CCS Report: PART I

Overview of Center for Computational Sciences

Summary of Activities 2004 – 2007

October 2007

Center for Computational Sciences

University of Tsukuba

Table of Contents

1. Introduction

This report summarizes the main events and activities of the Center for Computational Sciences, University of Tsukuba, since its foundation in April 2004 to the present. The report has been prepared for a review of the Center, scheduled from 30 October to 1 November of 2007.

The purpose of the review is to receive an outside examination of the research activities and their outcomes at the Center in view of the founding objectives, and to incorporate the recommendations from the review into future developments of the Center.

Since details of the research results are prepared as a separate report, this report focuses on an overview, which includes a brief overview and the mission of the Center (Section 2), a chronology (Section 3), organizational aspects (Section 4), and a brief summary of the research activities and collaborations of the Center (Section 5).

More details of the research activities and results of each division and group are described in CCS Report: PART II. The future plan and vision are described in CCS Report: PART III.

2. Mission and Overview of the Center for Computational Sciences

The mission of the Center of Computational Sciences is to promote scientific discovery by computational science through the application of advanced computing technologies, and to support research of computational science in Japanese universities and institutes by operating leading-edge computing systems. The Center for Computational Sciences was founded in April 2004 as an inter-university research facility for computational science by restructuring and expanding the Center for Computational Physics (April 1992-March 2004). The Center aims to carry out research on critical issues in fundamental science, material science, life science and environmental science by performing large-scale simulations and large-scale data analyses. To realize this goal, the Center conducts research and development of high-performance computing systems and networks, and advanced studies in computer and information science. Because the Center is an inter-university facility, it thus functions as an international as well as a national center for computational sciences.

High-performance computing systems and a high-speed network infrastructure are essential tools for carrying out successful computational science research. To develop computational science, it is vital to establish an organization that combines the forefront of science research with that of computer science and information science. The Center for Computational Sciences has been striving to carry out such collaborative research. For example, by collaboration between physicists and computer scientists, we performed R&D of a massively parallel computer CP-PACS (ranked as the No. 1 system in the Top 500 List of November 1996) by collaboration between physicists and computer scientists. Large-scale computations were carried out on CP-PACS resulting in significant progress in particle physics and astrophysics. In July 2006, a new massively parallel cluster PACS-CS started operation. This machine was built using special funds for education and research from the Japanese Government. We aim to develop computational sciences for a wide range of scientific disciplines, from fundamental science to material, life and global environmental sciences by making the best use of PACS-CS.

3. Chronology of CCS

3.1 Brief history prior to 2004

The chronology of the Center for Computational Sciences goes back to 1992, when the Center for Computational Physics (CCP) was founded at the University of Tsukuba. The purpose of the CCP was (i) to carry out research and development of parallel computers suitable for large-scale computational physics calculations, and (ii) to carry out research with the developed system in the area of particle physics, astrophysics, and condensed matter physics. In particular, CCP was to serve as the base for the project entitled "Research of Field Physics with Dedicated Parallel Computers" (FY1992-FY1996) funded by the Ministry of Education of the Japanese Government. This project developed a massively parallel system CP-PACS (Computational Physics with Parallel Array Computer System). This system achieved 368.2 Gflops for the Linpack Benchmark in September 1996, and was ranked as the No. 1 system in the November 1996 Top 500 List.

CCP had a faculty of 10 researchers in four divisions: Computational Particle Physics, Computational Astrophysics, Computational Condensed Matter Physics and Parallel Computer Engineering. The simultaneous existence of physics and computer science faculties within CCP, and actual close collaborations between them for the development of parallel computer systems and their usage, marked the unique feature of the Center. In fact, this interdisciplinary approach goes back to the early 1980s, when research and development of parallel computer systems started at University of Tsukuba under Professor Tsutomu Hoshino.

From 1996 to 2005, CP-PACS served as the main computing facility of CCP. In the late 1990s, large-scale calculations using CP-PACS produced a number of well-known results. The major scientific achievements are as follows:

1. Calculation of the quenched light hadron spectrum in lattice quantum chromodynamics (QCD). (S. Aoki et al., Physical Review Letters 84 (2000) 238)
2. First systematic lattice QCD calculation including light dynamical up and down quarks, showing that up and down quark masses are much lighter than previously thought. (S. Aoki et al., Physical Review Letters 85 (2000) 4674)
3. First astrophysical radiation hydrodynamical calculation of the reionization of the Universe including interaction of radiation and matter. (Monthly Notice of the Royal Astronomical Society 321 (2001) 593)
4. First many-body quantum mechanical calculation of the phases of solid hydrogen. (H. Kitamura et al., Nature 404 (2000) 259)

3.2 Reorganization in 2004

In April 2004 the Japanese national university system, of which University of Tsukuba is a member, underwent a major transition. While previously the national universities were part of the Japanese government and were strictly controlled by the Ministry of Education, Science, Culture and Sports, their legal status was changed to that of independent institutes. While the budget still came from the government, each university was granted much wider freedom of action on its own. The reason behind this change was pressure toward reformation of the Japanese government, including not only a reduction of employees and government spending, but also reformation of the university system to be more effective in the era of globalization and worldwide competition.

Preparations for the transition started in FY2002 at all national universities across Japan. The Center for Computational Physics considered the transition as a welcome opportunity to reexamine its future plan. While the Center for Computational Physics, with its small faculty of a dozen members, had functioned well in pursuing research projects within a limited area of fundamental physics, it was strongly felt that the interdisciplinary approach toward computational physics pursued at the Center could be extended to wider areas of science, and that the Center had a potential to significantly expand its activity by doing so.

Discussions with the Executive Office of the University on a possible reorganization and expansion started in the early summer of 2002. The Executive Office basically welcomed the Center's proposal, and provided strong support during negotiations with the Ministry of Education, Science, Culture and Sports to secure governmental approval from the winter of 2002 to spring of 2003.

The Center for Computational Physics was formally reorganized as the Center for Computational Sciences on 1 April 2004. The faculty expanded threefold from 11 to 31 academic members, and the following reorganization and expansion of divisions were accomplished:

- Division of Particle Physics and Division of Astrophysics were combined into a single division with an increased faculty of 7 members.
- Division of Condensed Matter Physics and Division of Biophysics were combined and significantly expanded to 10 faculty members in the Division of Materials and Life Sciences.
- A new Division of Global Environment and Biological Sciences was introduced with 3 faculty members.
- Division of Parallel Computer Science was expanded from 3 to 5 faculty members, and was renamed Division of High Performance Computing Systems.
- A new Division of Computational Informatics with 6 faculty members was set up to carry out research on computational intelligence and media.

Of the 20 members added to the original 11 for the Center for Computational Sciences, 14 were faculty members who were actively working in various areas of computational science at graduate schools of the university, while the remaining 6 were approved by the university and filled by new recruitments in 2004-2005.

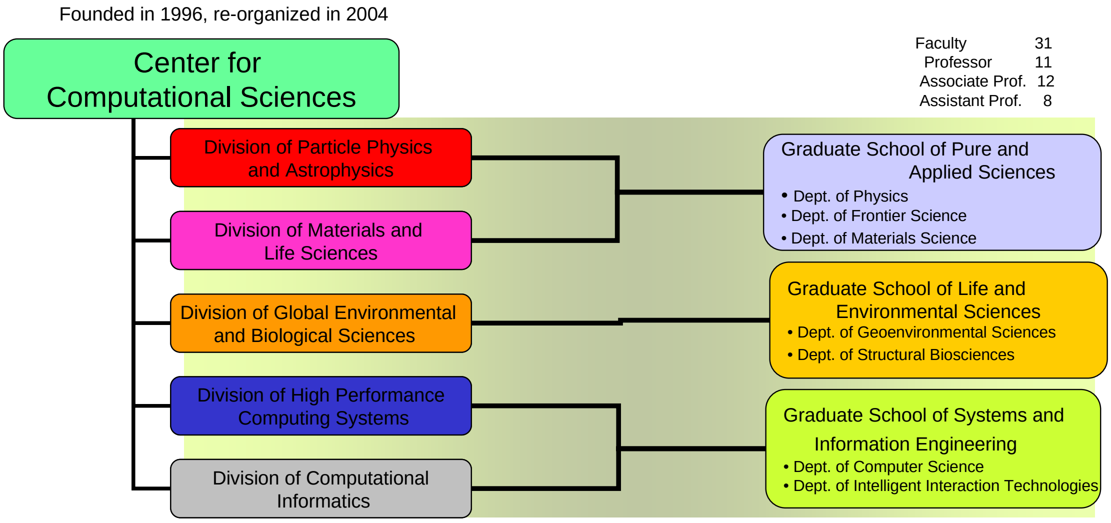


Figure 3.1: Overview of CCS Organization

3.3 The PACS-CS Project

Since advances in high-performance computing systems are rapid, planning toward developing the successor to the CP-PACS system was started immediately after its completion in 1996. One effort was the “Development of Next-Generation Massively Parallel Computers" project of “Research for the Future Program" (FY1997-FY2001) funded by the Japan Society for Promotion of Sciences. This project led to two important results: (1) the introduction of SCIMA, an on-chip memory architecture for controlling the memory wall problem in large-scale science and engineering calculations, and (2) the first realization of a heterogeneous multi-computer system to deal with calculations which involve both local as well as long-range forces necessitating completely different calculation schemes. This result later developed into the FIRST project.

