Center for Computational Sciences, University of Tsukuba

筑波大学
University of Tsukuba

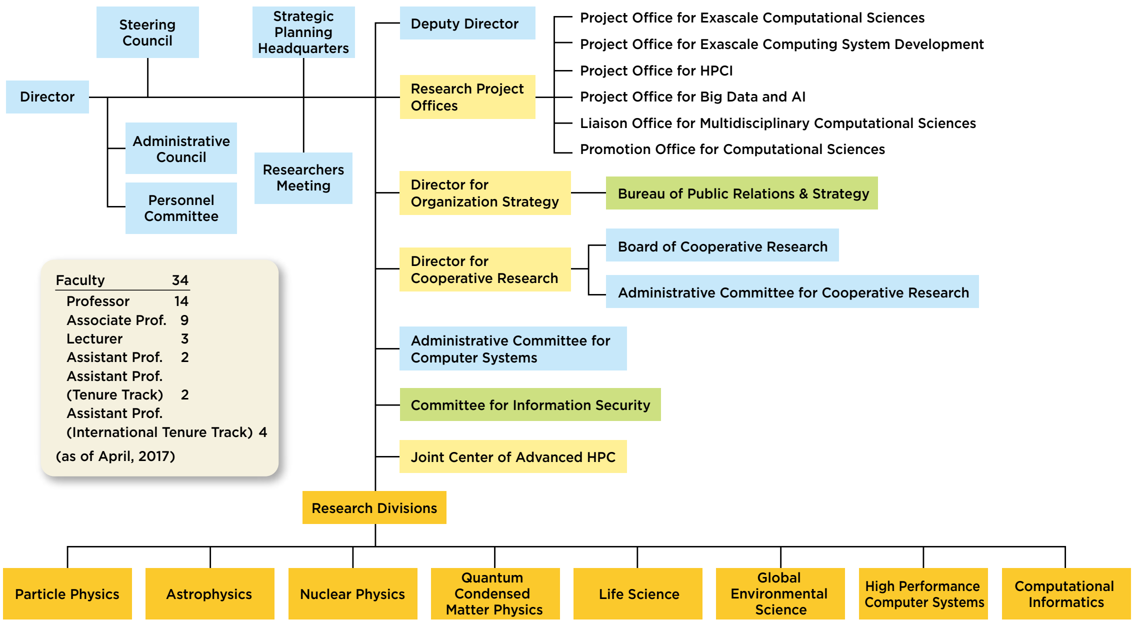
Overview

The mission of the Center for Computational Sciences (CCS) is the promotion of “Multidisciplinary Computational Science” through enhanced cooperation between, and the fusion of, computational and computer sciences. To that end, the CCS works toward the development of high-performance computing systems and networks, conducts sophisticated simulations in a variety of scientific research fields, and endeavors to expand the frontiers of Big Data analysis and innovative information technology. The scientific research areas of our Center encompass particle physics, astrophysics, nuclear physics, nano-science, life science, environmental science, and information science.

Originally formed as the Center for Computational Physics (CCP) in 1992, the CCS was reorganized and relaunched under its current name in April 2004. A massively-parallel supercomputer CP-PACS, which was completed in September, 1996, was ranked as No. 1 on the Top 500 World Supercomputer List. Currently, the CCS is endorsed as a leading center of advanced research for the Support and Development of Strategic Initiatives in University of Tsukuba. In 2013, we joined with the University of Tokyo in establishing the Joint Center for Advanced HPC (JCAHPC) as the first interuniversity joint-use center in Japan, which installed Oakforest-PACS as the fastest supercomputer in Japan in 2016. The CCS possesses 8 research divisions and 34 faculty members, and organizes 6 research project offices and a bureau of public relations to strategically promote and spread “Multidisciplinary Computational Sciences”. Also, a priority issue and exploratory challenges on Post-K computer are propelled under FLAGSHIP 2020 Project in Japan. Furthermore, a wide variety of multidisciplinary cooperation has been accelerated in Joint Institute for Computational Fundamental Science (JICFuS) and Organization for Collaborative Research on Computational Astrobiology (CAB).

The CCS is playing a significant role as a notable joint-use facility for outside researchers with providing computational resources broadly. Since 2010, the CCS has been approved as a “national core-center” under the Advanced Interdisciplinary Computational Science Collaboration Initiative (AISCI) launched by the Ministry of Education, Culture, Sports, Science and Technology (MEXT) of Japan. Under Multidisciplinary Cooperative Research Program (MCRP), the CCS assists nationwide researchers to promote scientific projects and encourages collaborations through financial supports for meetings or staying.

Organization of CCS



Message from the Director

Masayuki Umemura

Director of Center for Computational Sciences,
University of Tsukuba

Computational science, which is defined as the exploration of science by means of computers, is an indispensable research methodology in the basic and applied sciences, and contributes significantly to the progress of a wide variety of scientific research fields.

If computational science is compared metaphorically to music, “instruments” are computers, “scores” are programs, and “performances” are calculations. With common instruments, a wide variety of music can be created, including “Fusion”. Performances for common scores can be done with different instruments. In the CCS, programs in various fields are performed with a common instrument of supercomputer, and state-of the-art computers are developed for more sophisticated performance. Also, a common instrument of supercomputer provides a potential to synthesize different fields of science. In that sense, computational science is a powerful tool which brings invaluable possibilities towards the future sophistication and diversification in science.

The CCS has promoted multidisciplinary computational science based on the collaboration of computational and computer sciences. It is a pioneer of “Co-design”, which is currently common in the world. This co-design has brought the pre-eminent scientific outcomes in a lot of fields, and demonstrated the potential to nurture the fusion and collaboration between different research fields.

The CCS, by accelerating international collaborations, aims to become a hub institute for multidisciplinary computational science through enhanced collaborations between computational and computer sciences.

CCS Vision of "Multidisciplinary Computational Science"

Computational science is explored by large-scale simulations with high-performance computing resources as well as the high-bandwidth networks. The pivot for computational science is the collaboration between wide fields of computational scientists and computer scientists having expertise of computer hardware, software, algorism, and programming. This collaboration allows us to develop computers best suited for scientific exploration. We define such a "co-design" as "Multidisciplinary Computational Science".

Through a co-design, the CCS developed the massively parallel supercomputer named the Computational Physics by Parallel Array Computer System (CP-PACS) in 1996, which was ranked as the No. 1 system on the Top 500 List of November 1996. Large-scale computations carried out on CP-PACS have resulted in significant progress in particle physics and astrophysics. Since then, a large-scale cluster system named the Parallel Array Computer System for Computational Sciences [PACS-CS (2006)], and a special-purpose parallel system for astrophysics, the Cosmo-simulator FIRST (2007), have been developed. In 2011, another co-design project for the Highly Accelerated Parallel Advanced system for Computational Sciences (HA-PACS) was launched.

The CCS has been striving to carry out collaborative research with computer scientists in a field of fundamental science for more than thirty years. Currently, in addition to fundamental science (particle physics, astrophysics, and nuclear physics), applied fields are spread to materials science, life science, and global environment. As a result, a wide variety of collaborations among different fields have been initiated. This is a significant potentiality of "Multidisciplinary Computational Science".

Collaborations and Alliances

As for nationwide alliances, the CCS has entered the T2K alliance, which is an alliance aimed at the acquisition of a T2K supercomputer system. In 2013, we joined with the University of Tokyo in establishing the Joint Center for Advanced HPC (JCAHPC) as the first interuniversity joint-use center in Japan. This alliance between two universities allowed us to construct an unprecedentedly large-scale computational facility, and installed a novel many-core-architecture supercomputer, Oakforest-PACS, which was ranked as the fastest supercomputer in Japan in 2016. Furthermore, a wide variety of multidisciplinary collaborations has been accelerated in Joint Institute for Computational Fundamental Science (JICFuS) and Organization for Collaborative Research on Computational Astrobiology (CAB), and new collaborative activities with computational informatics or medial science have been initiated. Also, under the alliance with RIKEN Advanced Institute for Computational Science (AICS), the technology for high-performance computing has been explored. Besides, since our university is located in Tsukuba Science City, which is home to many government research organizations, we already have firm connections to a number of major research institutions located there. These include the High Energy Accelerator Research Organization (KEK), the Advanced Institute for Science and Technology (AIST), the National Institute for Materials Science (NIMS), the Meteorological Research Institute (MRI), and the National Institute for Environmental Studies (NIES).

International collaborations and alliances in computational science research are important factors for promoting and accelerating multidisciplinary computational science. To that end, we have strengthened international collaborations through alliances with The University of Edinburgh in the UK and Lawrence Berkeley National Laboratory in the US. With Korea Institute of Science and Technology Information (KISTI), we organize a winter school and a workshop for advanced computational science every year. Additionally, CCS computational material scientists collaborate with Vanderbilt University and Washington University in the US, under a bilateral program sponsored by the Japan Society for the Promotion of Science (JSPS).

The International Lattice Data Grid (ILDG) is an international project aimed at the development of data grids for sharing lattice quantum chromodynamics (QCD) configurations worldwide. The construction of regional ILDG grids has been finalized in the US, UK, Germany, Australia, and Japan [where it is known as the Japan Lattice Data Grid (JLDG)]. The JLDG is supported by the "Cyber Science Infrastructure Project" carried out by the National Institute of Informatics as a part of grid infrastructure developments for academic research between the universities and research institutions.

