CCS Report: PART III

Strategy and Future Plans of Center for Computational Sciences

February 2014

Center for Computational Sciences
University of Tsukuba

1 The Strategy of CCS

1.1 Introduction

This document, CCS report: PART III, describes the strategy and future plans of the Center for Computational Sciences, University of Tsukuba. The strategy focuses on a time frame of 2014-2020. The report has been prepared for the review of the Center scheduled from February 18th to 20th. The purpose of the review is to receive the evaluation from outside on the research activities and their outcomes of the CCS in the light of the founding objective, and to make recommendations from a viewpoint of future advances. Since the details of research outcomes are presented in a separate report, this report concentrates more on the strategy and future plans of the CCS.

1.2 Mission and Role of CCS

The mission of the CCS is to promote scientific researches by means of computational methodology, through the development of leading-edge computing systems and their applications to advanced sciences by nationwide researchers.

The CCS carries out researches in natural science, life science, and environmental science using large-scale numerical simulations and data analyses. To advance these researches, the CCS carries out the Research and Development in high performance computing and networking systems, and conducts applications of novel information technologies. The CCS is an inter-university facility open to researchers throughout Japan. In Japan, the CCS is a unique "multidisciplinary" organization, in that scientific researchers tightly collaborate with computer scientists, and also scientific researchers of various research fields intimately communicate and produce the synergy. Computational Science in each discipline is done by university labs and institutes specific to its discipline, but we conduct not just computational science in each discipline, but also "Multidisciplinary" researches to integrate many fields. Our center is not just for computer sciences, but also for computational sciences, in contrast to the institutes that are organized focusing on computer sciences: For example, National Institute of Informatics (NII) focuses on Information Science, neither computational science nor development of high performance computer system. In Japan, there are Supercomputer Centers in major universities, which focus on just operation and service on computing facilities, and not researches on computational science. From the viewpoint of development of scientific research within our university, our center is the topmost research center. Our university provides strong support with respect of budgets, faculty position and facilities. Also, the faculty of CCS belongs to graduate schools and contributes to the education of computational science.

1.3 "Multidisciplinary Computational Science" as the Vision of CCS

Computational Science, which enables us to explore uncharted fields of science through applications of high performance computing, is a third paradigm of scientific research which has become indispensable for the development of science and technology in the 21st century. The methods of large-scale numerical analyses that form the pillar of computational science are common over a wide range of scientific disciplines, from fundamental science to material, life and geo-environmental sciences. This common base brings mutual intimate connections among various scientific disciplines and allows us to approach science as a whole from a global perspective. This in turn leads to a global point of view over Nature, Life and Environment, which is indispensable for a harmonious advance of science and technologies and consequently of mankind. Furthermore, the progress of computational science will help produce the next generation of scientists that carry out research from global perspectives.

Development of computational science cannot be satisfactorily achieved solely by scientists who use computers. A close collaboration and an ensuing synergy with computer scientists with the expertise on computer hardware, software, algorithm and programming, and also with information scientists on data and media engineering and technologies, are indispensable. Therefore, in order to establish a solid base for development of computational science, it is necessary to build up a system which integrates the forefront of scientific research with that of computer science and information science.

Computational Science has been established in almost areas such as mathematics, biology, finance, physics, chemistry, or social science. For example, physics has developed "computational physics". So far, most researchers of computational science make use of existing "supercomputing center" to conduct their jobs and sometimes it may be a short-term project which have nothing to do with other fields of computational sciences. Some knowledge, models and algorithms, however, can sometimes be shared among different fields of computational sciences. In the view of problem solution, wide knowledge and integration of various fields should be required.

Computational science is currently a cutting-edge and indispensable area for the development of science and technology in the 21st century. In our center, we define "**Multidisciplinary Computational Science**" by two aspects as follows:

1) Integration and collaboration of computational science and computer science:
   - A high performance computing system will be getting bigger and more

complex in configuration. HPC technologies are indispensable to make the best use of it.

– Continuous development and investment are required to enable the next generation of computational science.

2) The common base of computational science brings mutual intimate connections among various science disciplines and allows us to approach science as a whole from a global perspective.