By 2004, when the Center for Computational Sciences was founded, the CP-PACS system was in its eighth year of operation. The needs to significantly enhance the computational facility of the Center were dire both due to the aging of the CP-PACS and the expanded faculty and research areas of the Center.

The PACS-CS project was an attempt to meet these needs. An intensive discussion by a small group to formulate a basic architecture took place in the summer of 2003. In view of the rapid progress of commodity technologies, a cluster approach based on a commodity CPU and network was considered suitable for quick development of the system necessary to meet the computational requirements of the Center’s researchers. At the same time, the system design had to achieve a good balance of floating point performance, memory throughput and network throughput in order to secure a high overall sustained performance for large-scale scientific calculations.

The basic design was drawn at the end of the summer of 2003. An initial presentation of the project to the government was made in the winter of 2004. A formal funding request from the university was made in the summer of 2004, and the government decision process ran through the fall of 2004, and included a review by the Committee for Science and Technology Planning (CSTP). CSTP is the highest office of the government for planning science and technologies. The Committee recommended the funding of the project to start from FY2005, and a formal announcement from the government was made in December of 2004.

The entire process was not trivial, since 2004 was the first year after the change of the national university system; so, the entire funding system for research was cast into a new form, and our proposal had to go through this new system.

Formally, the project has been funded by the ``Special Fund for Education and Research for National Universities" for the period of FY2005–FY2007. The official title of the project is “Discovery, Synthesis and Emergence of Novel Knowledge through Computational Sciences." The goal of the project is to carry out leading-edge research in computational sciences through a close collaboration of researchers of various science disciplines and computer science. In particular, the project plans to foster an interdisciplinary style of research in the area of materials and life sciences, and global environment and biological sciences, which were either strengthened or newly introduced with the reorganization of the Center. As a basic tool to carry out such research, the project proposed to develop a massively parallel cluster system. The system is named Parallel Array Computer System for Computational Sciences, or PACS-CS.

The project formally started in April 2005. A governmental bidding procedure was followed to decide the manufacturer of the system, and Hitachi Ltd. was selected as the main contractor of the system hardware and software in July 2005, and Fujitsu Ltd. was selected to develop special network software in August 2005. The development of PACS-CS was carried out by a close collaboration of the researchers of the Center and the two vendors.

The PACS-CS system consists of 2560 nodes, each carrying a 5.6 Gflops Intel Xeon processor and a 2 GBytes of memory. The nodes are connected by a 3-dimensional hypercrossbar network, each link consisting of a dual Gigabit Ethernet, with a total of 750 MByte/sec bandwidth for each node. The Linpack Benchmark achieved 10.35 Tflops, ranking 34th on the June 2006 Top 500 List. The full system started operation on 1 July 2006, and a formal commissioning was made on 3 September 2007. The system is now fully saturated and running a variety of applications.

1992 April	Founding of Center for Computational Physics (CCP) (10 year term / 10 faculty members and 3 visiting faculties) development of massively parallel computer CP-PACS begins
1996 October	Massively parallel computer CP-PACS completed
November	Ranked as No. 1 in the Top 500 World Supercomputer List
1997 April	JSPS research for the Future Project “Computational Science” 「Development of Next-Generation Massively Parallel Computers」 begins
2002 April	The Second 10 year term of Center for Computational Physics begins (11 faculty members and 3 visiting faculties)
2003 July-Dec.	Planning on reorganization and expansion of CCP
2004 April	Founding of Center for Computational Sciences (CCS) (31 faculty members and 3 visiting faculties)
2005 April	Development of Massively Parallel Cluster PACS-CS in the project 「Discovery, Synthesis and Emergence of Novel Knowledge through Computational Sciences」 begins （3years, FY2005～FY2007)

Figure 3.2: Brief chronology of CCS

3.4 Building

Another serious problem which arose from the expansion of the Center was the shortage of office space. A budget request for an expansion of the main research building was submitted to the government in the summer of 2005. The request was approved in the supplementary budget of the government for FY2005. The research building, after a complete remodeling, was completed in March 2007. The new building provides floor space of 2356 m^2, which is more than double the space of 1090 m^2 of the old building.

Figure 3.3: Photo of CCS building

4. Organization and Administration

4.1 Organization

The organization of the Center is shown in Fig. 4.1. The Center consists of five research divisions, a Division for Inter-university Activity and the Administrative Office under the Director.

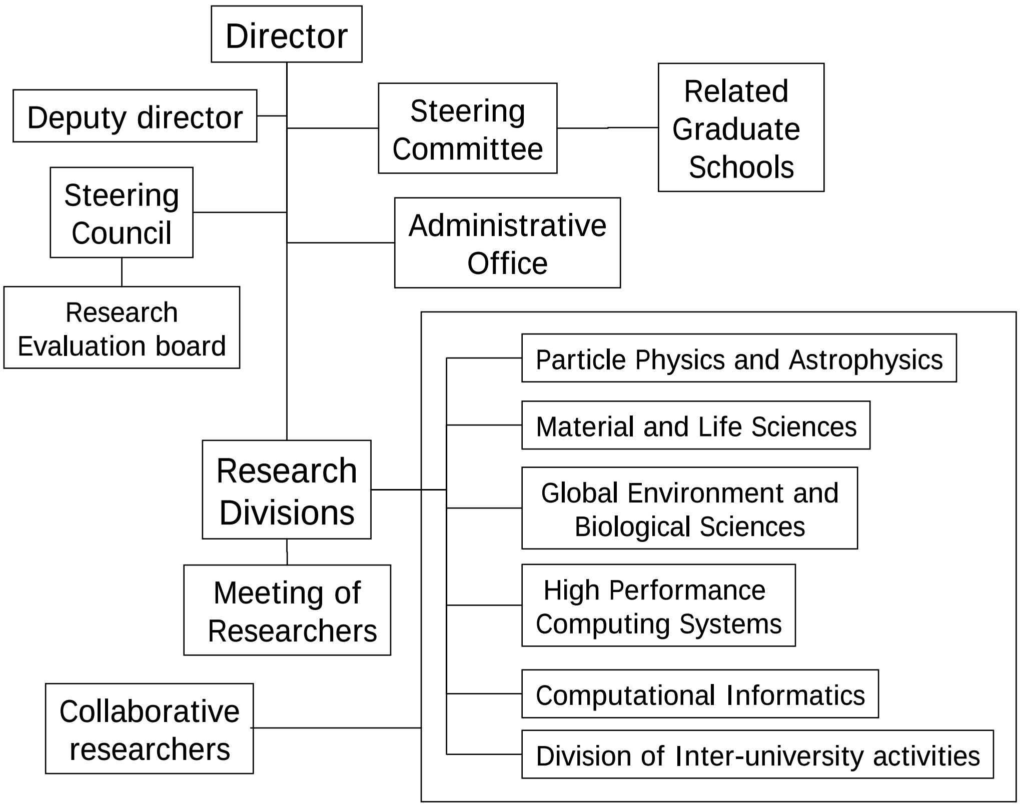


Figure 4.1: Organization of the Center for Computational Sciences

The Steering Committee consists of full professors of the Center and representatives from the three graduate schools to which the faculty members of the Center belong (these are the Graduate School of Pure and Applied Sciences, Systems and Information Engineering, and Global environment and Life Sciences). This committee supervises the day-to-day running of the Center.

The Steering Council consists of outside experts in various areas of computational sciences appointed by the Director of the University, the Director and the division heads of the Center. It supervises and coordinates the activities of the Center from a wider perspective of computational sciences.

4.2 Director

The Director of the Center has to hold the rank of professor of University of Tsukuba. The Director is appointed by the President of University of Tsukuba upon recommendation from the previous Director; in practice, a candidate is selected by a ballot of the Center faculty. The appointment is for two years and can be repeated up to six years.

The past directors are Prof. Yoichi Iwasaki (physics) from April 1992 to March 1998 and Prof. Akira Ukawa (physics) from April 1998 to March 2007. The current director since April 2007 is Prof. Mitsuhisa Sato (computer science).

4.3 Faculty of the Center

At University of Tsukuba, all faculty members belong to one of seven graduate schools. The faculty members of the Center ``belong" to a graduate school and ``work" at the Center. The affiliation of a faculty member is written as ``Graduate School (Center for Computational Sciences)".

The faculty members as of 1 October 2007 are listed in Appendix A.

4.4 Running of the Center

The research activities of the Center are coordinated by the Director through the following three meetings, and support is provided by the Administrative Office. The organization and the roles of the three meetings are as follows.

- Meeting of Researchers

  This meeting consists of the entire Center faculty and the Associated Research Fellows, who are collaborators of other universities and research institutes. This meeting is chaired by the Director of the Center and is held every month.

  At the meeting, all aspects of research are discussed, such as the status of ongoing projects, procurement of equipment and operation of the Center computer system.

- Steering Committee

  The Director of the Center chairs the committee, which holds meetings every month.

  The committee discusses important issues for running the Center, which include matters related to the organization of the Center, selection of faculty members, budget planning and confirmation of expenditures.

- Steering Council

  The council is held once a year, and is chaired by the Director of the Center.

  The council hears annual reports of the Center research activities, and discusses the direction of research of the Center and matters related to inter-university use of the Center facility. Under the Steering Council, a Research Evaluation Board is organized to evaluate the research activities annually.

4.5 Faculty Selection

The Center appoints new faculty members when openings become available among the Center faculty positions. The selection procedure is as follows.

- Choice of field
  When an opening of a position becomes available, the field of the position is chosen by the Steering Committee based on considerations of the research purposes of the Center and the balance among research fields.