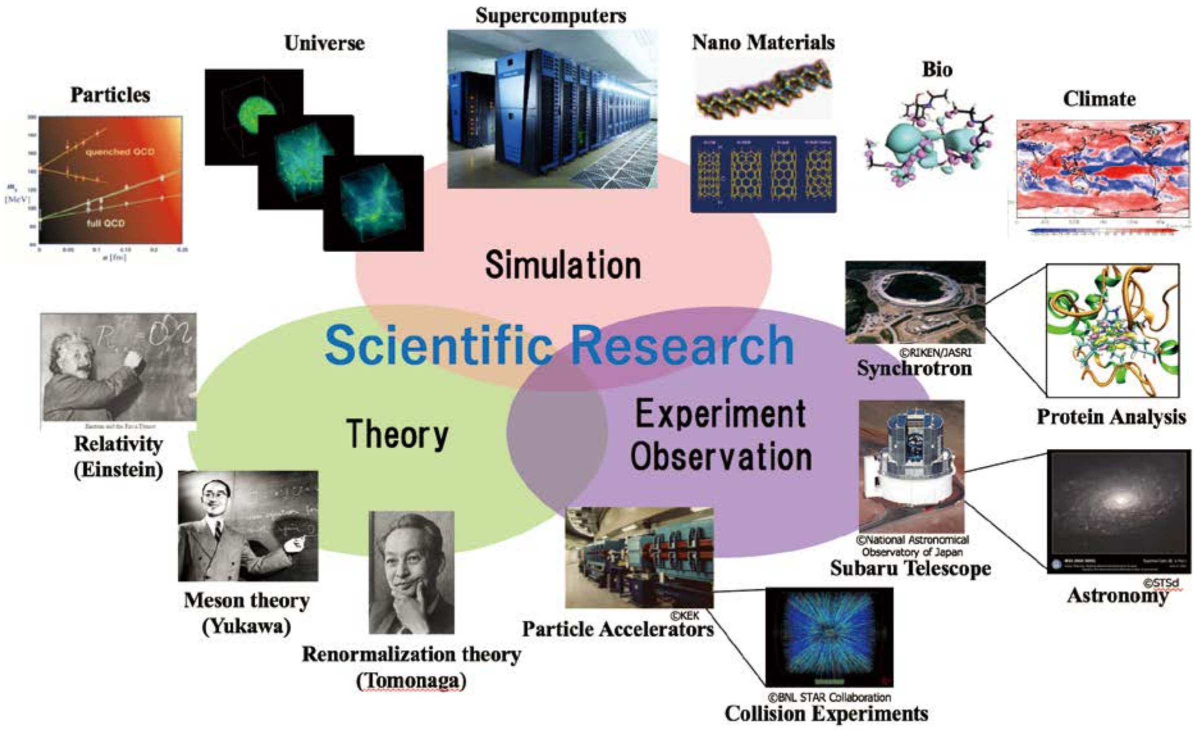
Chronology of CCS

1992	April	CP-PACS Project begins (5-year project). Center for Computational Physics (CCP) founded (10-year term).
1993	August	Computer building completed
1995	March	First research building completed
1996	September	CP-PACS (2048 PU) completed and installed
	November	Ranked as No. 1 on the Top 500 World Supercomputer List
1997	April	Research for the Future Program "Development of Next-Generation Massively Parallel Computers" begins (5-year term)
2002	April	Second 10-year term of the Center for Computational Physics begins
2004	April	CCP is reorganized, expanded and relaunched as the Center for Computational Sciences (CCS)
2005	April	Development of Massively Parallel Cluster PACS-CS in the project begins (3-year term)
2007	March	Second research building completed
	April	Cosmo-Simulator FIRST completed and installed
2008	June	Operation of T2K-Tsukuba begins
2010	April	Approved under the Advanced Interdisciplinary Computational Science Collaboration Initiative (AISCI)
		CCS is reorganized from five to seven divisions
2012	February	HA-PACS starts operation
2013	March	Joint Center for Advanced HPC (JCAHPC) established in alliance with the University of Tokyo
2014	April	COMA (PACS-IX) installed and started operations
2015	April	CCS is reorganized from seven to eight divisions
2016	December	Oakforest-PACS installed and started operations in JCAHPC

Cutting-Edge Research Areas

Simply speaking, "computational science" involves using computers to perform science. In the past decade, due to the extraordinary advances in science and technology that have been achieved as a result of dramatic increases in the power and availability of computers and their networks, most scientific disciplines are benefiting from computer modeling, analysis, and visualization.

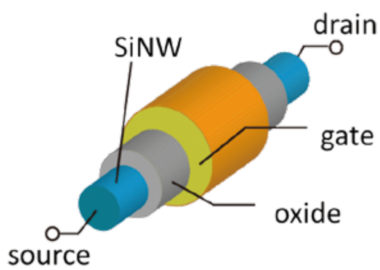
Computational science has shifted the scientific research paradigm to include simulation – along with experiment and theory – as fundamental methods of science. Computer simulation allows us to acquire scientific insights into problems that are too complex or difficult to study analytically using just "paper and pencil". It also enables the study of complex systems and natural phenomena that would be too expensive, dangerous, or which might even be impossible, to study by direct experimentation. As a result, computer simulation is now regarded as an equal and indispensable partner, alongside theory and experiment, in scientific research.



Awarded Gordon Bell Prize Two Years in a Row

The Gordon Bell Prize is an authoritative prize that recognizes papers presenting the most outstanding achievements in the application of parallel computing to science and technology.

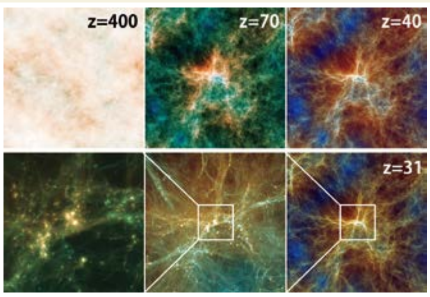
Appraised for the joint research conducted using the K Computer, University of Tsukuba's Center for Computational Sciences (CCS) was awarded the Gordon Bell Prize two years in a row.



2011 Gordon Bell Prize for Peak Performance

(University of Tsukuba/The University of Tokyo/RIKEN)

Atomic state simulation at actual semiconductor device scale. The electronic state of silicon nanowire materials, which are attracting attention as base materials of next-generation semiconductors, was calculated and quantum mechanical calculations were made for the electronic state of the nanowire at a scale of 100,000 atoms, which is close to the size of the actual material.



2012 Gordon Bell Prize

(University of Tsukuba/RIKEN/Tokyo Institute of Technology)

World's largest scale of a dark matter simulation. The "K computer" was employed to perform calculations related to the evolution of gravity for the early period of space consisting of about 2 trillion dark matter particles.

HA-PACS/TCA (PACS-VIII)

HA-PACS/TCA

The Highly Accelerated Parallel Advanced system for Computational Sciences with TCA (HA-PACS/TCA) is a GPU (Graphic Processing Unit) cluster that incorporates the latest CPU and GPU technologies. In addition to an ordinary InfiniBand interconnect, the system is also equipped with a specially designed interconnection network system named Tightly Coupled Accelerators (TCA) by FPGA (Field Programmable Gate Array) which is originally developed technology at CCS to realize the highest speed of GPU-to-GPU direct communication over computation nodes. A computation node is equipped with two sockets of Intel Xeon E5-2860v2 CPU (IvyBridge architecture) and four NVIDIA K20X GPU. The number of computation nodes is 64 and it started the operation on November 2013. TCA is a conceptual architecture to engage FPGA technology to both communication and computation to compensate the weakness of GPU cluster, and we implemented PEACH2 (PCI Express Adaptive Communication Hub ver.2) on Altera Stratix-IV FPGA. It enables 2.1μsec of minimum latency for GPU-to-GPU remote memory copy which was the most advanced technology at the time of HA-PACS/TCA installation. The theoretical peak performance of HA-PACS/TCA is 364 Tflops and the performance/power ratio of Linpack is 3518 Mflops/W to be ranked as #3 in the world at Green500 List on November 2013.

HA-PACS/TCA has been combined with the original part of HA-PACS named Base Cluster part (shutdown on March 2017), and their aggregated theoretical peak performance was 1.13 PFLOPS to provide the first PFLOPS-class supercomputer in CCS. HA-PACS/TCA is reconfigured and restarts its standalone operation from April 2017.

COMA (PACS-IX)

COMA

COMA (Cluster Of Many-core Architecture processor) is the 9th generation of PACS series supercomputer, and started its operation from April 2014. Intel Xeon Phi coprocessor enhances the performance of traditional multi-core CPU increasing the number of cores, and COMA is our second Pflops-class supercomputer with accelerators with 1.001 Pflops of theoretical peak, which was ranked as No. 51 in Top 500 list issued on June 2014. The system consists of Cray CS300 cluster with 393 of computation nodes and each node consists of two of Intel Xeon E5-2680v2 CPUs and two of Intel Xeon Phi 7110P (Knights Corner architecture) coprocessors. All the nodes are connected by full-bisection bandwidth of Fat-Tree network by InfiniBand FDR. It is equipped with 1.5 PByte of RAID6 Lustre shared file system.

CCS and Information Technology Center at the University of Tokyo introduced Japan's fastest supercomputer Oakforest-PACS and started its official operation from April 2017 under JCAHPC (Joint Center for Advanced HPC) which is a joint organization by two centers. Oakforest-PACS is equipped with Intel Xeon Phi 7250 (Knights Landing architecture) processors which is the 2nd generation many-core processor by Intel. Before Oakforest-PACS installation, COMA had been used for program development and performance improvement on many-core architecture processor. The software resource of COMA based on Knights Corner architecture is directly available on Knights Landing with much higher performance. COMA is used as standalone system as well as the preliminary software development platform for Oakforest-PACS.

Overview

The University of Tsukuba Center for Computational Sciences (CCS) established the "Joint Center for Advanced High Performance Computing (JCAHPC)" in order to design, operate and manage a next-generation supercomputer system jointly with the Information Technology Center (ITC), The University of Tokyo. JCAHPC was organized to handle the planning, installation and operation of Japan's highest class of supercomputer system. The first supercomputer under JCAHPC was installed at the ITC at the Kashiwa Campus of the University of Tokyo, named Oakforest-PACS which is the fastest supercomputer in Japan as on November 2016. It is believed that operating the Center through cooperation and collaboration will promote advanced computational sciences, and contribute to the promotion of academia, science, and technology in Japan.

Background and History

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. Although the K computer, operated at the RIKEN Advanced Institute for Computational Science, set a new world record in terms of speed since entering shared use in 2012, it was believed that closer cooperation between the ITC group furnishing the HPC platform and the attached Advanced Institute that operates the supercomputer would be necessary to establish a genuine world-class facility.

As a result, the institutions at both universities 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.

Mission

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 architect an advanced system that exploits many-core technology, which is believed to be the key to future 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. Based on this design and development, the institutions will jointly procure, operate, and administer the supercomputer. As the result of its first primary mission, we successfully procured and installed Oakforest-PACS as the fastest supercomputer in Japan. The establishment of such a joint organization and joint operation of a supercomputer is the first challenge in Japan in the history of HPC.

Oakforest-PACS

At JCAHPC, we started the full system operation of Oakforet-PACS from December 2016 as the fastest system in Japan. Its performance exceeds the former fastest supercomputer, K Computer at RIKEN AICS, both in the theoretical peak and in Linpack benchmark performance. It employs 8208 of computation nodes where each node is equipped with Intel Xeon Phi 7250 (Knights Landing architecture) which is the most advanced many-core architecture processor, and Intel Omni Path Architecture as the interconnection network. The processor on Oakforest-PACS is in the same family with that of COMA at CCS, however Knights Landing processor can work as standalone main CPU in the system while Knights Corner processor of COMA is an attached accelerator to ordinary Intel Xeon CPU. It is the largest Knights Landing system in the world as a PC cluster as well as the largest cluster with Intel Omni Path Architecture as on April 2017. It is also equipped with 26 PByte of Lustre shared file system as well as 960 TByte of high speed file cache known as burst buffer.

In TOP500 list on November 2016, Oakforest-PACS is ranked at No.6 in the world (No.1 in Japan) with 13.55 PFLOPS of Linpack performance out of 25 PFLOPS of peak performance. The many-core architecture is the most promised general purpose processor technology currently and near future, and wide variety of applications and system software will be developed toward next generation national flagship supercomputer. Oakforest-PACS plays a central role in development of application and system software toward Exascale computing.