University of Tsukuba and the Center for Computational Sciences have been making a long-standing effort to establish an international and nationwide research center for advance of computational science, taking advantage of the top-level research achievements produced and accumulated there. The CCS's vision is that **CCS aims to be a world-wide COE to develop "Multidisciplinary Computational Science" as a new discipline essential to 21st century advances in science and technology, and support it continuously from global and long-term perspectives.** The vision of CCS should be to further enhance and develop the close collaboration among various scientific areas, and computer and information sciences pursued at the CCS, which is quite unique in the world, and thereby establish a system which advances computational science from a global perspective and simultaneously produce the next generation of scientists who push forward science from global viewpoints. We aim to establish an organization for computational science research at the world's highest level through a close integration of science and computer and information sciences. On this basis, we aim to meet the grand challenges in various scientific fields such as fundamental, material, life and geo-environmental sciences. Simultaneously, the organization should function as an advanced educational system for educating the next generation of computational scientists.

1.4 Strategy and Plans

To realize our vision with accomplishment of our mission, we will take the following strategy and plans. The vision and this plan focus on a time frame of 2014-2020.

[Research & Development]

Integrate the forefronts of scientific research with those of computer science and information science, and thereby establish and promote new multidisciplinary computational science

【1】 Promote HA-PACS and COMA (PACS-IX) projects to execute inter-university "*Multidisciplinary Cooperative Research*".

【2】 Propel two next generation projects: one is JCAHPC Project to acquire the next generation large-scale many-core system and the other is "*Feasibility Study on Future HPC Infrastructure"* toward Exa-scale Computing.

【3】 Advance computational fundamental physics such as particle physics, astrophysics, and nuclear physics. For the purpose, continue and expand "*Joint Institute for Computational Fundamental Science*".

【4】 Found "*Organization for Collaborative Research on Computational Astrobiology*" to enhance the *Multidisciplinary Computational Science* among astrophysics, planetary science, and biology.

These projects are presented in the following sections.

[Education & Public Relations]

Educate and produce the next generation of scientists who push forward new multidisciplinary computational science from global viewpoints.

– Dual degree (double majors) program,
– Campus-wide courses on "computational science" for graduate students,
– HPC seminar series
– Workshops and symposium

Computational Science Dual Degree (double major) Program is to enable a graduate student in a doctoral program to simultaneously belong to a master program of a different Graduate School, and receive both a doctoral degree in science and a master degree in computer science, or vice versa, upon graduation. The program is intended to educate researchers who can push forward new multidisciplinary computational science from global viewpoints. We designed curriculum and courses for advanced computational science, and started this program in 2008. The expected combinations of majors are Physics in Doctor Course and Computer sciences in Master course.

Campus-wide courses on "computational sciences" for graduate students are other educational activities for computational science. Currently, we propose two courses:

・ Computational Science Literacy

・ High Performance Parallel Computing Technology for Computational Sciences (overlapped with HPC Seminar)

The lecture is given by the Faculty members of CCS, and it is accredited as "unit" in graduate courses. It started on summer in 2008. HPC Seminar presents knowledge, methodology and techniques for programming modern high performance computer systems, including recent microprocessors, and its performance turning, parallel programming. This is inter-university activity open for researchers outside the CCS, even including researchers in companies. It is held during 2 or 3 days in summer season. It is also broadcasted via internet. We will organize workshops and symposium. We have a plan of "***Long-term Computational Science Workshop***" where an advanced subject encompassing multiple disciplines of science and computer science is to be chosen, and participants who stay from a few weeks to a few months are encouraged to carry out multidisciplinary research collaborations. In addition to this, we have a plan to have an international symposium once in every year, which turn to a part of symposia series which are been held in various areas of computational science every year in Tsukuba.

[Collaborations with Other Institutes]

Promote alliance and collaboration, and establish international/national networks of researches on computational science

− Alliance with "supercomputer" centers of universities, the next-generation supercomputer center of RIKEN, and research Laboratories in Tsukuba

− Promotion of international collaborations by "Computational Science Researchers Invitation Program", and Support of virtual organization using Grid technologies.