- Selection of candidate
  Once the field is chosen, the actual selection process is handled by the Faculty Selection Committee under the Steering Committee.
  The opening is publicly announced to invite applications. Candidates are initially screened by a Search Committee made of five professors appointed by the Faculty Selection Committee. This screening includes reading the candidates' main papers and interviews. When the screening at the subcommittee converges toward a candidate, the conclusion is reported to the Faculty Selection Committee. If the Faculty Selection Committee approves the candidate, the result is reported both to the Steering Committee and the University Personnel Committee for formal approval.

5. Overview of Research Activities from 2004 to 2007

5.1 Overview

The reorganization of the Center in 2004 represented a major change in the way projects are organized and executed. While particle physics and astrophysics already had a long history of collaborating with computer science, other fields new to the Center, such as materials and life sciences and Global environment and biological sciences, had no such interaction. Thus, a common target that could be shared by these new areas of science and computer science had to be formulated and the two groups had to learn to work together.

In this regard, the PACS-CS project (2005–2007) occupied the central place in the research activities of the Center. The project aimed not only on developing a new cluster computer for computational sciences, but it also tried to foster interdisciplinary collaborations. The project involved all Center faculty members.

The research groups of the Center also pursued a number of large-scale projects of their own. These projects attempted to take advantage of the coexistence of science and computer science faculties to advance research in the respective science fields. The science projects that fall into this category are as follows:

- The FIRST project (2004–2007)
  This project developed a large-scale, heterogeneous multi-computer system, which integrates GRAPE-6, boards for gravity calculations into the node of a commodity cluster. Using this system, the project attempted to clarify the physics of formation of the first generation stars in the universe after the Big Bang.

- “Development of Nano-architecture through Computational Quantum Science” (2005–2009)
  This is a project in materials and life sciences which attempts to advance algorithmic and computational study of the possible principles which determine the relation between functions and spatial structure of nano- and bio-molecules. This project is supported by the JST-CREST program.

The Center has been involved in the development of peta-scale computing. There are two specific projects in this category:

- “Development of Element Technologies for the Next-generation Supercomputers” (2005–2007)
  With Hitachi Ltd., the project carries out research on possible CPU architecture for peta-scale systems. The Center is attempting to further develop the on-chip memory architecture along the line of SCIMA, and examine in more detail the low-power aspect of SCIMA as compared to vector architecture.

- “Development of the Next-generation Supercomputer” (2006–2012)

This is a national project to develop a next-generation supercomputer reaching 10 petaflops. RIKEN (Research Institute for Science and Chemistry) has been selected for executing the project. In September 2006, RIKEN and University of Tsukuba signed a collaboration agreement on the next-generation supercomputer project, and a group of computer scientists of the Center have been involved with the project as visiting fellows under this agreement.

In the following, we summarize the main results obtained up to now within these projects. We also summarize research activities carried out as interdisciplinary collaborations at the Center.

5.2 PACS-CS Project

The official title of this project is "Discovery, Synthesis and Emergence of Novel Knowledge through Computational Sciences." It is funded by the "Special Fund for Education and Research for National Universities" by the Ministry of Education, Culture, Sports, Science and Technology (MEXT) over three years from FY 2005 to 2007. The total amount is 2.3 billion Yen.

The project aims to advance the frontier of computational science through active interdisciplinary collaboration between various areas of science and computer science. The main component of the project is the research and development of the PACS-CS computer (Parallel Array Computer System for Computational Sciences) with which computations on various large-scale computational science applications in advanced scientific research are to be carried out.

The PACS-CS system is a massively parallel cluster system with 2560 computational nodes. Unlike ordinary HPC cluster systems, the PACS-CS system is designed with a clear view of the target applications.

This year is the last year of the project. The system itself has been completed and is under operation for various important applications working toward scientific results.

5.2.1 Design Concept of the PACS-CS System

In the conceptual design of PACS-CS, we took the view that it is the main computational engine to solve the fundamental issues of science in the areas covered at our Center, and designed the system as a semi-special-purpose system under the following concepts:

- The PACS-CS system is the follow-up system of our previous CP-PACS system (1996–2005), and is to be designed for large-scale applications with massively parallel algorithms.
- The system is based on commodity technology both for CPU and the interconnection network. However, we aim to realize an effective bandwidth for the memory and networking necessary for our important scientific calculations.
- The primary scientific target of the project is real-space density function theory for

material science and lattice QCD for particle physics, and the system is strongly oriented to the fundamental algorithms for these problems.

Based on the above concepts, we decided to design the system based on “real-space computational modeling” (see Fig. 5.1) with the following architectural features, which are different from traditional HPC clusters:

(1) Single processor node architecture
Each computational node is equipped with only a single CPU to utilize the full bandwidth provided by the memory and network on the node. Although this differs from ordinary dual-socket HPC server nodes, we keep the same density by packing two nodes on a 1U board in the system implementation.

(2) Multi-dimensional hyper-crossbar network with trunking of Gigabit Ethernet
For the interconnection network architecture, we selected the three-dimensional hyper-crossbar network (3D-HXB), which allows direct mapping of physical lattices to the array of nodes following real-space computational modeling. We applied a dual-link Gigabit Ethernet for each dimension of the network link, which is controlled by software. This inexpensive solution provides data transfer throughput similar to expensive SAN such as Myrinet and Infiniband.

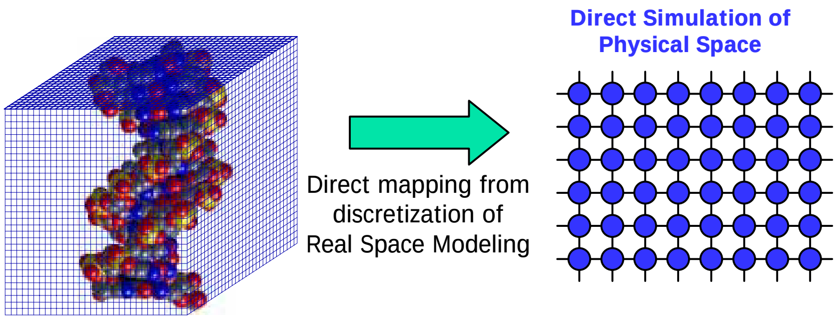


Figure 5.1: Physics simulation by real-space computational modeling in which the physical system is directly mapped onto a node array connected by a network.

5.2.2 Implementation of PACS-CS System

The basic specification of the PACS-CS system is as follows:

Table : Specification of PACS-CS

Number of nodes	2560 (16x16x10)
Peak performance	14.3 TFLOPS
Node construction	Single CPU / node
CPU	Intel LV Xeon EM64T, 2.8 GHz, 1 MB L2 cache
Memory	DDR2 400 MHz, 2 GB/node (5.12 TB/system)
Interconnection	3D-HXB, GbE dual-link trunking/dimension
Link bandwidth	250 MB/s/dim., 750 MB/s/3-D
Local HDD	160 GB/node (RAID-1 mirroring)
System size	59 racks
Power (peak)	545 kW (full UPS support)
Shared File-Server	10 TB RAID-5 + external 100 TB RAID-5
Software	Linux Fedora Core 3, SCore ver.5, Intel Compiler, YAMPI & MPICH, PM-Ethernet/HXB driver

Following the basic design, we developed a new motherboard to implement the single CPU/node configuration and a Gigabit Ethernet trunking to support the 3D-HXB interconnection network with the same system density as the traditional IA-32 based HPC clusters. Figure 5.2 shows the top-view of the motherboard (left) and the two-node implementation in the 1U-sized rack mountable chassis (right) with 12 Gigabit Ethernet ports.

Figure 5.2: PACS-CS motherboard (left) and mount on 1U chassis unit (right)

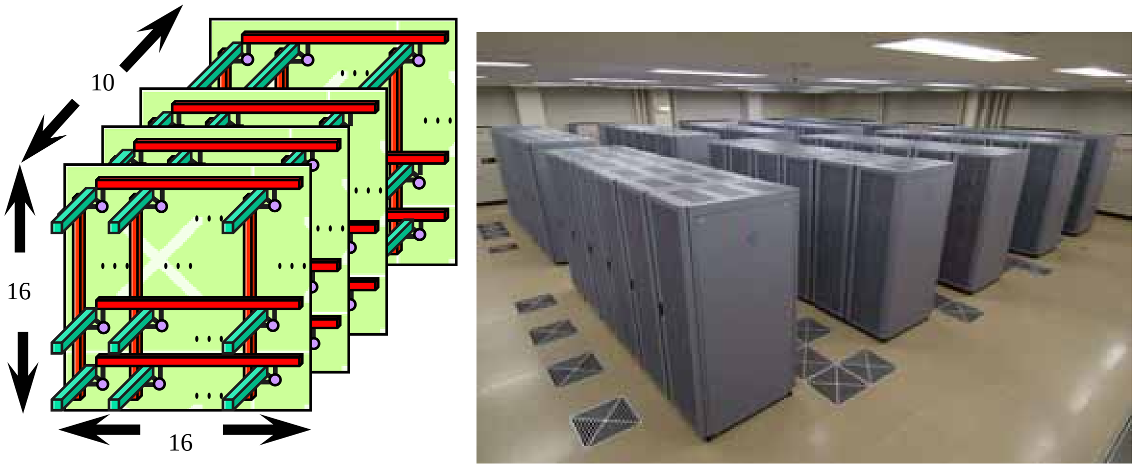


Figure 5.3: 3D-HXB conceptual view (left) and the view of entire system

Figure 5.3 shows the conceptual view of the 3D-HXB network and a photo of the entire PACS-CS system with 59 racks.