Oakforest-PACS

Provision of Computing Resources

The mission of the Center for Computational Sciences (CCS) focuses on promoting research efforts in computational sciences where scientists of various fields do not simply employ computers, but also work in close collaboration with computer scientists to develop computers that are most suitable for scientific investigations. Since 2002, the Center has been making computer resources available to collaborative research efforts in order to facilitate nationwide progress in computational sciences. Since 2007, these activities have been reinforced by enhanced links with computer sciences through the promotion of the Multidisciplinary Cooperative Research Program (MCRP). Since 2010, the Center has been recognized as a national core-center, Advanced Interdisciplinary Computational Science Collaboration Initiative (AISCI), through which it has been active in the MCRP, while also providing cooperative assistance and support in the areas of research meetings, visitor invitation, cooperative research travel and short-term employment.

The MCRP consists of the following programs: (1) Multidisciplinary Pioneering Program (MPP) (2) Priority Subjects Promoting Program (PSPP) (3) Cooperative Research Promoting Program (CRPP).

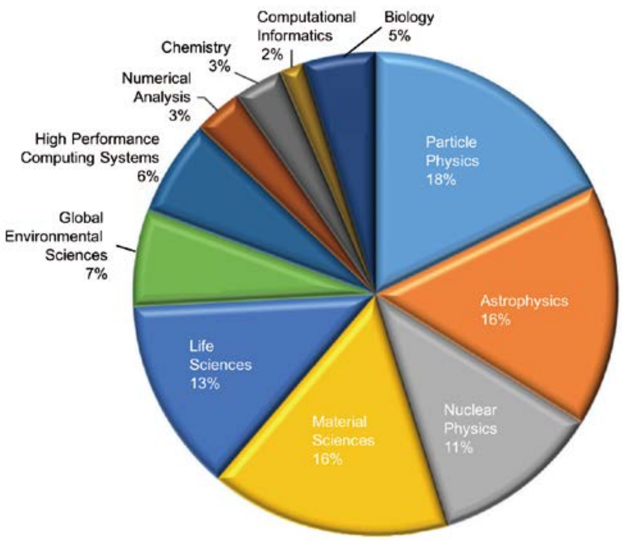
The MPP promotes combining different fields, while the PSPP is expected to promote computational science subjects via large-scale computations. The CRPP aims at promoting advancements in computational approaches to sciences and technologies through close collaboration between researchers inside and outside the Center. The Center has been soliciting proposals for the MCRP in the fields of computational sciences, including particle and nuclear physics, astrophysics, material sciences, chemistry, life sciences, global environmental sciences, and biology, as well as in the fields of computer sciences including high performance computing systems, computational informatics, and numerical analysis. Computational facilities that can be used under the MCRP include the Parallel Array Computer System for Computational Sciences [PACS-CS (2007-2011)], FIRST (2009-2011), T2K-Tsukuba (2008-2013), the Highly Accelerated Parallel Advanced system for Computational Sciences [HA-PACS (2013-)], COMA(PACS-IX) (2014-), and Oakforest-PACS (2017-).

The number of MCRP-approved projects conducted over the last ten years is shown in the table. Approximately 30 to 60 projects are approved each year. A breakdown of the 2016 projects by research fields is shown in the graph, and demonstrates how the projects extend across a variety of natural science and engineering fields.

The number of MCRP-approved projects

Year	# of projects	Computer
FY2007	13	PACS-CS
FY2008	36	PACS-CS, T2K-Tsukuba
FY2009	53	PACS-CS, T2K-Tsukuba, FIRST
FY2010	24	PACS-CS, T2K-Tsukuba, FIRST
FY2011	31	PACS-CS, T2K-Tsukuba, FIRST
FY2012	48	T2K-Tsukuba, HA-PACS
FY2013	59	T2K-Tsukuba, HA-PACS
FY2014	41	HA-PACS, COMA
FY2015	51	HA-PACS, COMA
FY2016	62	HA-PACS, COMA

A breakdown of the 2016 projects by research fields



Past symposiums organized by the Center
(including MCRP report meetings)

8th symposium on "Discovery, Fusion, Creation of New Knowledge by Multidisciplinary Computational Sciences"
Oct. 17-18, 2016, University of Tsukuba

7th symposium on "Discovery, Fusion, Creation of New Knowledge by Multidisciplinary Computational Sciences"
Oct. 19-20, 2015, University of Tsukuba

6th symposium on "Discovery, Fusion, Creation of New Knowledge by Multidisciplinary Computational Sciences"
Oct. 21-22, 2014, University of Tsukuba

5th symposium on "Discovery, Fusion, Creation of New Knowledge by Multidisciplinary Computational Sciences"
Nov. 5-6, 2013, University of Tsukuba

4th symposium on "Discovery, Fusion, Creation of New Knowledge by Multidisciplinary Computational Sciences"
-- Report Meeting on Multidisciplinary Cooperative Research Program (MCRP)
Oct. 25, 2012, University of Tsukuba

3rd symposium on "Twenty years anniversary of Center for Computational Sciences, University of Tsukuba" -- Development of Multidisciplinary Computational Sciences towards Exa-scale
Sept. 7, 2012, International Congress Center Epochal Tsukuba

2nd symposium on "Discovery, Fusion, Creation of New Knowledge by Multidisciplinary Computational Sciences"
-- Progresses of Computational Sciences by PACS-CS and Developments towards Next-generation Computing
Sept. 12-13, 2011, University of Tsukuba

1st symposium on "Discovery, Fusion, Creation of New Knowledge by Multidisciplinary Computational Sciences"
-- Development of Multidisciplinary Computational Sciences towards Post Peta-scale Computing
May 5-6, 2010, University of Tsukuba

Particle Physics Group

Chief: Yoshinobu Kuramashi, Professor, Ph. D. **Member**: Naruhito Ishizuka, Associate Professor, Ph. D. / Yusuke Taniguchi, Associate Professor, Ph. D. / Tomoteru Yoshié, Associate Professor, Ph. D. / Hiroshi Ohno, Assistant Professor, Ph. D. / Shinya Aoki, Visiting Researcher, Ph. D. (Director, Joint Institute for Computational Fundamental Science)

Overview

There are four fundamental forces in nature: gravity, the electromagnetic force, the weak force, and the strong force. Of these, the strong force is the energy source of twinkling stars in the sky, and makes up the nuclei in the atoms that constitute the myriad molecules forming all the matter. The strong force acts on the quarks, which are the smallest constitutive particles of matter (the elementary particle), and causes a characteristic phenomenon called "confinement" due to the non-perturbative effect: Experimentally observed is the bound state of multiple quarks called the hadron and quarks cannot yet be observed individually. Thus, some kind of non-perturbative method is necessary to investigate the strong force. The purpose of lattice quantum chromodynamics (QCD) is to define the QCD theory on the four-dimensional lattice, which consists of the discretized three-dimensional space and one-dimensional time, and then to study quantitatively, by first-principle calculations on a supercomputer, the realm of 10^{-15} m where the strong force reigns.

Research Topics

- Precision measurement of hadron spectra
- Precise determination of fundamental parameters in QCD (strong coupling constant and quark masses)
- Resonances and hadronic decays
- Direct construction of nuclei from quarks
- Determination of effective interactions between baryons based on QCD
- Investigation of QCD phase structure including high-temperature states (the beginning of universe) and high-density states (inside a neutron star)
- Application of tensor network scheme to lattice gauge theories

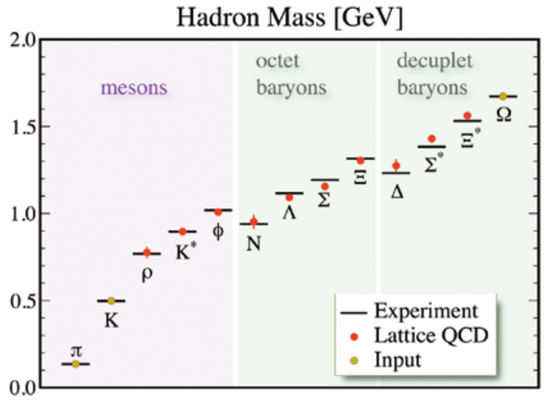


Fig.1 Hadron masses with lattice QCD in comparison with experimental values

Latest Accomplishments

Since the physical point simulations with the physical quark masses have been made possible thanks to algorithmic improvements and increasing computational resources in recent years, lattice QCD simulations are now in the stage of precision measurements at 1% error levels. This is a significant improvement from the previous 10% error stage. In the latest studies, the results for the hadron masses obtained by our lattice QCD simulation had almost reproduced the experimental values (Fig.1). Another important aspect to understand the physics of the strong interactions is the knowledge of QCD phase structure at finite temperature and density. Recently we have successfully determined the critical endpoint of finite temperature phase transition of three-flavor (up, down, strange quark masses are same) QCD at zero chemical potential for the first time in the world (Fig.2).

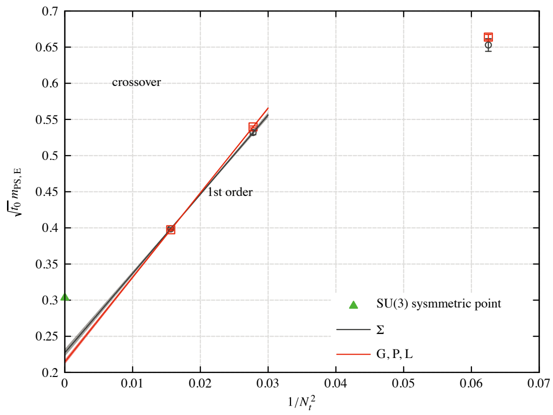


Fig.2 Critical endpoint of finite temperature phase transition of three-flavor QCD

Chief: Yoshinobu Kuramashi

Dr. Kuramashi graduated from the Department of Physics, Graduate School of Science, the University of Tokyo, in 1995 with a Ph.D. (Sciences). He assumed his present position after posts as an assistant professor at the Institute of Particle and Nuclear Studies, High Energy Accelerator Research Organization, and as a Lecturer and Associate Professor at the Center for Computational Sciences, University of Tsukuba. Concurrently, Dr. Kuramashi serves as the Field Theory Research Team Leader at the RIKEN Advanced Institute for Computational Science.

Astrophysics Group

Chief: Masayuki Umemura, Professor, Ph. D., Director of CCS **Member**: Masao Mori, Associate Professor, Ph. D. / Kohji Yoshikawa, Lecturer, Ph. D. / Alexander Wagner, Assistant Professor, Ph. D. / Kenji Furuya, Assistant Professor, Ph. D. / Naohito Nakasato, Visiting Associate Professor, Ph. D.

Overview

The Universe is thought to have been born 13.8 billion years ago with the occurrence of the Big Bang, but it wasn't until 0.38 million years later that hydrogen atoms formed. There were neither stars nor galaxies at that time, but there were density fluctuations with contrasts of 1/100,000. Moving ahead to 0.4 gigayears after the Big Bang, the Universe was reionized by unknown ultraviolet sources. Then, a number of newly born galaxies formed around 1 gigayears (Fig.1). Yet the era from 0.38 million years to 0.4 gigayears is often referred to as the "Dark Age of the Universe", and is enshrouded in mystery.
It is believed that, in this Dark Age, the first generation stars were born and the primordial galaxies formed. Thereafter, the merger of small galaxies led to the formation of massive galaxies, as well as galaxy clusters, and a large-scale structure came into being. For the cosmic structure formation, dark matter plays a key role.
In this research division, the formation processes of first stars, galaxies, massive black holes, and the large-scale structure of the Universe itself are investigated through numerical simulations that take into consideration dark matter, atoms, and radiation.