Our university is located in Tsukuba Science City which has many government research organizations. We already have connection to the major research institutions in Tsukuba (High Energy Accelerator Research Organization (KEK), Advanced Institute for Science and Technology (AIST), National Institute for Materials Science (NIMS), Meteorological Research Institute (MRI), and National Institute for Environmental Studies (NIES)). The strategy should be to strengthen research connections among the institutions in Tsukuba on the research of computational science.

2 Future Projects

2.1 COMA Project

2.1.1 Motivation and Objective

As described in Section 5.1 in this report, CCS is focusing on the accelerated computing technologies for the future computational platforms, and has been introducing GPU cluster HA-PACS or researching extremely SIMD architecture in the Feasibility Study toward exascale computing. Looking for other possibility on accelerated computing devices, we also focus on the many-core architecture. At present time, the most powerful and practical solution on many-core accelerator is Intel Xeon Phi series processor, which provides tens of simple CPU cores in a chip to realize “throughput core” collection to accelerate the computation in HPC problems while traditional general purpose CPUs such as Intel Xeon have been seeking the highest performance on each core (so called “latency core”). The performance/cost effectiveness on the peak performance of Intel Xeon Phi is almost comparable with that of NVIDIA’s latest GPU of Kepler generation. Therefore, we also have to examine the performance of many-core processor as a component of the large scale parallel processing system.

Based on this concept, CCS is going to introduce a new PC cluster with many-core processors as the acceleration engine in the end of March 2014. The system is named “COMA” (Cluster Of Many-core Architecture processors). As the high peak performance systems in CCS, compared with general purpose supercomputers such as T2K-Tsukuba, COMA is introduced as the 9th generation of PACS/PAX series system, and it is also coded as “PACS-IX”. (From this machine, we will change our tradition to give different names with “PACS/PAX” suffix/prefix such as CP-PACS, PACS-CS or HA-PACS, and just use the name of “PACS” with generation suffix.)

Another reason to introduce many-core architecture technology is for the next plan on our general purpose supercomputer. As shown in Section 5.5 in this report, we have launched a new organization JCAHPC under collaboration with University of Tokyo to share the national top-level supercomputer facility. Currently, we consider the general purpose stand-alone CPU (not as accelerator) with many-core architecture is the strongest candidate for the component of this system. It is planned that such a stand-alone many-core processor appears on the market on 2015, and that time frame fits to our requirement on the machine at JCAHPC. In order to port current computational scientific codes in CCS smoothly to the many-core architecture, we need a leading time to examine and port these codes to many-core system. COMA will be used for this purpose.

2.1.2 System Overview

The overall specification of COMA (PACS-IX) is shown in the table below.

Computation node	CPU	Intel E5-2670v2 (IvyBridge-EP) 2.5GHz x2
	# of cores	20 (10 cores / CPU)
	MIC	Intel Xeon Phi 7110P 61 core x2
	Main memory	64 GB (DDR3 1866MHz x 8 channel, 119.4GB/s)
	MIC memory	16 GB (8GB/MIC, 352GB/sMIC)
	Peak performance	400 GFLOPS (CPU) + 2147 GFLOPS (MIC)
	Network HCA	InfiniBand FDR
	Peak network b/w	7 GB/s
Number of nodes		393
Interconnection configuration		Fat-Tree with full bisection b/w
Peak performance		1.001 PFLOPS (CPU: 157 TFLOPS, MIC:844 TFLOPS)
Network bisection b/w		2.75 TB/s
Shared file system		Lustre file system
File system capacity		1.5 PB (user space)

2.1.3 Operation

In the end of March 2014, COMA will be replaced with T2K-Tsukuba which will finish its operation in the end of February 2014. As described above, the main purpose of COMA is to provide a test-bed for many-core accelerating technology for wide variety of applications in CCS. However, CCS is also responsible to provide massively parallel general purpose systems continuously to nation wide computational science researchers on the Collaborative Multidisciplinary Program and HPCI Program by MEXT. To balance these purposes, we are planning to introduce several types of system partitioning and job control.

There are three types of system utilization from user's viewpoint.