The 3D-HXB network can be configured as a 3-D torus of an arbitrary size that is appropriate to map the real-space computational modeling. In actual operation, the entire system is partitioned into multiple rectangular shapes to fit the logical node space required by the problem size, and multiple user jobs are performed simultaneously. The multi-link trunking in each dimension, the multi-dimensional simultaneous data transfer, and the routing between different dimensions are performed by a specially developed network driver for PACS-CS named PM-Ethernet/HXB. The maximum performance of the driver on 3-D simultaneous burst data transfer is up to approximately 80%. On MPI (YAMPI) user-level communication, however, transferring messages over 100 KB is needed to hide the latency caused by the Gigabit Ethernet protocol.

The implementation and installation of the hardware and software of the PACS-CS system, including the first version of the PM-Ethernet/HXB driver, was completed at the end of June 2006, and its operation began in July 2006. The SCore cluster middleware employed for the system has since been updated to include the check-pointing/restarting feature and improvement of PM-Ethernet/HXB performance. The system went into full-specification operation in the summer of 2007.

5.2.3 Operations of the PACS-CS System

We have been operating the PACS-CS system for more than one year, since July 2006. In order to avoid system failure and emergency system shutdown during the ordinary operation time, the system is maintained every month mainly for pre-replacement of memory and hard disk drives based on system logging information. With this effort, the actual failure is a very low rate of 1~3 times per month on average.

While the system can be split into multiple partitions with various sizes, the basic partition is a 256-node size (1.4 TFLOPS) x 10 partitions. Depending on the demand, we configure 512 or 1024 node partitions by combining the basic ones or 64 or 128 node partitions by subdividing them.

Since October 2007, the resource allocation of PACS-CS to users is regulated under the Interdisciplinary Computational Science Promotion Program. The partition size is changed on a weekly or monthly basis to fully incorporate the demand for large-scale simulations required by the program. Such fine-tuning of the system partitioning allows us to support large-scale jobs that are difficult to execute at conventional supercomputer centers in Japan. Because of the fine-tuned scheduling, the system always runs with a 100% workload.

5.2.4 Scientific Research and Results using PACS-CS

Research and results are as follows:

- Lattice QCD in particle physics

  Lattice QCD calculation aims to elucidate the physics of the strong interactions based on fundamental quarks and gluons. This field has been pursued since the early 1980s, and a significant body of results already exists. However, one of the serious limiting factors so far has been the rather heavy quark mass in the range of 50~100 MeV used in the simulations. This necessitated a long chiral extrapolation to the physical up and down quark mass of 3 MeV with ensuing systematic errors in the lattice QCD predictions.

  The specific goal of the PACS-CS project is to realize a realistic lattice QCD calculation in the sense that (i) the dynamic effects of all three light quarks, up, down and strange, are incorporated, and (ii) the masses of the three quarks, especially those of the lightest up and down quark, are reduced to their physical value. In order to achieve this goal, recent algorithmic developments based on domain decomposition and multi-time step methods are incorporated, and a new set of lattice QCD codes using the Wilson-clover quark formalism and optimized for PACS-CS are developed. The PACS-CS calculations have already succeeded in reducing the up and down quark mass from 70 MeV to 6 MeV on a large lattice of 3.2 fm with encouraging results for the chiral behavior and hadron spectrum. Further efforts are underway to reduce the quark mass to the physical value.

- Real-space density functional theory in materials science

  We are developing a real-space density functional theory (RSDFT) method as a promising computational method for describing phenomena in real materials with a very large number of atoms, e.g., 10,000 or more, from the first principles of quantum theory. RSDFT introduces a lattice in real space and calculates all quantities, such as electron wave functions at each lattice point. This method has several advantages for next-generation supercomputing: heavy all-to-all communications such as FFT are unnecessary, and flexible boundary conditions on wave functions can be imposed at the boundaries of the computational cell, thereby expanding its applicability to various materials. A newly developed code is now being fine-tuned on PACS-CS. Calculations of ionization energies and electron affinities of 10,000-atom clusters are being processed with the goal to pave the way toward a unified approach for molecules, clusters and bulk materials.

- Real-time density functional theory in materials science and many-body theory
  We have succeeded in a first-principles calculation of the electron dynamics for laser-induced breakdown of dielectrics. When an ultra-intense laser field is irradiated to the dielectrics, a large number of electron-hole pairs are excited even for a visible light which should be transparent in large-gap dielectrics. These excitations make the response of the dielectrics metallic, and are employed for laser machining and surgeries. We have shown, for the first time, that this process of optical dielectric breakdown can be naturally described by solving the time-dependent Kohn-Sham equation. The result shows the energy transfer from the laser pulse to the electrons in diamond as a function of the maximum intensity of the laser pulse. Around 10^{15} W/cm^2, a substantial increase of the energy transfer is seen where the dielectric breakdown occurs. A portion of this calculation is achieved by PACS-CS.

- Global circulation model analysis on PACS-CS
  We exchanged a research contract with the Center for Climate System Research (CCSR) of the University of Tokyo in order to collaborate on the development of the next-generation cloud resolving non-hydrostatic icosahedral general circulation model (NICAM). In the NICAM of CCSR/FRCGC, the dynamic core of the model is formulated specifically for massively parallel processing using MPI, which fits perfectly with the PACS-CS. The NICAM can extend the model resolution to a 3.5 km global mesh with cloud resolving physical processes. The testing phase with an aqua planet model (no topography) has been completed successfully, and full terrain has just been installed in the model. Using the latest version of the NICAM with topography, near real-time prediction experiments are being conducted on PACS-CS using the real-time GPV/JMA data archive developed and maintained at the Center.

- Regional weather model analysis on PACS-CS
  The Weather Research and Forecasting (WRF) regional model was progressively developed under the PACS-CS project. Coupled with the real-time GPV/JMA data, the real-time regional weather prediction system was constructed. A test run was conducted for the explosive cyclogenesis event that occurred on 7 January 2007 to confirm that the system is useful for research as well as for educational purposes.

- Phylogenetic multi-gene analyses on PACS-CS

The MPI version of a phylogenetic search program, Tree-Puzzle, was developed for PACS-CS. This program has been utilized for multi-gene analyses under separate model conditions. By using MPI-Puzzle, the exact ML trees will be exhaustively selected from all possible trees, and subsequently compared with the trees that are heuristically searched for.

5.3 FIRST Project

This project is a collaboration between astrophysicists and computer scientists, aiming at an elucidation of the evolution of first-generation objects through large-scale radiation hydrodynamic (RHD) simulations with a high-performance hybrid computer system. The project is funded by the Specially Promoted Research in Grants-in-Aid for Scientific Research over four years (2004~2007) with a budget of JPY 329.5 million (US $2.8 million), approved by the Ministry of Education, Culture, Sports, Science and Technology (MEXT) in Japan. Under this project, we have developed a new type of hybrid computer dedicated for astrophysical RHD, called the FIRST simulator, in a collaboration with the Division of High Performance Computing Systems.

5.3.1 FIRST Simulator

The FIRST (<u>F</u>usional <u>I</u>ntegrator for <u>R</u>adiation-hydrodynamic <u>S</u>ystems in <u>T</u>sukuba University) simulator is a hybrid PC cluster, in which a newly developed board for gravity calculations, called Blade-GRAPE, is embedded in each node. The Blade-GRAPE is composed of four GRAPE-6 chips which have dedicated pipelines for binary gravity calculations, and is designed for a PCI-X bus in PC clusters. The theoretical peak performance of a single Blade-GRAPE is 136.8 GFLOPS. Each board has 16 MB memory and can calculate the self-gravity up to 260,000 particles. The Blade-GRAPE is directly connected via PCI-X bus, and occupies the space of two PCI-X bus slots. The electric power supply is from the PCI-X bus (3.3 V) as well as from the cluster server board, +12 V (54 W). Each server PC is equipped with multi-port Gigabit Ethernet NIC for connection to a special interconnection network with commodity Ethernet switches.

The first version of Blade-GRAPE was 32 bits and 33 MHz (PCI). It has been improved to a 64 bit and 100 MHz version (PCI-X), Blade-GRAPE X64 (Fig. 5.4). Using Blade-GRAPEs, we have constructed a 256-node hybrid PC cluster system, the FIRST simulator. The system possesses 16 Blade-GRAPE boards and 224 Blade-GRAPE X64 boards. The node of the host PC cluster is a 2U-size 19-inch rack-mountable server PC (HP ProLiant DL380 G4) that has two dual Xeon processors in SMP configuration. The peak performance of the FIRST simulator is 36.1 TFLOPS, of which the host PC cluster contributes 3.1 TFLOPS and the Blade-GRAPEs 33 TFLOPS. All nodes are connected uniformly with each other via multi-port Gigabit Ethernet interconnect switches. The total memory of the FIRST simulator is 1.6 TB. The Gfarm Grid file system, which is a commodity-based distributed file system that federates the local disk of each node (http://datafarm.apgrid.org/index.en.html), is installed. With Gfarm, the storage of 22 TB is available as a seamless file server. In Fig. 5.5, the 256 node FIRST simulator is shown.