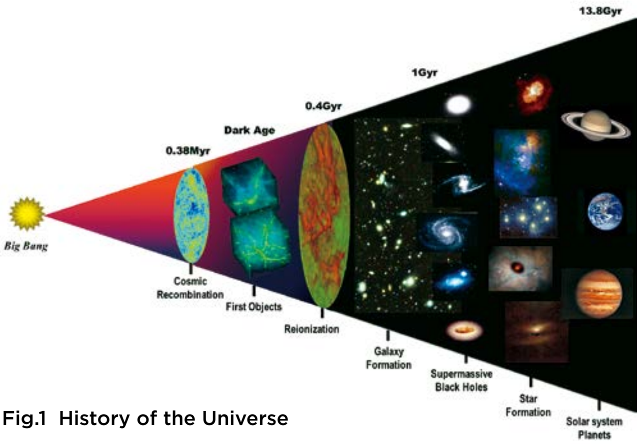


Fig.1 History of the Universe

Research Topics

● **Formation of first generation stars**

The formation of first generation stars is explored with three-dimensional (3D) radiation hydrodynamic simulations, where radiation transfer calculations are coupled with hydrodynamics. (Fig.2)

● **Galaxy collision and merger**

N-body simulations of the interaction between an accreting small galaxy and the Andromeda galaxy are performed. (Fig.3)

● **Formation of primordial galaxies**

Large-scale numerical simulations of dark matter and baryons are confronted with the observations of newly born galaxies.

● **Formation of massive black holes and the evolution of active galactic nuclei**

The growth of massive black holes (BHs) is investigated with general relativistic *N*-body simulations and relativistic radiation hydrodynamics, in relation to gravitational wave emissions recently discovered.

● **Formation of clusters of galaxies and a large-scale structure**

Hydrodynamic simulations are conducted coupled with detailed thermal processes including chemical enrichments.

● **Intensive numerical simulations of radiation hydrodynamics**

Methods of accelerated radiative transfer (RT), general relativistic RT, SPH-based RT, and resonant line transfer are developed.

● **Development of dedicated computers and exploitation of computational technique**

Novel techniques for numerical hydrodynamics and computers optimized for radiation hydrodynamics are explored.

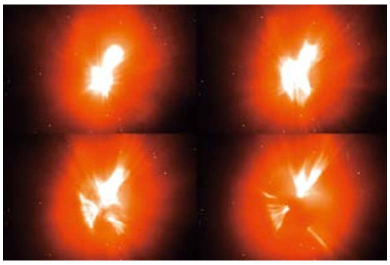


Fig.2 Successive formation of first stars in the early universe

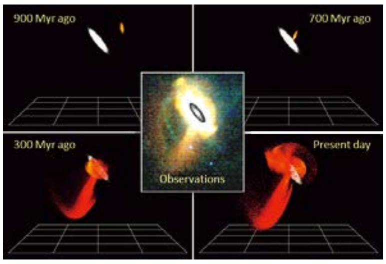


Fig.3 An accreting small galaxy and the Andromeda galaxy

Chief: Masayuki Umemura

Dr. Masayuki Umemura, graduated from Department of Physics in Hokkaido University in 1987 following the publication of his doctoral thesis entitled "The Formation of Stellar Shells and X-Ray Coronae around Elliptical Galaxies". Following graduation, he initially served as a postdoctoral fellow at the Yukawa Institute of Theoretical Physics in Kyoto University. In 1988, Dr. Masayuki Umemura was hired as an assistant professor in National Astronomical Observatory of Japan (NAOJ). In 1993, he moved to the Center for Computational Sciences (CCS) in the University of Tsukuba to assume a position as an associate professor. Dr. Masayuki Umemura became a full professor at the university in 2002, and is serving as the director of CCS since 2013.

Nuclear Physics Group

Chief: Takashi Nakatsukasa, Professor, Ph. D. **Member**: Kazuhiro Yabana, Professor, Ph. D. / Yukio Hashimoto, Lecturer, Ph. D. / Nobuo Hinohara, Assistant Professor, Ph. D.

Overview

Nucleus is a microscopic object composed of two kinds of fermions, protons and neutron, bound by the strong interaction. Theoretically, it is described by the many-particle quantum mechanics and the field theory. Nuclear structure shows a variety of different aspects, depending on its time and energy scales. These rich and quantum nature of nuclei has been fascinating researchers.
Nuclei are fuel of the stars and carry all the mass of materials. Properties of nuclei ultimately control the origin of elements. The burning process of nuclear fuel in the stars depends on nuclear reaction and structure, which determines brightness and destiny of the stars, species of produced elements, and so on.
Nuclear physics has been advanced with strong cooperative relationship between experiments using accelerators and theories using computers. The numerical calculation is indispensable in many-particle quantum problems such as nucleus. In Division of Nuclear Physics, we are developing theories/models/numerical methods, based on quantum dynamics, and aim at solving mysteries in nuclear structure, nuclear reaction, structure of stars, and origin of elements in the universe.

Research Topics

Density functional theory (DFT) has been developed for universal and quantitative description of nuclei. Figure 1 shows a chart of nuclear deformation in the ground state, obtained with the DFT calculation. Furthermore, the time-dependent density functional theory (TDDFT) enables us to study response and reaction of nuclear systems. We have developed numerical codes to study photonuclear reaction, giant resonances, low-lying elementary modes of excitation, and heavy-ion collision. From these numerical calculations, we have succeeded to achieve a number of new insights into microscopic mechanisms of nuclear reactions, spontaneous breaking of symmetry, and quantum fluctuations. In addition, these results contribute to understanding element-synthesis process behind explosive stellar phenomena, such as supernova.
Many attempts for synthesis of new elements have been performed using collisions of two heavy nuclei in accelerator facilities in the world. Recently, the naming right is awarded to a team in RIKEN, leading to the first element name by Japanese, “Nihonium”, of element 113. Figure 2 shows a study on possible reaction producing element 120. In most of heavy nuclei, protons and neutrons are paired and condensed in the ground state (pair condensation). This was confirmed in the calculation of Fig.1. This leads to nuclear superfluidity and significantly affects many properties of structure and reaction. However, its effects on nuclear reaction, such as pair transfer and dynamical shape evolution, have not been well understood. We are currently developing real-time simulation in the 3D space for collisions of superfluid nuclei, and microscopic determination of nuclear reaction path based on theories of large amplitude collective motion. These researches may reveal mysteries of heavy-ion reaction and nuclear fission phenomena.

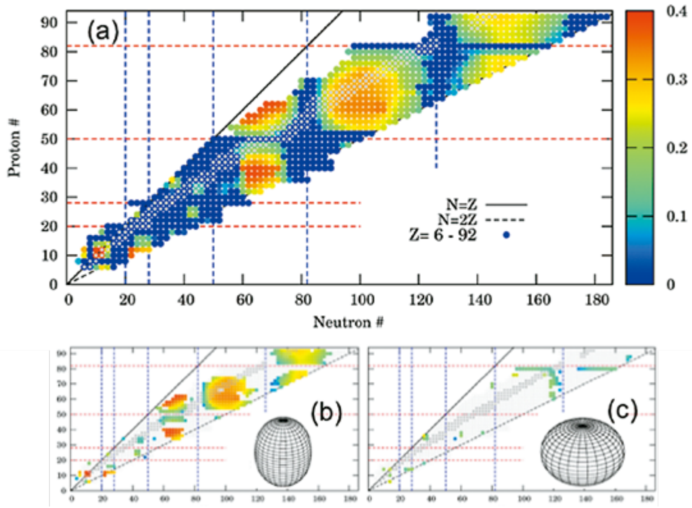


Fig.1 (a) Chart of nuclear deformation. Among those with relatively large deformation, (b) prolate shapes, and, (c) oblate shapes.

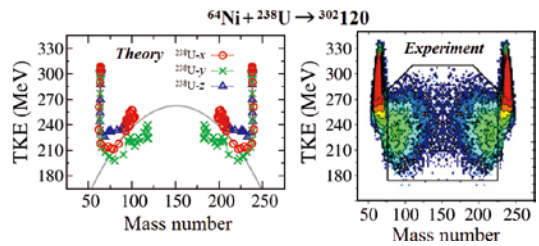


Fig.2 Distribution of mass and total kinetic energy of fragments produced by nuclear collision of Nickel and Uranium. Result of numerical simulation (left) and experimental data (right)

Chief: Takashi Nakatsukasa

Ph. D., Kyoto University, 1994. Postdoctoral Research Associate in Chalk River Laboratory (Canada, 1994), in University of Manchester Institute of Science and Technology (UK, 1996), and in RIKEN (1999). Assistant Professor in Tohoku University (2001), Lecturer in University of Tsukuba (2004), Associate Chief Scientist in RIKEN (2007), Current position since 2014. He is major in the theoretical nuclear physics, with extensive researches in nuclear many-body problems in structure and reaction.

Quantum Condensed Matter Physics Group

Chief: Kazuhiro Yabana, Professor, Ph. D. **Member**: Hiroyasu Koizumi, Associate Professor, Ph. D. / Xiao-Min Tong, Associate Professor, Ph. D. / Tomoya Ono, Associate Professor, Ph. D. / Nobuya Maeshima, Lecturer, Ph. D. / Atsushi Oshiyama, Visiting Professor, Ph. D.

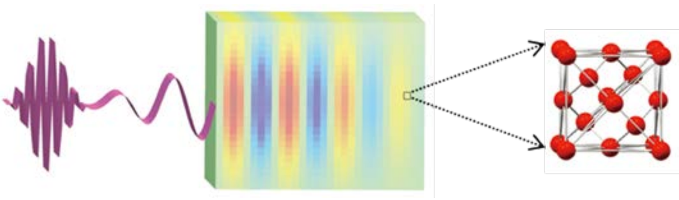
Overview

All the materials around us are composed of atoms, and atoms are composed of nuclei and electrons. Materials exhibit various properties reflecting their composition and structures and they are widely used in today's science and technology. In this division, we study quantum many-body systems--the substances coupled by Coulomb interaction--by solving quantum mechanical equations of motion numerically. Our goals are to elucidate various properties of materials, to find devices of new functions, and to search a way to control the dynamical processes. Such researches are the foundation for the future technology.

Research Topics

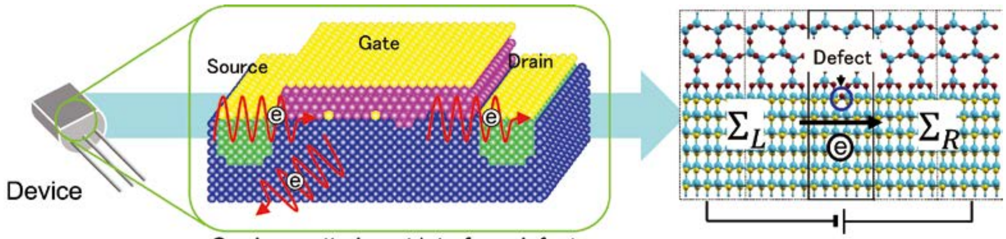
Light-matter interactions

Lights have been used to measure the properties of materials accurately. Recently, in optical sciences, a strong ultrashort pulsed light is used to measure the fast electronic motion in real time and to control the electron motion. We develop a simulation code based on the first-principles calculations to investigate the electronic dynamics and to understand the mechanism of the light-matter interactions.