(1) General Purpose Partition
(2) Accelerator Partition
(3) Mixed Partition

The General Purpose Partition is dedicated to the users who want to use the general purpose CPU cores only. On the other hand, the users of Accelerator Partition can use many-core accelerators (Intel Xeon Phi card) to port, evaluate and run their applications to fit to this new technology. Finally, in the Mixed Partition, the user can utilize entire computational resources on the node including Intel Xeon CPUs and Intel Xeon Phi cards for the aggressive challenge to utilize all the resources in a hybrid/heterogeneous computing manner. In each partition, the users can reserve a set of multiple nodes to run their parallel codes based on MPI.

To realize such an operation, we will allow a job-mixing on the computation nodes to support General Purpose Partition and Accelerator Partition simultaneously. Since each computation node consists of 20 of CPU cores by Xeon and two of Xeon Phi cards, we provide 16 cores of Xeon CPU for General Purpose Partition, and 4 cores of Xeon CPU and two cards of Xeon Phi for Accelerator Partition. It is logically possible to mixture two jobs in these partitions with certain computational resoruce assignment such as memory capacity under control of SLURM batch scheduler. And then, there is an individual set of computation nodes for Mixed Partition. It is quite simple because the nodes belonging to this partition are just assigned to a job which can occupy all the resources on the assigned nodes.

For the operation in FY2014, HPCI users can only use General Purpose Partition while the Collaborative Multidisciplinary Program users can access three of them for aggressive program development and high performance execution.

2.2 JCAHPC Project: *Acquisition of the next generation large-scale many-core system*

This JCAHPC project is to acquire a large-scale many-core supercomputer system for the next-generation high performance computing platform under co-operation with the University of Tokyo Information Technology Center. The University of Tsukuba Center for Computational Sciences (CCS) and the University of Tokyo Information Technology Center jointly established the "Joint Center for Advanced High Performance Computing (JCAHPC)" in order to design, operate and manage a next-generation supercomputer system using many-core processors.
JCAHPC has been organized to install and run a supercomputer system, designed (for the most part) by the faculties of both organizations, at the Information Technology Center (ITC) at the Kashiwa Campus of the University of Tokyo. Operating the Center through cooperation and collaboration will promote advanced computational sciences, and contribute to the promotion of the advanced computational science and technology in Japan.

To run JCAHPC, Mitsuhisa Sato, Professor of Center for Computational Sciences, University of Tsukuba is appointed to the director, and Yutaka Ishikawa, Professor, of Information Technology Center, University of Tokyo, is appointed to Deputy Center Director.

2.2.1 Background and Motivation

The advancement of computational sciences through cutting-edge high performance computing (HPC) platforms is vital to maintaining a world-leading position in science and technology in the 21st century. In Japan, although the K computer, operated at the RIKEN Advanced Institute for Computational Science (AICS), set a new world record in terms of speed since entering shared use in 2012, we claim that further cooperation between the University supercomputer centers running their own HPC platform and the AICS that operates the K computer would be necessary to keep potential of computing by continuous development of world-class HPC facilities in Japan.
Based on these background of Japanese HPC community, the centers at both universities, which have been running large-scale supercomputers, joined to establish "JCAHPC," and tasked the organization with conducting joint design and development, and joint operation and administrative management of the next-generation supercomputers, as well as to promote advanced computational science by facilitating research in various disciplines.

2.2.2 Mission and Plan

The objective of the JCAHPC mission is to design and develop of a large-scale HPC system worthy of becoming the hub of Japan's computational sciences, and to design an advanced system that exploits many-core technology, which is expected to be the key to the coming HPC systems. Furthermore, such research and development will proceed in establishing alliances with other organizations for the operating system, programming languages, numerical computation libraries, etc., that comprise the technologies at the heart of the system software, as shown in Figure 1. Based on this design and development, the institutions will jointly acquire and run the supercomputer.

