant completed the extension curriculum).

Bioinformatics Series (6 sessions: 2013 January 19 and 26)

An introductory Bioinformatics Series focused on applications for medical care and life

sciences research, including data analysis and parallel computing techniques, was offered to graduate students through the Graduate School of Engineering Science at Osaka University. This series was approved for course credit by Osaka University this year. Total participants numbered 5 (2 graduate students earned university credit, and 2 participants completed the extension curriculum).

Collaboration Seminar with Industry and Academia: K computer for Drug Discovery and Medical Care

Industry-academe collaboration seminars were held in Osaka on December 19 2012 (83 participants) and in Tokyo on January 25 2013 (73 participants). At both venues, current K computer users presented their research activities, and industrial researchers wishing to use of the K computer described their research plans. Our SCLS supercomputer system and the peer-reviewed system for research themes on the use of SCLS Supercomputer System were introduced at the both sessions.

II-1-3 RIKEN, HPCI Strategic Program Field1 Planning and Coordination Group

Lectures

1-1) The Planning and Coordination Group presented lectures on computational life sciences in collaboration with the Graduate School and Faculty of Pharmaceutical Science, Kyoto University, the Center for Advanced Medical Engineering and Informatics, Osaka University, the Faculty of Human Development, Kobe University, and the Graduate School of Pharmaceutical Sciences, Tokyo University of Science. Total participants numbered 346.

It is remarkable that the Kobe University Faculty of Human development students were most impressed to learn of the importance of collaboration between biologists and those trained in the quantitative sciences (e.g., mathematics, physics, and chemistry. They were also struck by the fact that supercomputers and K computer in particular, are not just computing machines but are versatile and applicable to daily life.

1-2) Educational outreach for high school students

1. Much of research in the life sciences today utilizes tools coming from physics, chemistry, and mathematics. The Planning and Coordination Group made on-site presentations to high school students, highlighting the importance of such

interdisciplinary approaches and presented work on simulations of biological systems using K computer. Participant feedback showed that the students gained a much broader view of the potential impact of supercomputing in biology. Lectures were held at high schools in Fukuoka, Tochigi, and Hyogo prefectures, where participants totaled 168. We also explained the importance of interdisciplinary in Computational Life Science to high school biology teachers in Fukuoka July 1 2012 to 40 participants.

2. The Planning and Coordination Group organized exhibition booths at the “Science Fair in Hyogo” in Kobe on January 20 2013 and at the “Kagaku no Koshien: Science Olympic” in Nishinomiya city on March 24 2013. At both venues, we introduced computer simulations of biological macromolecules using a DNA base sequence puzzle and three dimensional Hemoglobin and Myoglobin puzzles.

II-2 Establishment of Human Networks

1) Dissemination *via* Symposia

The Planning and Coordination Group held symposia at Tohoku University, Okayama University, and Kyusyu University to foster better understanding of the HPCI and computer simulations in life sciences. Total participants numbered 408.

At the Tohoku University, we provided selected applicants for “Five minutes session for graduate students” with travel support to give short themed presentations on “What do you utilize it for life sciences if you use the K computer?” and “What do you expect of the K computer in life sciences”. Following the symposium, collaboration discussions were initiated between a faculty member at Tohoku University School of Medicine and one of the selected graduate student presenters.

We also organized a symposium at the annual meeting of the Biophysical Society of Japan (1,500 participants) and a session at the 2013 Joint Conference on Informatics in Biology, Medicine and Pharmacology (621 participants).

2) Installation of the SCLS supercomputer system

We introduced a K compatible supercomputer system: SCLS supercomputer system to support use by external biologist and bioengineers (on a peer-reviewed basis) to promote computational life science research.

SCLS Supercomputer system: PRIMEHPC FX10 Supercomputer

[Specifications]

Processor: SPARC64 IXfx

Number of compute nodes: 48

Theoretical peak performance: 10.1TFLOPS

Total memory capacity: 1,536GB

Shared file sized limit: 128TB

SCLS Access Proposals for Research Themes

The FY2012 first call for research themes was launched December 3 2012 and closed after about one month. In all, 14 research theme applications were granted to use computer resources by the SCLS Committee. Access to the SCLS supercomputer system was launched on March 1 2014.