Phenomena at the surface and interface of materials and their application to devices

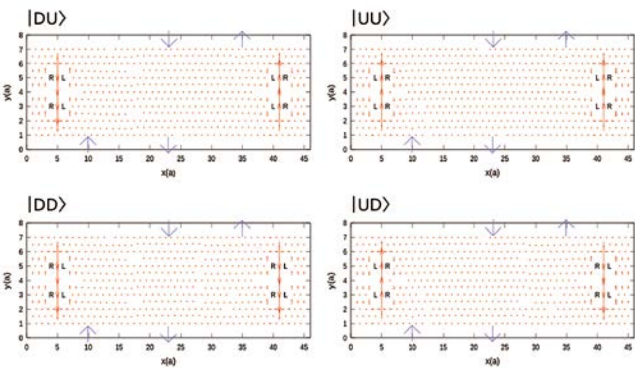
Electrons at a surface and interface behave differently from their counterpart inside material. Functions of devices are mainly decided by the motion of electrons at the surface or interface. We explore the mechanism of the electron motion at the surface/interface, search a way to improve the functions of devices, and develop a new-type functional device by numerical simulations.



Carrier scattering at interface defects

Strongly correlated material and topological material

Strongly correlated materials or topological materials whose properties depend on the shape of the material exhibit interesting properties that cannot be explained by the band theory. We develop a numerical method to study properties of these systems including electronic states, phase transitions, optical responses, and perform a research toward developing new quantum information devices. The right figure shows four states of two quantum bits realized by spin-vortex induced loop currents.



Chief: Kazuhiro Yabana

Professor K. Yabana graduated from Kyoto University in 1987, with a doctor degree in theoretical nuclear physics. He joined the Faculty of Science, Niigata University as an assistant professor in 1988, moved to Institute of Physics at the University of Tsukuba as an associate professor in 1999, then a full professor since 2002. He specializes in computational material sciences and nuclear theory and works on first-principles calculations of electron dynamics and interactions of strong pulsed light with materials.

Biological Function and Information Group

Chief: Yasuteru Shigeta, Professor, Ph. D. **Member**: Mitsuo Shoji, Assistant Professor, Ph. D. / Megumi Kayanuma, Assistant Professor, Ph. D.

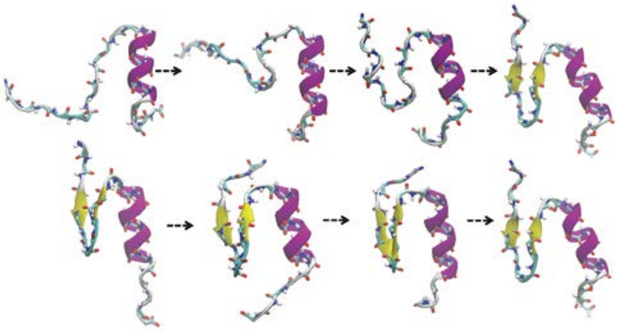
Overview

Phenomena expressing in life are dominated by a series of chemical reactions driven by macromolecules such as proteins, nucleic acids, lipids, and sugars. Therefore, the fundamental molecular mechanisms of biological phenomena can be clarified by investigating the electronic structure change and the spatial arrangements of atoms accompanied by the chemical reactions. In our group, dynamic structure-function correlations of biomolecules are explored by using first-principles and classical molecular dynamics simulations.

Research Topics

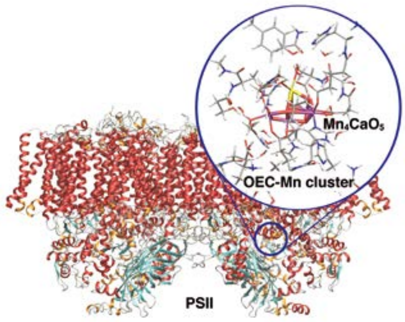
Structural transitions of proteins for understanding its function

We have developed an efficient sampling method to induce structural changes of proteins, which are extremely relevant to protein functions such as protein folding, domain motion, induced-fit, and protein complex formation processes. This method is a very suitable method for massively parallel computer environment.



Enzymatic reaction analyses by using hybrid QM/MM calculations

Photosystem II has a unique reaction active center composed of manganese, calcium, and oxygen atoms, where oxygen molecules are generated from water molecules by multi-step chemical reactions using light energy. We have clarified the reaction mechanisms of a series of water decomposition reactions by using the hybrid QM /MM method.



Origin of amino acids and its enantiomeric excess in space

Since some of the amino acids in life are also found in the meteorite, there is a possibility that an origin of life exists in the interstellar space. In collaboration with the Division of Astrophysics, our group has studied molecular evolution and symmetry breaking processes of the amino acids in space.

Chief: Yasuteru Shigeta

Dr. Yasuteru Shigeta graduated from Department of Chemistry, Osaka University in 2000. Following his graduation, he initially served as a postdoctoral fellow of Japan Society for the Promotion Science working at the University of Tokyo. He served as an assistant professor in the University of Tokyo (2004), a Lecturer in University of Tsukuba (2007), an associate professor in University of Hyogo (2008), and an associate professor in Osaka University (2010). Since 2014, he joined the Center for Computational Sciences (CCS) in the University of Tsukuba as a full professor.

Molecular Evolution Group

Group Leader: Yuji Inagaki, Professor, Ph. D.

Overview

● Building the global phylogeny of eukaryotes

All living organisms on Earth are believed to have evolved from a single common ancestral cell, eventually diverging into the three “domains,” of Bacteria, Archea (Archaebacteria), and Eukarya. Needless to say, biological evolution has never stopped, and has resulted in the creation of countless numbers of living organisms. One of the most important and difficult fields of biological study involves the evolutionary relationship amongst all the life forms on earth – building the “Universal Tree of Life”.

The central focus of our research is working to gain insights into the origin and early evolution of eukaryotes (members of the Eukarya domain). From the results of pioneering studies conducted to date, it is now believed that the vast majority of eukaryotes belong to any of ten major assemblages. One of the goals of this research is reconstructing the relationship amongst the major taxonomic groups in Eukarya, and this issue has been tackled by using molecular phylogenetic techniques.

Research Topics

● Analyzing ‘phylogenomic’ data comprising >100 gene sequences

Until recently, phylogenetic trees were constructed from the information of a single gene or a few genes. However, the information of a single gene is insufficient to make robust phylogenetic inferences related to ancient events such as the separations of major eukaryotic groups. To counter the difficulties of single-gene analyses, sequence data comprised of more than 100 genes have taken center stage in more recent phylogenetic analyses. These ‘phylogenomic’ analyses have provided successful insights into the relationship between major eukaryotic assemblages.

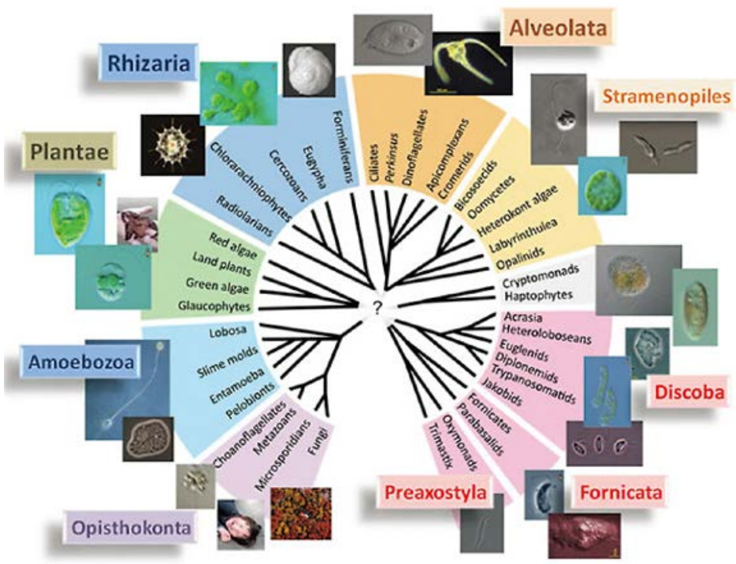


Fig.1 Tree of eukaryotes

Current ongoing projects

We are specifically interested in several eukaryotic groups, such as cryptophytes (and their close relatives), Discoba, and Fornicata, as these may hold the keys to understanding eukaryotic cell evolution, particularly the evolutions of two important organelles – mitochondria and plastids (or chloroplasts). Cryptophytes are photosynthetic eukaryotes bearing plastids, but recent studies have indicated that cryptophytes and various non-photosynthetic lineages form a previously identified monophyletic group. Thus, the group represented by cryptophytes can be used as a model group to study the birth and death of plastids. Discoba is known as the group containing a species with the most ancestral mitochondrion, while many members of the Fornicata group lack classical mitochondria. Thus, we expect that these two groups will provide important insights into study of mitochondria evolution. Currently we are engaged in the phylogenomic analysis of the organisms described above. Since a reliable phylogenetic inference simultaneously requires numerous genes and species, large-scale analyses using high performance computers play a key role in our study.

Group Leader: Yuji Inagaki

Doctor Yuji Inagaki began his professional career as a Postdoctoral Fellow in the Program of Evolutionary Biology at the Canadian Institute for Advanced Research in 2000. In 2004, he became a lecturer at the Nagahama Institute for Bioscience and Technology before moving to University of Tsukuba as an Assistant Professor in 2005. Dr. Yuji Inagaki was awarded the Young Scientists Prize by the Ministry of Education, Culture, Sports, Science and Technology (MEXT) in 2007, and received the Young Scientist Initiative Award from the Society of Evolutionary Studies, Japan in 2008.

Global Environmental Science Group

Chief: Hiroshi L. Tanaka, Professor, Ph. D. **Member**: Hiroyuki Kusaka, Professor, Ph. D. / Mio Matsueda, Assistant Professor, Ph. D.

Overview

In the Group of the Global Environmental Science, there are three faculties of Prof. Hiroshi L. Tanaka, Prof. Hiroyuki Kusaka and Asst. Prof. Mio Matsueda. There is one collaborative staff of Prof. Hiroyuki Ueda (Dept. of Life and Geoenvironmental Science) and three Researchers of Dr. Doan Quang Van, Mr. Ryosaku Ikeda, Mr. Akio Yamagami. We study global-, synoptic-, and local-scale weather and climate, using a general circulation model NICAM and a regional model WRF. Advanced technology of the super computer is used to enhance the accuracy of the prediction.

Research Topics

● NICAM (Non-hydrostatic ICosahedral Atmospheric Model)

NICAM is the most promising cloud resolving general circulation model, originally developed by CCSR, the University of Tokyo and by FRCGC in JAMSTEC, and recently installed at the T2K-Tsukuba and Coma systems in CCS. Using NICAM, we start investigating tropical cyclones, extra-tropical cyclones, arctic cyclones, and predicting blocking anticyclones, stratospheric sudden warming, and the Arctic Oscillation in the global atmosphere.