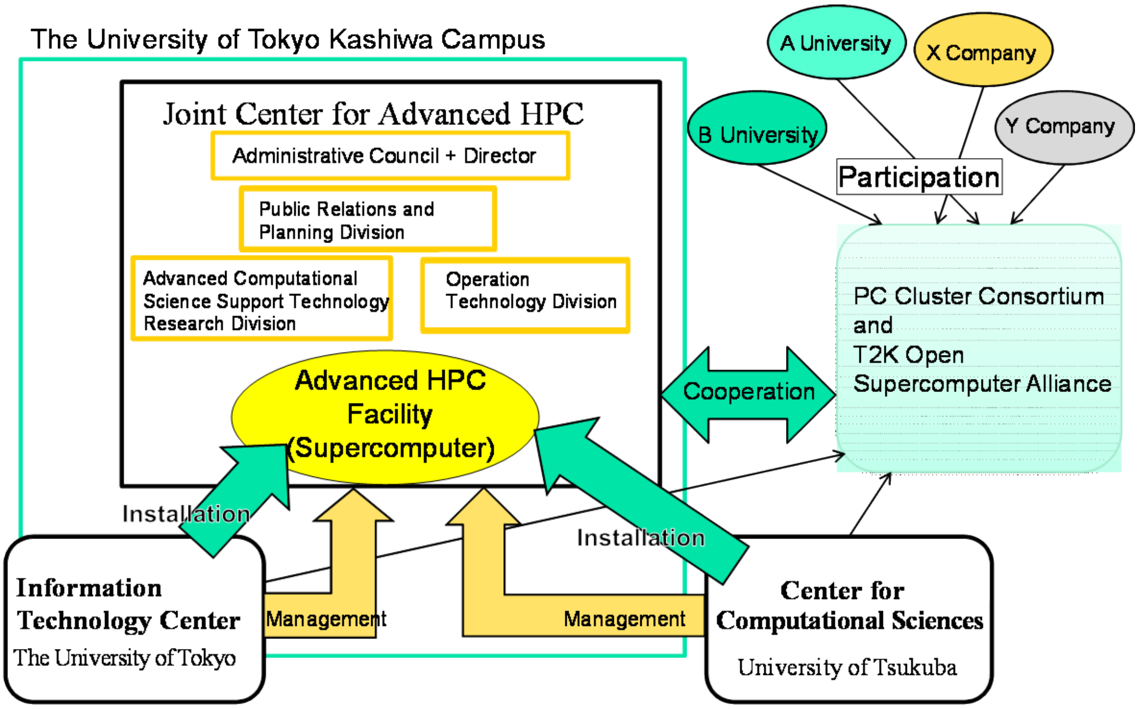

Figure 1. Organization and Structure of JCAHPC

After the system is operational, both institutions will distribute the system proportionally based on computation volume, operate their portions separately, and offer services to each user based on the programming used. This arrangement not only reduces administrative costs and the like, but also enables computing at a larger-scale than the case where each institution independently owns a supercomputer system.
This effort represents the first attempt to create such a facility in Japan, as well as the first attempt in Japan to jointly operate and administer a supercomputer.

This system is scheduled to be installed for operation and management in 2015. We expect the system to be installed will have more than 20PF in theoretical peak performance. Figure 2 shows the overall schedule of acquisition and operation of our system.