The SCLS Committee membership is as follows:

Chair: Minoru Kanehisa (Kyoto University, Professor)

Shigeo Wada (Osaka University, Professor)

Akinori Kidera (Yokohama City University, Professor /RIKEN HPCI Program,
Vice Program Director)

Yukihiro Eguchi (RIKEN HPCI Program, Vice Program Director)

Number of External Users: 51 (As of March 1 2013)

SCLS User Workshop

We held a workshop for beginners to support new external users of the SCLS supercomputer system at the CBRC, AIST on March 27 2013. The workshop was also open to users based at RIKEN AICS, who attended *via* video conference. Total participants numbered 8.

II-3 Dissemination of Research Outcomes

The Planning and Coordination Group disseminated its activities and research programs for the HPCI Strategic Program Field1 *via* improved websites, newsletters, brochures, and exhibitions.

Websites

The Planning and Coordination Group improved the website to reflect our expanding activities. Specifically, to be more visible and more usable, we included banner displays and an analytical tool that records website access logs. In addition, to expand our communication networks, Twitter and Facebook accounts were set up to disseminate information about our efforts, including AICS and other HPCI Five Strategic Programs.

Publications

The Planning and Coordination Group released a newsletter (semi-annual) collaborating with the Next-Generation Integrated Living matter and a brochure for researchers. We also created a brochure (annual) to provide the general public with an easy-to-understand explanation of the program.



From left to Right: BioSupercomputing Newsletter Vol.7, Vol.8, Brochure front covers for the general public and researchers (Back: Japanese; Front: English).

In addition, we introduced and explained our research activities by contributing articles to professional journals.

Booth presentations

The Planning and Coordination Group presented our research project and activities at booths for the general public, academic researchers, and industrial scientists.

Major activities were as follows:

- RIKEN Open Day: We participated six times a year in Open Days organized by regional RIKEN centers. At the Open Day, the AICS (Kobe), we presented the research project and demonstrated molecular origami. Participants enjoyed making a paper model of an icosahedral virus, with which they learned about macromolecular shapes. Total participants numbered ~3,500.

The Planning and Coordination Group hosted exhibit booths at scientific meetings and events to disseminate our project research and activities as follows:

For industry:

- Bio Japan 2012 (October 10 to 12 2012, Yokohama). Total participants numbered 12,369.
- RIKEN Friends in Industry (February 14 2012, Tokyo). Total participants numbered 445.

For researchers:

- Conference on Computational Physics 2012 (October 14-18 2012, Kobe). Total participants numbered 404.
- Supercomputing Conference 2012 (November 12-15 2012, Salt Lake City, USA). Total participants numbered 9,822.
- The 1st Computational Materials science Visualization Symposium (March 5 2013, Tokyo). Total participants numbered 136.

Seminar for the public at large

The Planning and Coordination Group organized a seminar on April 20 2012, hosted by the Senri Life Science Foundation, describing the potential role to be played by the K computer in benefiting Japanese society. In the seminar, the design concepts underpinning the architecture of the K computer, its performance during the commissioning period, and research plans for medical care and drug discovery were presented and expectations for the utilization of the K computer were discussed. Total participants numbered 116.

Academia-industry joint project

The Planning and Coordination Group worked to develop a joint academia-industry project using our K computer application, MP-CAFEE. Our overarching goal was to garner mainstream recognition that the K computer represents an effective tool for drug discovery. This project is led by Professor Yasushi Okuno, Kyoto University, and consists of 11 pharmaceutical companies, two IT companies, a university, and two research organizations.

II-4 Interdisciplinary Projects

Workshops by HPCI Five Strategic Programs

The Planning and Coordination Group collaborated workshops for researchers on July 9 2012 and January 16 2013 to exchange technical information and share issues beyond professional discipline to promote effective use the K computer. Dr. Hisashi Ishida (JAEA) and Dr. Takeshi Yamashita (The University of Tokyo) presented on July 9 2012 and Professor Satoru Miyano (The University of Tokyo) and Dr. Kazuya Shimizu on October 3. Total participants numbered 83 and 77, respectively.