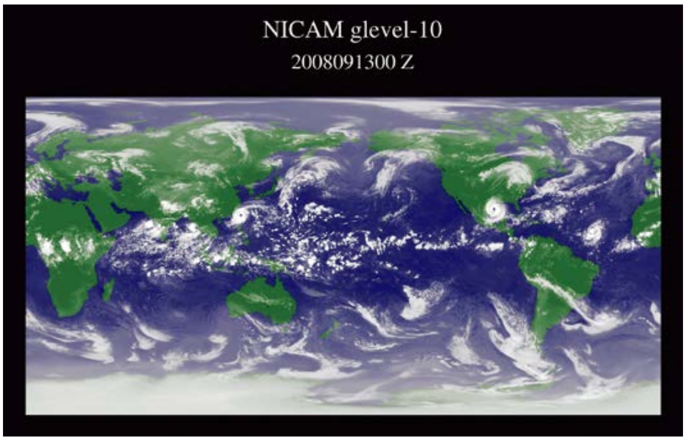


Fig.1 Numerical simulation of the general circulation of the atmosphere produced by 7-km resolution NICAM. NICAM-based modeling accurately predicted the evolution and movements of Typhoon Sinlaku and Hurricane Ike in 2008.

● WRF (Weather Research and Forecasting)

WRF, which is a compressible, non-hydrostatic regional model, is a collaborative development of the National Center for Atmospheric Research (NCAR), the National Centers for Environmental Protection (NCEP), National Oceanic and Atmospheric Association (NOAA), and the Association of Fish & Wildlife Agencies (AFWA) of the US, is now installed in the CCS T2K-Tsukuba supercomputer system. Using WRF, we investigate heavy rains and strong winds resulting from mesocyclones, urban heat island effects, and the recent record heat wave experienced in Kumagaya and Tajimi. Urban climate predictions associated with global warming is the main research focus of WRF modeling.

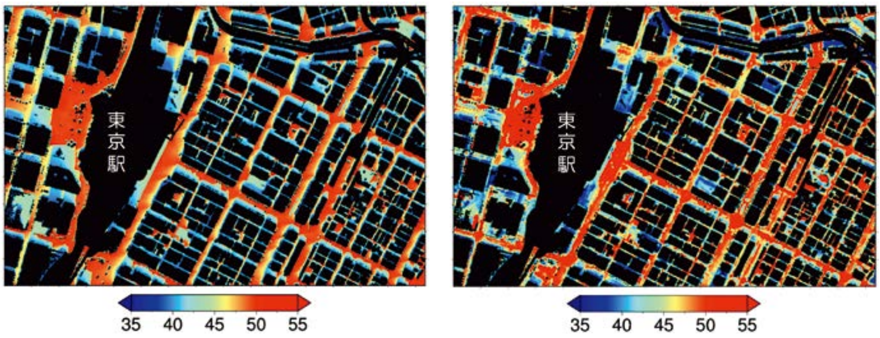


Fig.2 Road skin temperature distribution estimated by the model (left) and helicopter observation (right). Black indicates buildings.

Chief: Hiroshi L. Tanaka

Professor Hiroshi L. Tanaka of the Faculty of Life and Environment Sciences originally received his Ph. D. from the University of Missouri-Columbia, USA, in 1988. His research fields include general circulation, blocking and Arctic Oscillation.

High Performance Computing Systems Group

Chief: Taisuke Boku, Professor, Ph. D., Deputy Director of CCS **Member**: Daisuke Takahashi, Professor, Ph. D. / Osamu Tatebe, Professor, Ph. D. / Kawashima Hideyuki, Associate Professor, Ph. D. / Hiroto Tadano, Assistant Professor, Ph. D. / Ryohei Kobayashi, Assistant Professor, Ph. D. / Toshihiro Hanawa, Visiting Associate Professor, Ph. D.

Overview

In order to respond to demands for cutting-edge, ultra high-speed, and large capacity computation resources for the computational sciences, the High Performance Computing Systems (HPCS) Division in the Center for Computational Science (CCS) is investigating a wide variety of high performance computing (HPC) hardware and software systems. Through collaborative work with other application divisions in the Center, we are researching the creation of ideal HPC systems that are most suitable for application to real world problems.

Our research targets, which are spread across various HPC technologies, include high performance computing architecture, parallel programming language, massively parallel numerical algorithms and libraries, accelerated computing systems with GPU or FPGA, large scale distributed storage systems, and grid/cloud technology. The followings are among our more recent research topics.

Research Topics

● Tightly Coupled Accelerators architecture (TCA)

TCA is a novel concept that combines accelerating computing devices such as GPUs with low level communication facilities such as PCI Express to provide very low latency communication that directly connects accelerating devices for large scale parallelism with strong scalability. Basic network infrastructure, PCI Express Communication Hub Ver. 2 (known as PEACH2) has been developed as a part of the Highly Accelerated Parallel Advanced system for Computational Sciences (HA-PACS) supercomputer project. This concept extends the PCI Express Adaptive and Reliable Link (PEARL) network in order to employ PCI Express as the node-to-node interconnection for device-to-device direct communication among nodes.

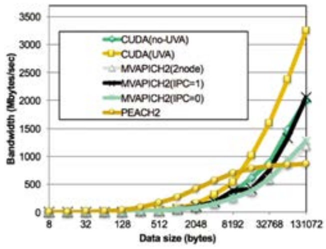


Fig.1 PEACH2 test board (left) and basic performance in bandwidth (right)

● XcalableMP

XxcalableMP is a next generation large scale parallel programming language. In future supercomputer generations, which are expected to have millions of cores and distributed memory architecture, traditional message passing programming would strongly reduce software productivity. To maintain high levels of performance tuning in large-scale parallel programming ease, we have designed and implemented a new language named XcalableMP. This language provides OpenMP-like directive base extension to C and Fortran to permit a global view model of data array handling in the manner of Partitioned Global Address Space (PGAS) concept as well as local-view modeling when describing highly tuned parallel programs. We are also developing an extension of XcalableMP for accelerating devices named XcalableACC in order to cover, for example, large-scale GPU clusters.

● Gfarm

Gfarm is a large-scale wide area distributed file system. In order to utilize computing resources spread widely throughout the world, high performance large-scale shared file systems are essential to process distribution freedom. Gfarm is an open-source distributed file system developed in our division that has the capability to support thousands of distributed nodes, tens of petabytes of distributed storage capacity, and thousands of file handling operations per second. With carefully designed system construction to ensure the metadata servers do not cause performance bottlenecks, it also provides a large degree of scalability for client counts. Gfarm is officially adopted as the High Performance Computing Infrastructure (HPCI) shared file system and provides nationwide access to and from any supercomputer in Japan.

● High performance and large-scale parallel numerical algorithms

Fast Fourier Transform (FFT)-E is an open-source high performance parallel FFT library developed in our division that provides an automatic tuning feature that is available from PC clusters to MPP systems. Our recent research into the Block Krylov subspace iterative method resulted in the introduction of the newly developed Block BiCGGR method, which provides both high precision calculation and low iteration counts for multi-vector linear equation solving. This method is currently used to solve large scale quantum chromodynamics (QCD) in the Center.

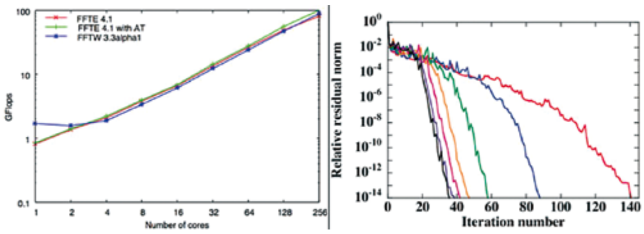


Fig.2 3D-FFT result on T2K-Tsukuba (left) and the convergence characteristics of Block Krylov subspace method under preconditioning with Jacobi method (right)

Chief: Taisuke Boku

Dr. Taisuke Boku got his Master and Ph. D. degrees from Department of Electrical Engineering, Keio University. After his career as an Assistant Professor in Department of Physics, Keio University, he moved to the University of Tsukuba and has been continuously working at Center for 25 years from its establishment. He has participated in the development of most of the supercomputer systems in CCS such as CP-PACS, FIRST, PACS-CS and HA-PACS as a HPC system researcher. All of these systems were designed and developed through discussion and collaboration with researchers in other Center application divisions. Dr. Boku's research interests include high performance interconnection networks, large scale cluster system design, parallel programming and tuning for real applications, and most recently, GPU and FPGA accelerated computing.

Database Group

Chief: Hiroyuki Kitagawa, Professor, Dr. Sc. **Member**: Toshiyuki Amagasa, Professor, Ph. D. / Hiroaki Shiokawa, Assistant Professor, Ph. D.

Overview

Big Data management and utilization are very important issues in various computational science fields. The Database Group is working on a wide range of Big Data analysis, management, and application problems from a data engineering perspective (Fig.1). Specifically, we are focusing on the following research topics: data processing frameworks for integrating heterogeneous and real-time data, scalable data analysis techniques for large-scale data, knowledge acquisition techniques for large-scale social and scientific data, and open data management techniques. Besides conducting basic research on algorithms and systems for Big Data, we are also collaborating with Divisions of Global Environment Science, Particle Physics, and Life Science in the Center for Computational Sciences, and other research institutes such as International Institute for Integrative Sleep Medicine for further contribution to a wider range of computational science applications.

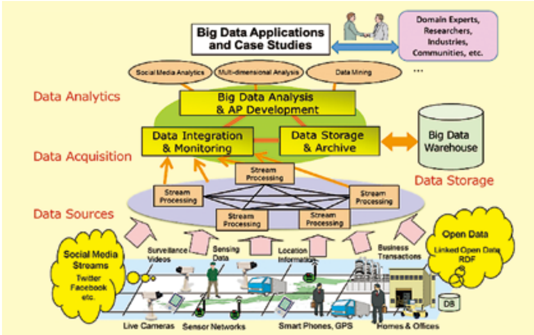


Fig.1 Research topic overview for Big Data management

Research Topics

Big Data Processing Frameworks

We are developing the following data processing systems and algorithms for Big Data management and utilization addressing the 3V properties of Big Data (Volume, Variety, and Velocity): (1) data processing frameworks for integrating and processing stream data obtained from sensors, social streams and other data sources, (2) scalable Big Data analysis techniques using massively parallel processing hardware such as GPUs, Intel Xeon Phi, and multi-core CPUs, (3) privacy-preserving and secure data processing schemes for Big Data management, and (4) data processing frameworks for open data including RDF and LOD. Specifically, we have developed a stream processing framework JsSpinner and several query optimization techniques. Furthermore, we have built an OLAP system for streams, named StreamOLAP, based on JsSpinner to support interactive analysis of massive stream data from multi-dimensional perspectives. These systems are utilized in Big Data use case studies in several research projects collaborating with Tsukuba city and Fujisawa city.