Fig 5.4: Blade-GRAPE

Fig 5.5: FIRST Simulator (256node, 1TFLOPS)

5.3.2 Performance

With the FIRST simulator, we have investigated the acceleration of gravity calculations by Blade-GRAPEs. First, we tested the two types of Blade-GRAPEs. The main difference between Blade-GRAPE and Blade-GRAPE X64 is the bus clock; Blade-GRAPE works at 33 MHz and Blade-GRAPE X64 at 100 MHz. The dependence of performance on the number of particles for a single board is shown in Fig. 5.6. If 260,000 particles are calculated with a single board, the performance of Blade-GRAPE is 93% of the peak speed, and that of Blade-GRAPE X64 is 98%. This weak dependence shows that, for this number of particles, the communication with the host computer is negligible compared to the force calculations in GRAPE chips. The performance is reduced, however, with a decreasing number of particles. For 16,000 particles, the performance of Blade-GRAPE is 44%, and that of Blade-GRAPE X64 is 74%. For this number of particles, the communication with the host computer is noticeable, and therefore Blade-GRAPE X64 with a three times faster bus has a roughly double performance over Blade-GRAPE.

Next, in a simulation using 256^3 particles, we measured the run time with and without Blade-GRAPEs. The results are shown in Fig. 5.7. In this simulation, the dominant part of the calculations is the self-gravity calculations. The acceleration turns out to be 5 times with Blade-GRAPE, and 10 times with Blade-GRAPE X64. In this simulation, 10,000 particles are sent to each Blade-GRAPE board on average. Therefore, the performance with Blade-GRAPE X64 is approximately twice that with Blade-GRAPE due to the communication bandwidth.

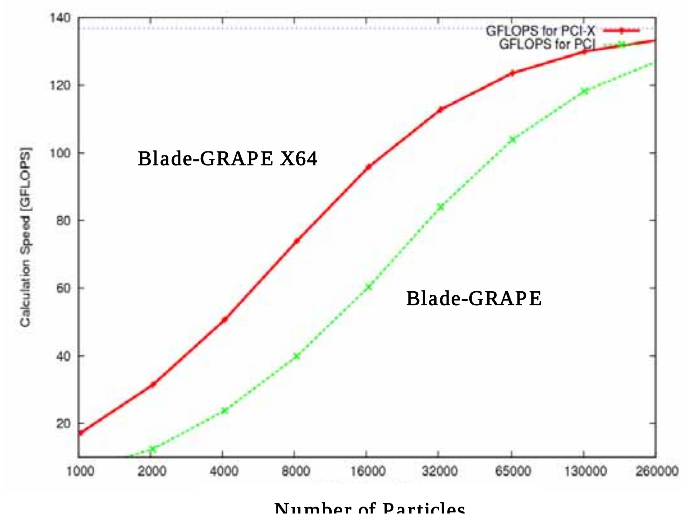


Figure 5.6: The dependence of performance on the number of particles in a board is shown for Blade-GRAPE and Blade-GRAPE X64.

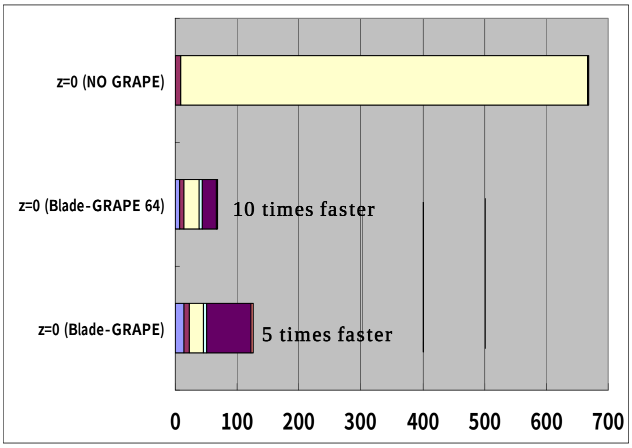


Figure 5.7: The acceleration of calculations for 256^3 particle simulations.

5.4 ILFTNet and ILDG Project

The ILFTNet (International Lattice Field Theory Network) project (FY2004–FY2005) aimed to construct a research network among leading institutes in Japan, USA, UK, Germany and other countries in the field of lattice quantum field theories through promotion of international collaboration, a chain of workshops and seminars, and researcher exchange. The infrastructure of the network was to be provided by the International Lattice Data Grid (ILDG) for sharing gluon configurations and lattice data. The project was funded by JSPS and ran for two years, from April 2004 till March 2006. The hub institute in Japan was the Center for Computational Sciences, Univ. of Tsukuba.

For more details, refer to http://www.rccp.tsukuba.ac.jp/projects/ILFTNet/.

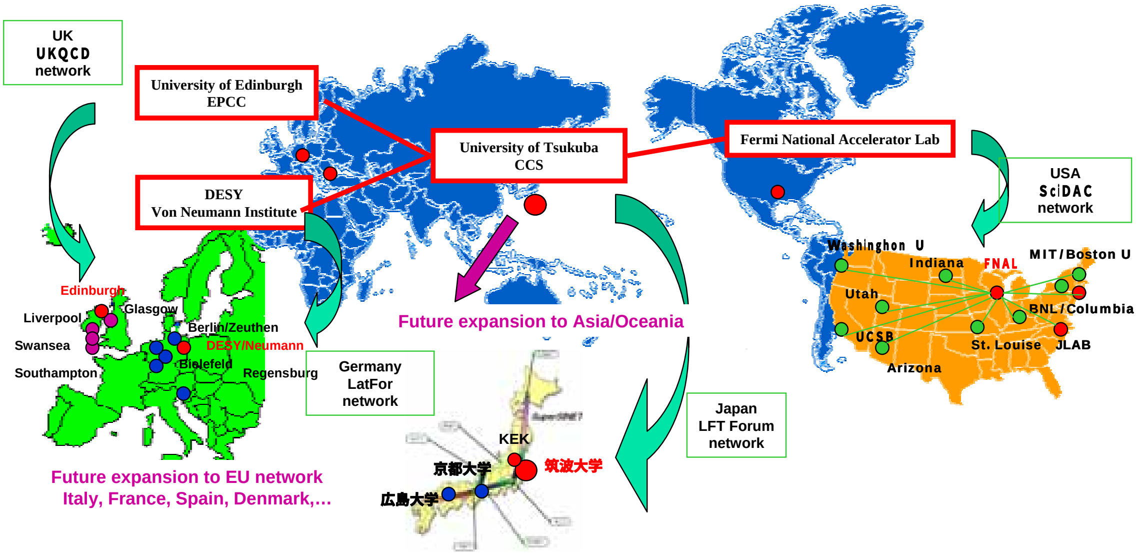


Figure 5.8: Research network of ILDG

This activity has continued in FY2006 and beyond with the support from the CSI (Cyber Science Infrastructure) project of the National Institute of Informatics (NII). The activity involves constructing the lattice QCD archive and JLDG, the national data grid for the lattice QCD community in Japan.

5.4.1 ILDG: International Lattice Data Grid

ILDG is an international project to develop a grid of data grids for sharing lattice QCD configurations worldwide. An XML-based markup language, QCDml, which describes metadata for QCD configurations and ensembles (sets of configurations with common physics parameters) have been developed. Middleware interfaces among collaborating grids are defined with WSDL. The construction of regional grids was finalized in US, UK, Germany, Australia and Japan. JLDG works as the ILDG Japan grid. The interoperability of the regional grids has been achieved for download operations, and valuable configurations have already been archived in the grid.

For more details, refer to http://www.lqcd.org/ildg

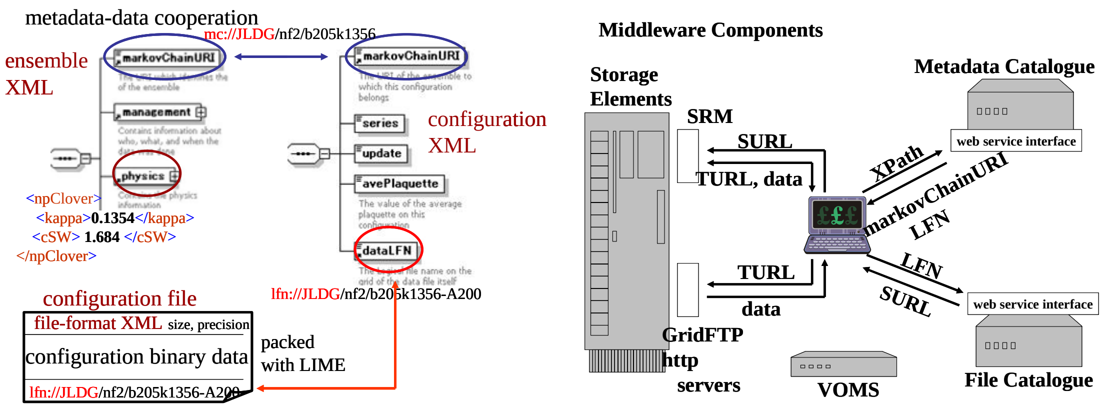


Figure 5.9: QCDML and overview of ILDG architecture

5.4.2 LQA: Lattice QCD Archive

LQA is a database of QCD configurations maintained by the Center for Computational Sciences (CCS) since December 2003. The archive currently stores i) two-flavor full QCD configurations generated by the CP-PACS parallel computer at CCS (about 8000 files stored in 1.5 TB disk space) and ii) 2+1 flavor full QCD configurations generated by the CP-PACS and JLQCD collaborations (about 21000 files stored in 6 TB disk space) and makes them available to the lattice QCD community worldwide. Configurations for much lighter quarks, which will be generated with the PACS-CS computer, will be added to the archive. One can use the ILDG standard interface to search ensembles and configurations and to download configurations, or use an interactive Web interface. The LQA was designed to serve as a Japan gateway to/from other sites of ILDG. The system will be restructured as a gateway between JLDG and ILDG in 2007.