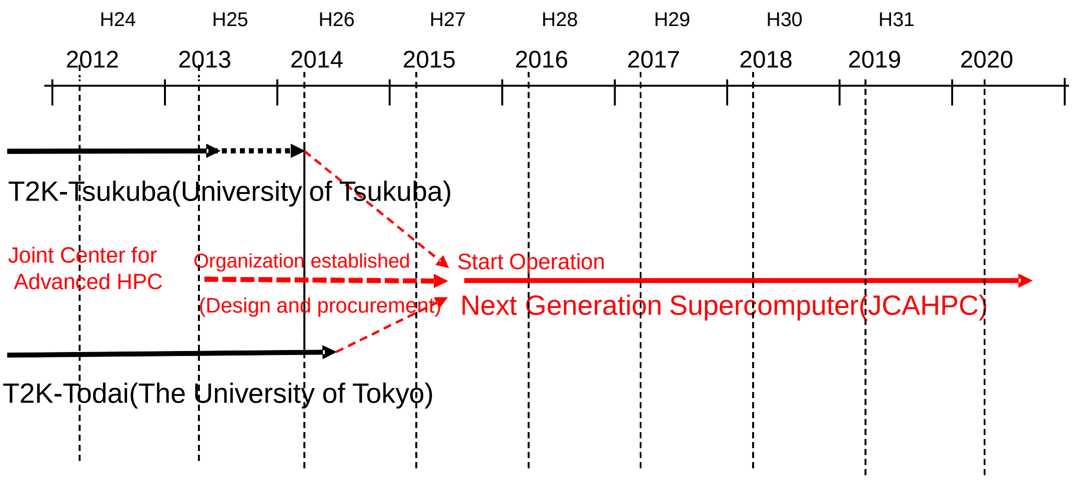

Figure 2. Schedule of JCAHPC

2.3 Toward Exa-scale Computing: *"Feasibility Study on Future HPC Infrastructure"*

Europe, the US, Japan and China are racing to develop the next generation of supercomputer – exascale machines - capable of a million trillion calculations a second by around 2020.
In 2012, MEXT initiated the "Feasibility Study on Future HPC Infrastructure" projects to study the architecture of post-petascale systems following the K computer for Japanese exascale system. As four projects have been accepted including us, together with Hitachi Ltd. and several researches in universities, we have been conducting the project "Study on exascale heterogeneous systems with accelerators" to exploit accelerated computing for future exascale systems.

To realize exascale systems, there are many challenges and issues including the limitation of power consumption and architectures to realize strong-scaling. We claim that one of promising approaches is an accelerated computing which uses specialized hardware, such as GPU, to speed up certain computational tasks, offering users energy efficiency, high performance for strong scaling. In this study, we are interested in the following topics, but not limited to:

- Architecture of accelerators, core and memory architecture
- Direct connection between accelerators in a group
- Power estimation and evaluation
- Programming model and computational science applications
- Requirement for general-purpose host system and system overall architecture

Figure 3 shows a straw man architecture of our study. We are designing the "extreme SIMD" architecture called PACS-G, which consists of huge number of PEs working with PE local memory in a SIMD manner. We also propose a dedicated network for direct connection between accelerators, which have been already studied in TCA (Tightly Coupled Accelerator) technology of HA-PACS project.

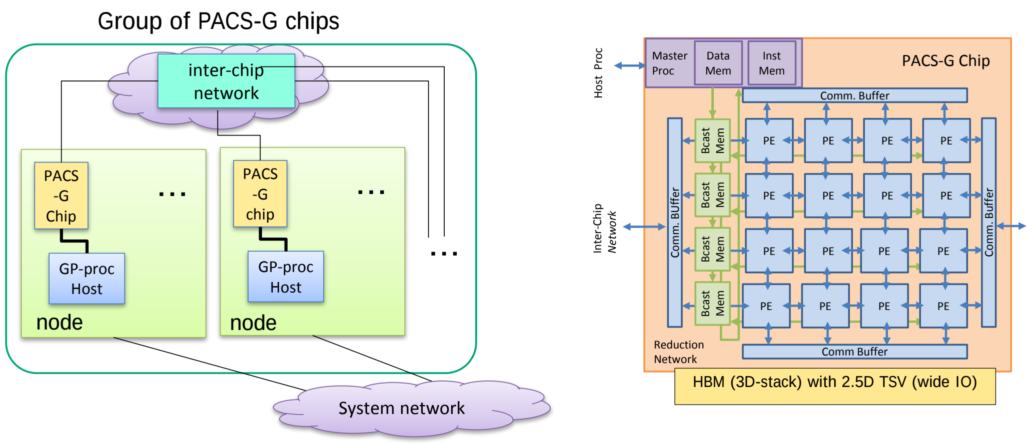

Figure 3. PACS-G strawman architecture: system and PACS-G processor

In 2014, the Japanese government is about to launch the national project ("Exascale coming Project") to develop a exascale computer system. RIKEN AICS, the organization which currently runs the K computer, will undertake the project to design and develop the exascale system. For the development, the output and results from "Feasibility Study on Future HPC Infrastructure" projects are expected to be used. We hope CCS will contribute not only to the designing of the system by the output of our exascale accelerated computing study, but also to the evaluation and performance improvement by development of real target application codes for the exascale system.