Data Mining Algorithms

We have developed various data mining and knowledge discovery techniques including (1) data analysis and mining algorithms for documents, images, and graphs, (2) social data analysis and mining methods, and (3) machine learning algorithms for biological and medical data analysis. In addition, we have proposed several efficient methods for analyzing large-scale graphs and social networks using general purpose computing on graphical processing unit (GPGPU) and many-core processors. The experimental results prove that our methods outperform the state-of-the-art algorithms running on a CPU by a factor of several orders of magnitude.

Scientific Data Management

To deal with rapidly increasing big scientific data, research has been conducted on the following topics: (1) development and operation of meteorological databases, such as the GPV/JMA Archive and the Japanese 25- (55-)year ReAnalysis (JRA-25/55) Archives (Fig.2), (2) development and operation of the Japan/International Lattice Data Grids (JLDG/ILDG), which enable researchers in particle physics to share and exchange lattice QCD gauge configurations, and (3) machine learning algorithms for effectively analyzing biological and medical data. Specifically, we have developed a novel sleep stage analysis algorithm MASC for mice in collaboration with International Institute for Integrative Sleep Medicine in University of Tsukuba. MASC automatically classifies states of mice into the REM sleep, Non-REM sleep, and wake stages with accuracy of more than 95%.

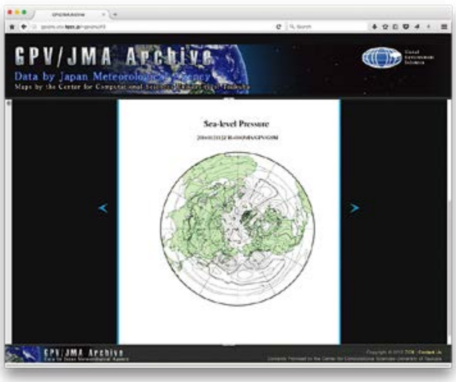


Fig.2 GPV/JMA archive

Chief: Hiroyuki Kitagawa

Hiroyuki Kitagawa is a full professor at Center for Computational Sciences, University of Tsukuba. He received the Dr. Sc. degree in computer science from the University of Tokyo in 1987. His research interests include databases, data integration, data mining, and information retrieval. He is a fellow of IPSJ and IEICE, and an Associate Member of the Science Council of Japan.

Computational Media Group

Group Leader: Yoshinari Kameda, Professor Ph. D. **Member**: Itaru Kitahara, Associate Professor, Ph. D. / Hidehiko Shishido, Assistant Professor, Ph. D.

Overview

Computational media are advanced information media on which high sensing functionality and huge computing resources are elegantly unified over computer networks. We aim to supply appropriate information to everyone wherever and whenever it is necessary through computational media. Since such media stand on advanced and intelligent visual information processing technologies, our research area includes developing new technologies, such as mechanisms for searching appropriate sensory devices, mechanisms for searching and identifying information receivers, mechanisms for appropriate conversion to fit the properties of receivers, and mechanisms for preventing information interception, alteration, and/or unauthorized copying.

We also pursue the advanced applications based on our video processing technologies. We have been working on vision analysis and novel visualization on civilization engineering, sport analysis, support for athlete training, driver support in vehicle, safety assessment of passengers on autonomous vehicle, navigation for visually impaired, crowd sourcing, social imaging, etc.

Research Topics

- **Next generation sport browsing system by free-viewpoint virtual camera**

Viewers can freely fly through the sport field and see the game from arbitrary viewpoints.

- **Novel public application of surveillance cameras**

We pursue to add convenient and usable visualization technology to our society to let people recognize the positive value of the cameras.

- **Seamless unification of real world and virtual reality**

Our mixed reality research can promote smooth communication by the seamless unification of the two worlds.

- **Massive Sensing**

A large and long-term observation and recording are utilized to recognize human behavior analysis and support of our daily life.

- **Location Estimation by only a single snapshot on a street**

Our vision based approach does not need GPS and/or other sensors, hence it could be applicable to any situations.

- **Ultra-high Immersive visualization based on multiple cameras**

Our high resolution and smooth video switching approach can achieve outstanding immersive experience.

We have been working on visualization and natural camera operation of free-viewpoint camera on soccer game field. While our visualization technology realizes three dimensionally free motion of the virtual camera on a captured real game, it is not easy for ordinary people to control the camera to see what they want. We have invented three new user interface to solve this problem. The first approach is to attach the virtual camera to a player in the game (Fig.1). It is called first person view. The user can get direct immersive experience, but the camera motion should be carefully designed so as to prevent VR sickness. The second approach is to control the camera by two hands over a miniature of the soccer field (Fig.2). By setting up a horizontally placed display as a miniature of the soccer field, the user can glance the whole game from bird-eye viewpoint. The user has two sticks by their two hands. The end of the one stick corresponds to a position of the camera, and the endo of the other correspond to a point of interest. The view of the virtual camera is rendered in the center display. The third approach is to control the transition and rotation of the camera by tapping operation on a tablet display. We have proposed a new and natural tapping command system so that many users can control the virtual camera without detailed instruction and training.

These our new interface designs have been presented in international and domestic conferences and academic articles, and won high evaluation.

Fig.3 Tapping interface for camera rotation and motion

Fig.1 First person viewpoint in a soccer game

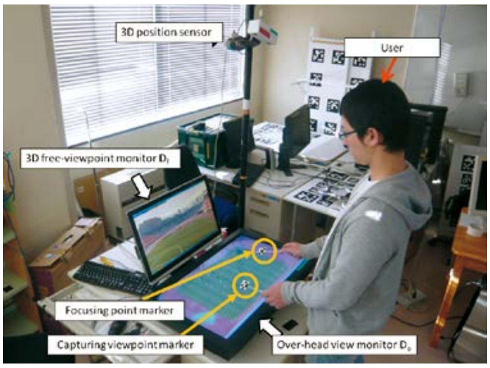


Fig.2 Two-hand camera operation over a miniature of the soccer field

Group Leader: Yoshinari Kameda

Yoshinari Kameda received his Bachelor of Engineering degree, his Master of Engineering, and his Doctor of Philosophy from Kyoto University in 1991, 1993, and 1999. He was an assistant professor at Kyoto University until 2003. He was a visiting scholar in AI Laboratory at MIT in 2001-2002. In 2003, he joined University of Tsukuba and is now a full professor. Dr. Kameda's research interests include intelligent enhancement of human vision, augmented reality, video media processing, computer vision, and sensor fusion.

Introduction of Research Projects Offices

Project Office for Exascale Computational Sciences

Develop Computational Sciences with the Full Performance of the Machine

Head: Kazuhiro Yabana, Professor, Ph. D.

Supported by the dramatic growth of computer power, the computational sciences have seen remarkable developments in recent years, and are now recognized – along with theory, experiment, and observation – as indispensable partners in the promotion of the cutting-edge scientific frontiers of the 21st century.

Nowadays, computers characterized by a new architecture are appearing in rapid succession and include large-scale systems equipped with Graphics Processing Units (GPUs) as accelerators, massively-parallel computers equipped with many-core processors, which may play a central role in future large-scale computing, to say nothing of ordinary massively-parallel computers combining a multitude of CPUs. Due to advances of such diverse computers, it becomes a difficult task for researchers to make computations with the full power of each machine.

By means of close collaborations among researchers of physics and those of computer sciences, the Center for Computational Sciences (CCS) has successfully achieved a number of breakthroughs by developing optimum computers for computational sciences in the fields of particle physics and astrophysics. Furthermore, the Center now has a Project Office for Exascale Computational Sciences dedicated to close collaborations among computational and computer scientists in a wide variety of fields, and to establishing cooperation among researchers belonging to divergent scientific fields.

The services of this Office are not restricted to the Center alone, but extend outside to promote nationwide collaborations. To date, it has conducted analyses and examinations of hot spots for major applications to ensure that they show high efficiency in the Highly Accelerated Parallel Advanced system for Computational Sciences (HA-PACS), which is a massively-parallel supercomputer equipped with GPU accelerators, and in COMA, which is equipped with processors of Many Integrated Core architecture, under close cooperation with the Project Office for Exascale Computing System Development, which is the organization promoting the development of new computers. Currently, developments and adjustments of computer codes that run efficiently at Oakforest-PACS in Joint Center for Advanced High Performance Computing (JCAHPC), the fastest supercomputer in Japan equipped with processors of Many Integrated Core architecture, have been a central issue at the Office.

Activities on Oakforest-PACS undertaken by the Project Office for Exascale Computational Sciences

	Scientific Target	Numerical calculations employing Many Integrated Core processor
Particle Physics	- High precision calculations of the standard model of particle physics - Multiscale physics - Physics at finite temperature and density - Physics beyond the standard model	- Iterative solver for linear equations with large sparse matrices - Dense matrix-matrix multiplication - Extraction of eigenvalues and singular values
Astrophysics	- Exploring the formation of the first generation of astrophysical objects in the early universe - Exploring the structure formation of galaxies, galaxy clusters, and the large-scale structures in the universe	- Radiation transfer and radiation hydrodynamic simulations using ray-tracing method - Vlasov simulation in 6 dimensional phase space
Nuclear Physics	- Exploring many-nucleon dynamics based on unified description of nuclear structure and reactions	- Projection and configuration-mixing calculations - Time-dependent density-functional theory calculations incorporating pair condensation
Material Science	- Exploring light-matter interactions and ultrafast electron dynamics in matters	- Time-dependent density functional theory calculations in real time and real space
Life Science	- Analyses of enzymatic reaction in living body - Large-scale phylogenetic analyses on eucaryote	- Fragmented molecular orbital method - Real space Car-Parrinello molecular dynamics method
Global Environmental Science	- Exploring arctic oscillation - Exploring urban climate and local wind	- Efficient solution of Poisson equation - Similarity retrieval of high-dimensional data
Computational Informatics	- Information management and knowledge discovery in massive scientific data	- Efficient processing of large graphs - Cluster analysis over large-scale scientific data
Mathematical modeling and algorithms	- Large-scale parallel computational methods in computational sciences	- Parallel algorithms for a generalized eigenvalue problem of dense matrices - Development of eigenvalue calculation software for sparse matrices – z-Pares, CISS

Empirical Research for Exascale Computing

Head: Taisuke Boku, Professor, Ph. D., Deputy Director of CCS

The theoretical peak performance of massively parallel supercomputers is represented as the processor performance of a single node and the number of those nodes. The performance improvement of supercomputers, to date, has been mainly achieved by the "scaling system", which refers to increasing the number of computing elements in a system. However, faced with limitations related to electric power consumption and/or the thermal or fault ratio of each part, "weak-scaling" strategies are facing their achievable limits. To overcome these limitations, it will be necessary for the next generation of Exascale computing to improve the single node performance by several tens TFlops, as well as to establish fault tolerant technology that will enable several million nodes to be incorporated into a system. For single node performance improvements, one of the most promised methods is using accelerators to reduce the time-to-solution, rather than enlarging the computation problem size. This is known as the "strong-scaling" problem.