For more details, refer to http://www.jldg.org/lqa/index.html.

5.4.3 JLDG: Japan Lattice Data Grid

JLDG is a data-grid infrastructure for the lattice QCD (LQCD) community in Japan. Several large LQCD collaborations in Japan have been working on lattice QCD simulations using supercomputers. Outputs of simulations called "QCD configurations" are valuable, because physicists can study various aspects of QCD using these configurations. JLDG enables the community to share configurations and other data distributed over distant sites. File sharing is realized with the GFarm global file system. GSI authentication is managed by VOMS. JLDG utilizes the NII Super SINET MPLS VPN, HEPnet-J/sc, as a hardware infrastructure. Part of the configurations can be accessed from all over the world through the ILDG interface. Full installation of the system was completed in FY2006. Mutual test operations are ongoing.

For more details, refer to http://www.jldg.org.

Figure 5.10: Conceptual view of JLDG

5.5 Toward Peta-scale Computing

In 2005 MEXT initiated the “Elemental Supercomputing Technology” project within a larger project of “R&D to Build Future IT Infrastructure.” The elemental technologies developed in these projects were expected to be used in future supercomputers.

Together with Hitachi Ltd. and University of Tokyo, we have been conducting the project “Low-Power and High-speed Device, Circuit and Logic for Next-generation Supercomputer Systems” of the “Elemental Supercomputing Technology” project. Our task in the project is to carry out research on “Research and Development on Fundamental Logic on Processor Architecture and Memory Hierarchy.”

We have been studying the on-chip memory architecture and computing acceleration mechanism for low-power and high-performance systems. In the next-generation supercomputer, power consumption is one of the most important issues in the system design. We proposed the on-chip memory architecture called SCIMA (Software-Controlled integrated memory architecture) for multi-core processors and accelerators to make arithmetic units more efficient. We considered the SIMD arithmetic unit and Vector processing unit as accelerators, and compared the performance and power efficiency. We hope these research results will be incorporated into the processor architecture of the next-generation supercomputer.

In 2006, the Japanese government launched the national project ("Next-Generation Supercomputer Project") to develop a peta-scale computer system, which has the performance of more than 10 PFLOPS (so-called "Keisoku" computer). The project spans seven years (2006–2012) and RIKEN (Research Institute for Science and Chemistry) has been selected to conduct the project.

In September 2006, RIKEN and University of Tsukuba signed a collaboration agreement for the "Next-Generation Supercomputer" project. Based on this agreement, several members of the Center for Computational Sciences have been appointed as visiting fellows of RIKEN and have been involved in the project.

The project is now in the stage of detailed designing. CCS will contribute not only to the designing of the system but also to the evaluation and performance improvement of real target application codes. The Center and RIKEN are setting up a research collaboration program under the General Agreement for tuning QCD, RS-DFT and FFT codes for the Next-Generation Supercomputer as peta-scale applications. We think that such a contribution is possible in the unique environment of CCS, where researchers of computer science and computational science are working together.

5.6 Summary of Interdisciplinary Collaborations in the Center

- As described in Section 5.2, the PACS-CS project is an interdisciplinary program. The Particle Physics Group, building upon their past experience in R&D of parallel computing, has been involved in the development of the PACS-CS system from the beginning with computer scientists in the High Performance Computing Group. It has contributed significantly in the initial testing and improvement of the PACS-CS system after the installation in July 2006. A new collaboration was also set up with the experts in algorithms and programming, which helped in the optimization of lattice QCD codes and exploration of new methods such as the 32 bit acceleration techniques.

  The Materials Science Group set up a working group with the High Performance Computing Group to develop the real-space and real-time density functional calculations on PACS-CS. The performance of the RS- and RT-DFT codes was analyzed and optimizations were carried out. The benefit was twofold in that computer scientists learned the key features of the RS-DFT method toward peta-scale computing.

  The Global Environment Science Group also set up a working group with computer scientists. In collaboration with the data-engineering experts in the Computational Informatics Group, they set up the real-time weather data archive GPV/JMA and have been using it in conjunction with global and regional weather analyses using PACS-CS.

Finally, the Biological Science Group has been working with the experts in distributed computing in the High Performance Computing Group to develop a parallelized phylogenetic search code in order to greatly expand the number of analyzed genes using PACS-CS

- As described in Section 5.3, the FIRST project is carried out through collaboration between the Astrophysics Group and the High Performance Computing Group. In addition to the systems development, the collaboration resulted in the installation of the Gfarm Grid file system, which had been developed in the High Performance Computing Group, in the FIRST simulator. As a result, the distributed storage has been integrated as a seamless file server.

- The ILDG (International Lattice Data Grid) project has been conducted by the Particle Physics Group and grid experts in the High Performance Computing Group since 2000. Jointly, they have contributed to a worldwide effort to standardize QCDml, an XML for lattice QCD configurations, and the middleware architecture for interfacing the regional lattice data grids and ILDG. They have also developed JLDG, the Japanese regional grid. ILDG and JLDG are now in operation mode.

- Within the Division of Material and Life Sciences, the Groups of Materials Science, Life Science and Quantum Many-Body Systems have a tight collaboration. Our stance is to recognize the common features in nano- and bio-materials, perform calculations based on quantum theory, and clarify and predict various phenomena in the two categories of materials from an integrated viewpoint. Collaboration with the Computational Life Science Group is therefore essential.

  Time-dependent density functional theory is an important methodology for the quantum many-body group. This scheme has common aspects with the RS-DFT code of the Materials Science Group. A considerable part of the source code of the real-time calculation is common to the real-space density functional code. Joint discussions, also involving researchers from the High Performance Computing Group, have helped to locate the critical paths in the two types of programs and to develop ways to optimize them.

- The Global Environmental Science Group has a close collaboration with the High Performance Computing Group and the Computational Intelligence Group under the common subject of constructing a large database of real-time weather data, named the GPV/JMA project. This goal of this project is to archive real-time weather data of the global spectral model (GSM), regional spectral model (RSM), meso-scale non-hydrostatic model (MSM) provided by the JMA. In addition to these model data, weekly ensemble forecast data and monthly ensemble forecast data are also archived and released to the public through the CCS web site. The weather map presented on Google Earth was provided by a collaboration of the Computational Intelligence Group.

- The groups in the Division of Computational Informatics organized the “Computational Informatics Seminar” in order to share awareness of the problems involved in the leading-edge field of “Computational Informatics.” The seminar members include all the faculty in the Computational Informatics Division and active researchers in related fields invited from other departments of the university and external organizations, such as the National Institute of Advanced Industrial Science and Technology (AIST).

- The Computational Media Group of Computational Informatics and the Grid Computing Group of the High Performance Computing Division have jointly planned a research proposal with other research groups of Kyoto University, etc. This activity has led to a new project entitled “Sensing Web,” which aims at developing the next generation of sensor grids and networking, for 2007–2009, and is supported by the Special Coordination Funds for Promoting Science and Technology.

6. Inter-university Activity, Education and Public Relations

6.1 Interdisciplinary Computational Science Promotion Program

The Center of Computational Sciences is an inter-university facility, open to researchers of universities and other research institutes in Japan. The Center solicits proposals for the Interdisciplinary Computational Science Promotion Program to encourage research activities of computational sciences. The computational power of the PACS-CS is provided to researchers throughout Japan through this program.

The Interdisciplinary Computational Science Promotion Program has two categories:

1. Interdisciplinary Collaboration Program
2. Large-scale Scientific Simulation Program.

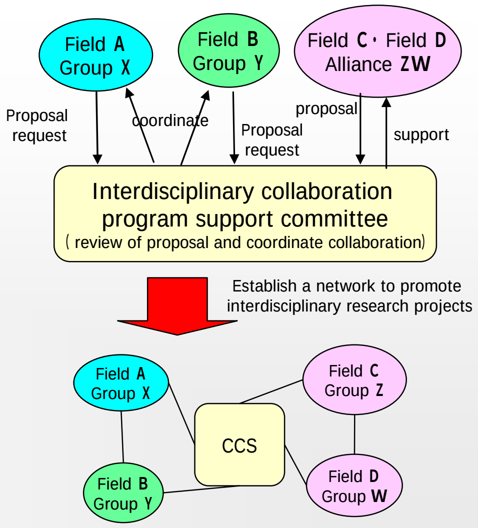
The Interdisciplinary Collaboration Program promotes interdisciplinary research activities of different disciplines. For example, trends in HPC architecture are such that, at the highest end, systems are expected to consist of a huge number of processors, with each processor containing multiple cores with small vector instructions. These features present a programmer with a number of different ways to exploit different types of parallelism within algorithms. Optimizing the performance and designing algorithms involve a number of challenges, including exploiting parallelism within codes and overlapping different types of operations. This requires tight collaboration of application scientists and computer scientists.

An area where innovative research may be expected from such a program is that of algorithm design. New modeling techniques enable researchers to take a more comprehensive view of physical phenomena stretching across disparate length and time scales. We expect that similar numerical algorithms and modeling might be applied to the problems in different fields.

A project can be proposed by a team that includes researchers from different fields. If one team needs partners for the proposed collaborative research and it is accepted, CCS is ready to coordinate appropriate partners for the project through the CCS Interdisciplinary Collaboration Program Support Committee. The fields inviting applications in this category are particle physics and astrophysics, material sciences, life sciences, global environmental sciences, biological science from application fields, and high-performance computing and computational informatics and numerical analysis from the computer science fields.