2.4 Joint Institute for Computational Fundamental Science (JICFuS)

2.4.1 HPCI Plan and Strategic Program Field 5

The innovative High Performance Computing Infrastructure (HPCI) plan, which was established with the "K" supercomputer at the core, was created to actualize an innovative computational environment capable of meeting diverse users needs, and aimed at promoting the exploitation of HPCI. As major policy objectives, building an organization for promoting computational sciences in major fields (HPCI Strategic Program), and producing revolutionary results through the exploitation of HPCI are cited.

In the HPCI Strategic Program, five potential fields have been identified as strategic fields that not only require K supercomputer resources, but can also be expected to yield significant social and scholarly breakthroughs. "Field 5: The origin of matter and the Universe" is one of these. This field deals with fundamental physics, primarily concerning elementary particles, the atomic nucleus, and astrophysics. The institution (strategic institution) that leads Field 5 research and development is the Joint Institute for Computational Fundamental Science (JICFuS), which is a joint research organization combining the University of Tsukuba's Center for Computational Sciences (CCS), the High Energy Accelerator Research Organization, and the National Astronomical Observatory.

2.4.2 Strategic Objective of Field 5

The history of the Universe is believed to have begun with the ultra-high-temperature, ultra high-density state called the Big Bang, which occurred 13.7 billion years ago. Baryons such as protons and neutrons were made as the bound states of quarks and gluons with the temperature drop following the event. Subsequently, protons and neutrons bonded, and light atomic nuclei were generated.

However, it is also postulated that unidentified dark matter exists in much larger quantities than baryons in the Universe. Furthermore, it is currently thought that dark matter coalesced under the influence of gravity and created a structure, to which normal baryonic matter was drawn, eventually forming the galaxies and stars of the Universe, which then evolved into its currently observed form. In those galaxies, stars eventually perish due to gravitational collapse and supernova explosion, while new stars are also actively being born. Through this process, heavier atomic nuclei are generated. Through this process, it can be seen that the history of the generation of matter has a close relationship to the history of the structural formation of the Universe.

The strategic objective of Field 5 is to understand, in a unified fashion, the context of the history of the Universe beginning with the Big Bang. This includes the origin and structure of matter and the Universe from elementary particles to elemental synthesis, to stars and galaxy formation, by scientific computational methods that connect the multiple hierarchical steps. Four research and development topics have been set toward the objective.

(1) Determination of interactions between baryons at the physical points by lattice QCD

(2) Nucleus property elucidation by large-scale quantum many-body computing and applications

(3) Elucidation of a supernova explosion and the birth process of black holes

(4) First-generation celestial body formation from dark matter density fluctuations

Research of these topics will proceed using the “K” supercomputer, which has a peak performance of 10.5 Pflops (calculations enabled at about 10 quadrillion times per second). Results have been yielded steadily, and the dark matter simulation performed on the “K” supercomputer won the Gordon Bell Prize, the most prestigious of its type in the field of computers, in November 2012.

In parallel with this research, the efficient use of computational resources in the field of computational fundamental science, personnel development, creation of a research network, and fostering cooperation across different fields have been pursued with the aim building a technology promotion organization for computational science within the field. As the core of these strategic institutions, the project office promotes the accomplishment of research and development topics and structuring of the technology promotion organization for computational science.

2.5 Organization for Collaborative Research on Computational Astrobiology (CAB)

In the last decade, the field of “Astrobiology” has attracted a significant deal of attention owing to advanced observations of extrasolar planets as well as interstellar molecules. This organization aims at the creation of a *computational astrobiology* by exploring key processes related to the origin of life in the universe through *ab initio* calculations based on collaboration among the Computational Astrophysics, Computational Biology, Computational Planetary Science, and Computer Science fields.

These research efforts are targeted on the potentials of interstellar molecular biology, planetary biology, and the astrophysics of star and planet formation. At present, 54 researchers from 22 institutes are participating in the CAB, which was formed at the initiative of the CCS, University of Tsukuba.

Currently, we are promoting two projects, the cosmic origin of amino acid homochirality, and the hydrodynamic and magneto-hydrodynamic turbulence.