Special Lecture at the Kobe University

The Planning and Coordination Group organized a seminar series, entitled “Special Lecture on Natural Environmental Science D - New science opened up by the K computer-”, in the second semester of FY 2012 collaborating with AICS and HPCI Five Strategic Programs. This omnibus session was themed on how the K computer is utilized to analyze the natural environment and how computational science can contribute to society.

Total participants numbered 22.

November 17 “Computing Machinery and the K computer in Society”

Dr. Toshiyuki Maeda (RIKEN AICS)

“History and Changes of the Magnificent Natural Environment Surrounding Us” <Field 5>

Professor Takaharu Otsuka, (The university of Tokyo)

December 1 “How to Assess the Severity of Energy Problems, and How to Overcome Them” <Field 2>

Dr. Osamu Sugino (The University of Tokyo)

“The Mystery of Microorganisms Coexisting with Humans”<Field 1>

Dr. Takashi Ishida

December 15 “The Environment Created by Humans, its Safety, and its Soundness” <Field 4>

Dr. Norihiro Nakajima (JAEA)

“ Roles of the K computer in the Study of Massive Ocean-trench Earthquakes and Disaster Mitigation” <Field 3>

Dr. Yoshiyuki Kaneda

Collaborative meetings with AICS, HPCI Five Strategic Programs, RIST and Next-Generation Integrated Simulation Living matter projects

AICS, which manages and operates the K computer, HPCI Five Strategic Programs, RIST, which promotes the utilization of the High Performance Computing Infrastructure that encompasses the K computer and other computational facilities at nine Japanese universities, and the Next-Generation Integrated Simulation Living matter projects, which develop research using the K computer, conduct collaborative meetings every several months to promote closer cooperation. At these meetings, progress and management situations of the K computer were reported by AICS and issues arising during use of K computer were discussed by participants.

Collaboration with Next-Generation Integrated Simulation Living Matter Project

As there are significant commonalities in researches topics between the Next-Generation Integrated Simulation Living Matter Project and the HPCI Strategic Program Field1, we have been actively promoting collaborative relationships to advance research in computational life science. We made various outreach efforts, including semi-annual release of BioSupercomputing Newsletter and hosting a booth presentation for CCP2012: Conference on Computational Physics 2012. The Planning and Coordination Group has ported software source codes made by the Next-Generation Integrated Simulation Living Matter Project to the SCLS supercomputer system for utilization by users. In addition, Dr. Ryutaro Himeno, Vice-Program Director of the Next-Generation Integrated Simulation Living Matter Project, serves as an observer at the monthly steering committee meetings of the HPCI Strategic Program Field 1.

Participation in the Working Group for Public Dissemination of Information on Computational Science

The working group focused on information dissemination in computational science to the public, established under aegis of the AICS and HPCI Five Strategic Programs collaboration, released a midterm report on March 2012. Since May 5 2012, the working group met with the Committee for Physical Sciences and Engineering Section of the Science Council of Japan and is due to hold a symposium hosted by the Science Council of Japan on June 21 2013.

Participation in Network Meeting for AICS and HPCI Five Strategic Programs

The second network meeting for AICS and HPCI Five Strategic Programs to promote information sharing and enhance institutional and programmatic collaboration was held at

the University of Tokyo, Hongo Campus on May 15 2012. During the meeting, the role of the group in the K Project, working-level guidelines for Mass Media, and future work were discussed. Periodic meetings to promote research using the K computer were planned.

Total participants numbered 17.

Workshop for Mass media

Workshops for Mass Media were held at the AICS under aegis of the AICS, RIST, and HPCI Five Strategic Programs collaboration to enhance dissemination of information regarding the K computer to the general public. This joint effort aims to foster better understanding of the research process, and effectively disseminate research outcomes. During the workshops, research themes, expected outcomes, research schedules, and advantages afforded by use of the supercomputer and the K computer were presented.

First workshop (November 6 2012). Total participants: ~40, including 12 members of the press.

Second workshop (February 6 2013). Total participants: 43, including 12 members of the press.