The Large-scale Scientific Simulation Program pushes forward the challenges in several fields of computational sciences by providing the computational power of the PACS-CS. Since this program solicits research proposals which are impossible to solve without the large amount of computing resources of PACS-CS, the proposal should describe the reason why the use of PACS-CS is indispensable. The fields inviting applications in this category are expected to be particle physics and astrophysics, material sciences, life sciences, global environmental sciences, biological science.

- Interdisciplinary collaboration program
  - Support to establish a network of interdisciplinary research projects and to encourage grand challenges of interdisciplinary computational science.
  - To promote interdisciplinary research projects of different disciplines.
    - Between Computer science and application fields (e.g. Applied Math and Particle Physics)
    - Between different application fields (e.g. Modeling of radiation in Astrophysics and Climate simulation)
  - Matchmaking of research groups from different fields
    - Review of Proposals by external reviewer of Interdisciplinary collaboration coordination committee
    - Coordinate research groups from different fields
    - Find partners to mach the request
    - Advice with expertise of different fields
  - Follow up the research activity produced by the interdisciplinary collaboration



- Large-scale scientific simulation program
  - Push forward the grand challenge of several fields in computational sciences by providing the computational power of the PACS-CS.
  - Review proposals and concentrate our computational power to make new scientific discoveries
  - Follow up the scientific results

Figure 6.1 shows the organization for inter-university facilities operations. In order to execute the Interdisciplinary Computational Science Promotion Programs, we organize the Inter-university Research Review Committee, including external members, to evaluate the proposals. We also organize the Interdisciplinary Collaboration Program Support Committee to review the proposals and coordinate collaborations between different fields. We report the policy, results and status of inter-university activities to the annual Steering Council meeting of the Center.

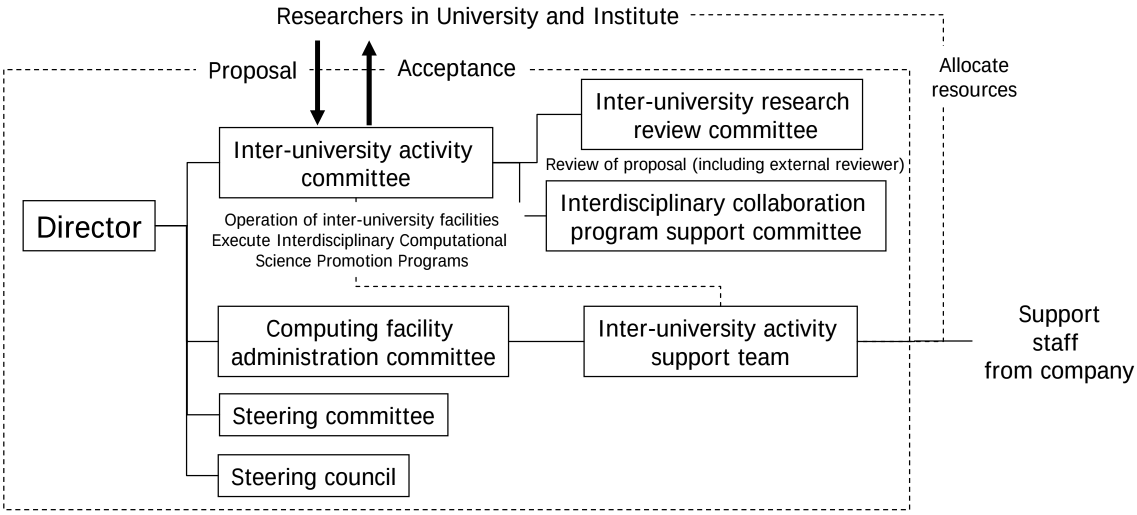


Figure 6.1: organization for Inter-university facilities operations

The Interdisciplinary Computational Science Promotion Program started in October 2007. Proposals from 13 research groups were accepted for the 2nd half of FY2007.

6.2 Other Inter-university Activities and Contributions to Computational Science Communities

- Symposiums, workshops and colloquia organized by CCS
  We organize an annual symposium on computational science, which covers all fields related to computational science. The Center also organizes international symposia and invites visitors from abroad in order to promote international exchange and collaboration of scholars in computational sciences Workshops in each field and colloquia are held occasionally.

- Operation and support of scientific databases and data grids
  Scientific databases are becoming increasingly important in computational science. We support the following two databases for particle physics research and climate research:
  - Lattice QCD archive, Particle Physics (open since Feb 2004), extended into Data Grid ILDG (2007)
  - GPV/JMA archive, Climate research (open since Jan 2005)

- Education, Outreach, and Public Relations
  All the faculty members of the Center participate in the Graduate and Undergraduate Program of University of Tsukuba, through which they provide education in various aspects of computational sciences. The Center also has been hosting seminars and lectures for computational science and HPC technology. We hope that these activities

educate the community to increase participation in advanced computing technology careers.
Every year we receive a large number of visitors from high schools and other guests. We attempt to inform society through the visitors about our activities and the impact of advanced computing in improving knowledge and the quality of life.
]

Appendix A. Faculty Members of CCS

Director: Mitsuhisa Sato
Deputy Director: Masayuki Umemura
Taisuke Boku

◆ Division of Particle Physics and Astrophysics (Division Manager: Masayuki Umemura)

Particle Physics Group (Group Leader: Sinya Aoki)

Faculty Members

Tomoteru Yoshie, Associate Professor

Graduate School:
Physics , Graduate School of Pure and Applied Sciences
Research topics:
Elementary Particle Physics

Naruhito Ishizuka, Associate Professor

Graduate School:
Physics , Graduate School of Pure and Applied Sciences
Research topics:
Computational studies on strong interactions using lattice field theories

Yoshinobu Kuramashi, Assoicate Professor

Graduate School
Physics , Graduate School of Pure and Applied Sciences
Research topics:
Theoretical and computational studies on strong interact ions using lattice field theories

Yusuke Taniguchi, Assistant Professor

Graduate School:
Physics , Graduate School of Pure and Applied Sciences
Research topics:
Lattice gauge theory

Akira Ukawa, Professor, Executive Advisor to the President

Graduate School
Physics , Graduate School of Pure and Applied Sciences ,
Research topics
Computational particle physics, in particular lattice QCD, and development of computers for such studies

Collaborative researchers

Sinya Aoki, Professor

Graduate School:
Physics, Graduate School of Pure and Applied Sciences
Research topics:
Elementary Particle Physics Theory, Lattice Field Theory

Kazuyuki Kanaya, Professor

Graduate School:
Physics, Graduate School of Pure and Applied Sciences
Research topics:
lattice field theory, parallel computers

Research staff

- Kiyoshi SASAKI
- Noriyoshi Ishii
- Naoya Ukita
- Daisuke Kadoh

Astrophysics Group (Group Leader: Masayuki Umemura)

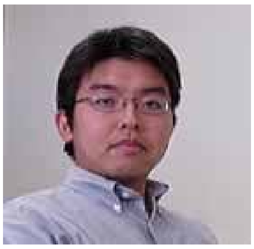
Faculty Members

Masayuki Umemura, Professor

Graduate School:
Physics , Graduate School of Pure and Applied Sciences
Research topics:
Theoretical Astrophysics.
In particular, the study with radiation hydrodynamics
on the formation of first generation objects and galaxies

Hiroyuki Hirashita, Assistant Professor

Graduate School:
Physics , Graduate School of Pure and Applied Sciences
Research topics:
Theoretical study of element production history
in galaxy formation and evolution



Kohji Yoshikawa, Assistant Professor

Graduate School:
Physics , Graduate School of Pure and Applied Sciences ,
Research topics
Astrophysics.
Theoretical studies on observational cosmology,
the formation of galaxies and galaxy clusters, and intergalactic medium

Junichiro Makino, Visiting Associate Professor

Graduate School:
Graduate School of Science, University of Tokyo
Research topics:
Computational Astrophysics,
Development of dedicated computers for computational science

Research Staff

- Yoshiaki Kato
- Tamon Suwa
- Takuya Akahori

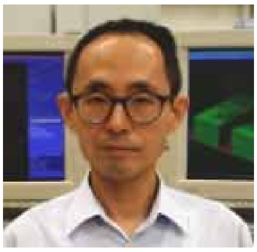
◆ Division of Material and Life Sciences (Division Manager: Atsushi Oshiyama)

Material Science Group (Group Leader: Atsushi Oshiyma)

Faculty Members

Atsushi Oshiyama, Professor

Graduate School:
Frontier Science, Graduate School of Pure and Applied Sciences
Research topics:
Nanoscience and Theoretical Condensed Matter Physics



Kenji Shiraishi, Professor

Graduate School:
Frontier Science , Graduate School of Pure and Applied Sciences
Research topics:
Nanoscience and Theoretical Condensed Matter Physics

Susumu Okada, Associate Professor

Graduate School:
Frontier Science , Graduate School of Pure and Applied Sciences
Research topics:
Nanoscience and Theoretical Condensed Matter Physics

Susumu Saito, Visiting Professor

Graduate School:
Department of Physics, Tokyo Institute of Technology
Research topics:
Nanoscience and Theoretical Condensed Matter Physics

Research Staff

- Jun'ichi Iwata

Life Science Group (Group Leader: Masaru Tateno)

Faculty Members

Masaru Tateno, Associate Professor

Graduate School
Physics , Graduate School of Pure and Applied Sciences ,
Research topics:
Computational analyses
of functional controle mechanisms of biological macromolecules

Yasuteru Shigeta, Assistant Professor

Graduate School
Physics , Graduate School of Pure and Applied Sciences ,
Research topics:
Theoretical studies on electron
and proton transfer reactions in biological systems

Collaborative researchers

Mauro Boero, Associate Professor

Graduate School:
Physics, Graduate School of Pure and Applied Sciences
Research topics:
First principles molecular dynamics simulations :
checmical and biochemical reactions of organic and inorganic materials
in liquid and solid phases

Research Staff

- Kamiya Katsumasa
- Yoshitaka Fujimoto

Quantum Many-Body Systems Group (Group Leader: Kazuhiro Yabana)

Faculty Members

Kazuhiro Yabana, Professor

Graduate School
Physics , Graduate School of Pure and Applied Sciences ,
Research topics:
Nuclear physics, computational sciences on atomic, molecular,and optical sciences

Yukio Hashimoto, Assistant Professor

Graduate School
Physics , Graduate School of Pure and Applied Sciences ,
Research topics:
Microscopic theory of nuclear collective motions

Hiroyasu Koizumi, Associate Professor

Graduate School:
Materials Science, Graduate School of Pure and Applied Science
Research topics:

Tong Xiao-Min, Associate Professor

Graduate School:
Materials Science, Graduate School of Pure and Applied Science
Research topics:
Atoms, molecules interaction with intense laser field and time-dependent density functional theory

Collaborative researchers

Kenichi Hino, Professor
Materials Science, Graduate School of Pure and Applied Science

◆ Division of Global Environment and Biological Science (Division Manager: Hiroshi Tanaka)

Global Environmental Science Group (Group Leader: Hiroshi Tanaka)

Faculty Members

Hiroshi L. Tanaka, Professor

Graduate School:
Geoenvironmental Sciences,
Graduate School of Life and Environmental Sciences
Research topics:
General circulation, dynamics and energetics of the atmosphere

Kusaka Hiroyuki, Assistant Professor

Graduate School:
Geoenvironmental Sciences,
Graduate School of Life and Environmental Sciences
Research topics:
Urban climate, Applied Meteorology,
Numerical simulationof mesoscale weather using the WRF model

Collaborative researchers

Fujio Kimura, Professor

Graduate School:
Geoenvironmental Sciences
Graduate School of Life and Environmental Sciences
Research topics：

Global Environmental Science Group (Group Leader: Tetsuo Hashimoto)

Faculty Members

Yuji Inagaki, Associate Professor

Graduate School:
Biological Sciences, Graduate School of Life and Environmental Sciences ,
Research topics
Molecular phylogeny of eukaryotes Investigation of lateral genetransfers
Estimation of protein functions by combining structural
and evolutionary parameters Artifacts in molecular dataanalyses

Collaborative researchers

Tetsuo Hashimoto, Professor

Graduate School:
Biological Sciences, Graduate School of Life and Environmental Sciences ,
Research topics
Molecular evolutionary studies
on the origin and early evolution of eukaryotes

Hideko Urushihara, Professor

Graduate School:
Functional Biosciences, Graduate School of Life and Environmental Science
Research topics
Studies on developmental programs described in the genome

◆ Division of High Performance Computing Systems (Division Manager: Taisuke Boku)

System Architecture Group (Group Leader: Taisuke Boku)

Faculty Members

Boku Taisuke, Professor

Graduate School:
Computer Science, Graduate School of Systems and Information Engineerin
Research topics:
High performance parallel computing,
cluster computing, hybrid parallel processing system,
grid computing

Daisuke Takahashi, Assoicate Professor

Graduate School:
Computer Science, Graduate School of Systems and Information Engineerin
Research topics:
High performance parallel computing,
High-performance numerical algorithms on parallel computers
and performance evaluation

Hiroshi NAKAMURA, Visiting Assoicate Professor

Graduate School:
Graduate School of Information Science and Technology, University of Toky
Research topics:
High-Performance and Low-Power Processor Architecture,
High-Performance Computing, Dependable Computer System

Collaborative researchers

Moritoshi Yasunaga, Professor

Graduate School:
Computer Science, Graduate School of Systems and Information Engineerin
Research topics:
VLSI Engineering, Evolvable Hardware, Dependable Systems

Kouichi Wada, Professor

Graduate School:
Computer Science, Graduate School of Systems and Information Engineerin
Research topics:
Numerical algorithms and simulation,
Mathematical software for GRID computing

Research Staff

- Toshihiro Hanawa

Grid Computing Group (Group Leader: Mitsuhisa Sato)

Faculty Members

Mitsuhisa Sato, Professor, Director

Graduate School:
Computer Science, Graduate School of Systems and Information Engineerin
Research topics:
High performance parallel computing,
compilers and performance evaluation, grid computing

Osamu Tatebe, Associate Professor

Graduate School:
Computer Science, Graduate School of Systems and Information Engineerin
Research topics:
High performance parallel computing,
Grid Computing, Distributed File System

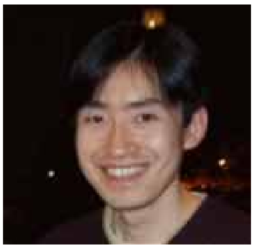
◆ Division of Computational Informatics (Division Manager: Yuichi Ohta)

Computational Intelligence Group (Group Leader: Hiroyuki Kitagawa)

Faculty Members

Hiroyuki Kitagawa, Professor

Graduate School:
Computer Science, Graduate School of Systems and Information Engineerin
Research topics:
Database systems, Data engineering Information integration,
WWW and databases, Knowledge discovery, XML databases,
Multimedia information retrieval, and DBMS architecture



Toshiyuki Amagasa, Assistant Professor

Graduate School:
Computer Science, Graduate School of Systems and Information Engineerin
Research topics:
Database Systems, Data Engineering.
XML Databases, Web Information Systems, Bioinformatics

Hideyuki Kawashima, Assistant Professor

Graduate School:
Computer Science, Graduate School of Systems and Information Engineerin
Research topics:
Database Systems and Data Engineering:
DBMS Architecture, Sensor Networks

Computational Media Group (Group Leader: Yuichi Ohta)

Faculty Members

Yuichi Ohta, Professor

Graduate School:
Advanced Engineering Systems,
Graduate School of Systems and Information Engineering
Research topics:

Yoshinari Kameda, Assoicate Professor

Graduate School:

Research topics:
Massive Sensing, Intelligent Video Making based on Scene Understanding, Model Based Vision,Coorperative Distributed Vision, Lecture Archiving and Distance Learning, Visual Surveillance, Human Interface to Virtual Reality

Itaru Kitahara, Assistant Professor

Graduate School:
Advanced Engineering Systems,
Graduate School of Systems and Information Engineering
Research topics:
Image media with ubiquitous sensor networks

Collaborative researchers

Tomonori Shirakawa, Professor

Graduate School:
Advanced Engineering Systems,
Graduate School of Systems and Information Engineering
Research topics:

Appendix B. Facilities of CCS

1. Computer Systems Overview

The computational facilities of the center mainly consist of a massively parallel cluster system PACS-CS and its front-end computer system, and the new generation of astrophysics simulator FIRST.

The front-end computer system consists of the system controlling servers to manage the PACS-CS cluster and the small-sized mini-PACS-CS for program development, Magellan (Hitachi SR11000J) for post-processing and analysis on generated data by PACS-CS, 100 TByte of large capacity file server to hold all data of these machines. There are additional medium to small size clusters for data analysis and general networking services. Beside of these main facilities in Computer Building, there are a number of graphic workstations and PCs to support daily research of researchers and students in Research Building. A central switch in Computer Building connects all computational facilities by Gigabit Ethernet for high-speed data exchange. It is also connected another central switch in Research Building via 10 Gigabit Ethernet to support high-speed data access among all resources in the center.

Main computational facilities in the center are shifting from vector machines to large scale high-end clusters including PACS-CS and FIRST to support various fields of computational sciences and computer science in all research divisions in the center.

Since the PACS-CS system is the main central facility in the center, the operation, job status and detailed system temperature such as CPU, chassis and network interfaces of each computational node are monitored in real-time. The status of the machine and air conditioners in Computer Building are remotely monitored to detect any failure.


New generation of astrophysics simulator
FIRST
Performance(256 nodes):Blade-GRAPE 33Tflops /
General purpose CPU 3.1Tflops
The massively parallel cluster
PACS-CS
Performance(2560 nodes):14.34Tflops
Perseus cluster
201.6Gflops
SR11000J1 Magellan
480Gflops
FileServer
100TB
Center LAN
Mini PACS-CS
Post-processing cluster
Flare
10Gbps Network
General-purpose
Workstations
Graphic Server room
PACS-CS pilot system
Corona
UPS
800KVA 5min

2. Network Environment

University of Tsukuba has been connected 10 Gbps of nation-wide network for research and education named SINET3 under MEXT since April 2007. In addition, the university is also connected to major research institutes in Tsukuba City by a high-speed WAN with 20 Gbps bandwidth named TSUKUBA-WAN. Our center is connected to SINET3 with 2 Gbps of general purpose network and three of 1 Gbps special purpose research network. Moreover, we are also connected to the nation-wide research network JGN2 with 10Gbps link to stimulate various research activities in the center. In such network environment, we share the valuable data computed by PACS-CS and other center facilities as well as high-performance Grid computing research toward new generation of computational sciences.