In the Project Office for Exascale Computing System Development, we have been researching the next generation of accelerated computing systems under the new concept of accelerated computing named Tightly Coupled Accelerators (TCA). The HA-PACS/TCA is an experimental testbed for TCA architecture, as well as the application development platform with the latest graphics processing unit (GPU) computing technology. Currently, we are extending the concept of TCA to more advanced one named Accelerator in Switch (AiS) where FPGA (Field Programmable Gate Array) is aggressively utilized both of computation and interconnect communication between all computation resources in a node and over nodes. In generic GPU clusters so far, the applicable applications are limited due to lack of flexibility, partially insufficient degree of parallelism, communication bottleneck (especially latency) among multiple nodes, etc. Under AiS concept, we employ FPGA for partial offloading of computation which is not suitable for GPU as well as computation tightly combined to inter-node communication. Here, we utilize FPGA for following purposes.

High speed inter-node communication

In the TCA, the communication among FPGA is performed on PCI Express protocol to treat it as the extension of intra-node GPU-to-GPU communication. In recent FPGA, however, it is available to provide 100Gbps class of communication link as hard-IP which can be applied for high bandwidth and low latency inter-FPGA communication.

Partial offloading of computation

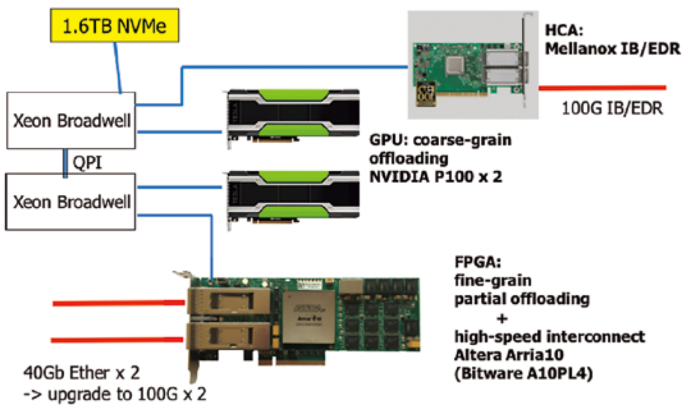
GPU is good at for wide SIMD-style computation with large degree of synchronized parallelism, however not all application has such a feature or its degree is not sufficient in some part of the application. It causes serious bottleneck on strong-scaling of HPC system where the performance of GPU does not contribute. We will (partially) offload such computation part to FPGA with flexible programming to compensate the flexibility of GPU and slow speed of CPU.

Unification of computation and communication

Implementing the high speed communication and partial offloading to an FPGA for computation-communication unification, we can realize a new style of accelerated computing for strong-scaling to release the performance bottleneck on ordinary accelerated cluster systems.

PPX (Pre-PACS-X)

Based on the concept of AiS, CCS is planning to introduce the 10th generation of PACS series supercomputer, PACS-X (PACS ver. 10). For a proof-of-concept system of AiS, we have built a prototype system of PACS-X, named PPX (Pre-PACS-X). PPX is equipped with two cards of NVIDIA TESLA P100 which is the fastest GPU to date, two sockets of Intel E5-2680v3 (Broadwell architecture), Intel/Altera Arria10 FPGA evaluation board, 1.6 TByte of NVMe local storage, as well as InfiniBand EDR interconnection HCA. The system consists of six computation nodes with 100G Ethernet switch. There are two channels of 40Gbps Ethernet link from Arria10 FPGA to provide multi-link high speed communication by Ethernet. All nodes are also connected by InfiniBand EDR (100Gbps link) in parallel with FPGA network. PPX is used for development of FPGA, system software, integrated language and library, and various applications toward PACS-X development.



PPX node configuration

Project Office for HPCI

Innovative Research Using the Flagship Supercomputer in Japan and Framework to Advance Computational Science and Technology

Head: Yoshinobu Kuramashi, Professor, Ph. D.

HPCI Plan and Strategic Program Field 5

The innovative High Performance Computing Infrastructure (HPCI) plan, which was established with the "K computer" 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, which had been operated from FY2011 to FY2015, five potential fields were identified as strategic fields that not only required K computer resources, but also were expected to yield significant social and scholarly breakthroughs. "Field 5: The origin of matter and the Universe" was one of these. This field dealt with fundamental physics, primarily concerning elementary particles, the atomic nucleus, and astrophysics. The institution (strategic institution) that successfully led Field 5 research and development for five years was 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 (KEK), and the National Astronomical Observatory of Japan (NAOJ).

Toward the Post-K Computer

The post-K computer development plan under the FLAGSHIP 2020 Project, initiated by the Ministry of Education, Culture, Sports, Science and Technology in 2014, has set the target of developing (1) the next generation flagship supercomputer of Japan (the successor of the K computer) along with (2) a wide range of applications that will address top 9 priority social and scientific issues. "Priority Issue 9: Elucidation of the fundamental laws and evolution of the universe" led by the CCS, University of Tsukuba and 10 other institutions is essentially the successor of "Field 5: The origin of matter and the Universe" aiming at new developments. The CCS also joins "Priority Issue 7: Creation of new functional devices and high-performance materials to support next-generation industries (CDMSI)". In addition to the priority issues, there are four exploratory challenges selected to be tackled using the post-K computer. The CCS joins two of them: "Exploratory Challenge 1: Frontiers of basic science: Challenging the limits" and "Exploratory Challenge 3: Elucidation of the birth of exoplanets (second earth) and the environmental variations of planets in the solar system". As a core institution of priority issues and exploratory challenges, the project office promotes the accomplishment of research and development targets.

K Computer

Toward Formation of the International Hub of Computational Sciences

Head: Daisuke Takahashi, Professor, Ph. D.

The Center for Computational Sciences (CCS) conducts research activities grounded in the central concept of "Multidisciplinary Computational Science" through collaboration and cooperation among various computer-related and scientific fields. The Liaison Office for Multidisciplinary Computational Sciences is a key part of the Center's efforts aimed at maintaining its position as an international hub for computational science information.

Cooperation among Different Fields

In order to promote multidisciplinary computational science, cooperation among different fields is essential. In 2011, using the research results of first-principles electronic state calculation for 100,000 atom silicon nanowires using K computer, a research group from RIKEN, the University of Tsukuba, the University of Tokyo, and Fujitsu Limited won the Gordon Bell Prize for Peak-Performance, which is recognized as an outstanding achievement in high-performance computing. This is just one of the results of cooperation among different fields that have taken place at the Center in recent years.

International Cooperation

As for international cooperation, partnership agreements have been concluded between University of Tsukuba and the University of Edinburgh in the UK, as well as with Lawrence Berkeley National Laboratory in the US. Furthermore, as part of the efforts to deepen the computational science research exchanges, the CCS and the University of Edinburgh Parallel Computing Center (EPCC) are currently hosting joint symposiums, and the Center is cosponsoring workshops with Lawrence Berkeley National Laboratory. Additionally, bilateral exchange joint research projects into computational materials science are being conducted with Vanderbilt University and the University of Washington in the US under the sponsorship of the Japan Society for the Promotion of Science (JSPS).

Multidisciplinary Pioneering Program

The Multidisciplinary Pioneering Program encourages the promotion of research efforts that require collaboration and cooperation among divergent scientific fields. For example, there is a current project underway that requires cooperation between the computational physics (science) and numerical analysis (engineering) fields in order to implement calculation code with high execution efficiency, and to perform the necessary large-scale simulations using the code. There are also projects that aim at new research deployments and developments by facilitating organic cooperation among different fields utilizing the same techniques in computational science. This Multidisciplinary Pioneering Program has been carried out in conjunction with the collaborative multidisciplinary program of the center.

Organization for Collaborative Research on Computational Astrobiology

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, 51 researchers from 20 institutes are participating in the organization, which was formed at the initiative of the CCS, University of Tsukuba.

Collaboration workshop between Tsukuba and Edinburgh universities

Promotion Office for Computational Sciences

Promote Social Contributions and Human Resource Development in Computational Sciences

Head: Hiroyuki Kitagawa, Professor, Dr. Sc.

The Promotion Office for Computational Sciences promotes the personnel development program associated with computational sciences in collaboration with the graduate schools, conducts activities related to campus-wide courses for graduate students, and contributes to society by disseminating information concerning the advanced research conducted at this Center.

Personnel Development

Graduate School Dual Degree Program

The graduate school consists of master's programs and doctoral programs. Doctoral candidates usually study a specialized field through both programs. However, since sophisticated computer skills and experiences are necessary to advanced research in scientific fields such as physics, global environment, and biology, a broad level of expertise in both science and computer technology is required for computational science doctoral candidates.

The Promotion Office for Computational Sciences promotes dual degree programs to meet this need. The dual degree program makes it possible to obtain a doctorate in a scientific field along with a master's degree of computer science simultaneously, by a doctoral program in scientific field and a master's program in computer science.

Computational Science English Program

In response to the increasing numbers of international students from overseas, the Computational Science English Program was established as a master's program in computer science that can be completed in English. As shown in the table, this program provides English lectures in 14 subjects, along with English language research guidance aimed at assisting master degree candidates in successfully obtaining their degrees.

Campus-wide Courses for Graduate Students

Since computer technology is the foundation of all research activities in graduate schools, classes in computational science literacy and high-performance parallel computing technology for computational science have been established as common subjects for all graduate students. These are open to outside researchers and students from other universities.

	Course Name
Special Subjects	Advanced Course in Computational Algorithms
	Special Lecture on Numerical Simulation
	Programming Environment
	Data Engineering I
	Advanced Course in High Performance Computing
	Statistical Analysis
	Basic Computational Biology
	Topics in Computational Science I
	Principles of Software Engineering
	Advanced Performance Evaluation for Computer and Communication Systems
	Adaptive Media Processing
	Experiment Design in Computer Science
Graduate School Common Courses	Computational Science Literacy
	High Performance Parallel Computing Technology for Computational Sciences

Social Contribution

Cooperation with other institutions

Domestically, research cooperation in the field of high performance computational technology is advanced under the T2K Alliance that connects University of Tsukuba with the University of Tokyo and Kyoto University, along with the close research cooperation ties with other research organizations within Tsukuba City. We have also built an international research cooperation framework through the International Lattice Data Grid (ILDG), which is an international data-sharing project in particle physics, with the University of Edinburgh (UK), Lawrence Berkeley National Laboratory (US), and others. We intend to further strengthen and develop the domestic and international research cooperation, and to utilize those relations as a bridge among researchers and exchange students to pursue collaborative research.

Mt. Tsukuba Project

This project supports research and educational activities, while contributing to society, by continuously observing, recording, and disseminating weather observations (temperature and humidity) from the 877m summit of Mt. Tsukuba.

Dissemination of Information

Our office produces three types of brochures. One aimed at high school students and above, another aimed at graduate students and above, and the third written in English to meet the needs of our diverse applicants and students. The office also coordinates visits from high school students within Japan and overseas university students, as well as "open house" events that are open to the public. Through these efforts, we work to deepen exchanges with people around Tsukuba City and in the Kanto region. In addition, the faculty members actively offer and promote off-campus classes and lectures.

Bureau of Public Relations and Strategy

The Bureau of Public Relations and Strategy performs activities aimed at improving relations with society in order to advance the mission of the Center for Computational Sciences (CCS) and to promote the computational sciences themselves.

Articles and the photos of press conference

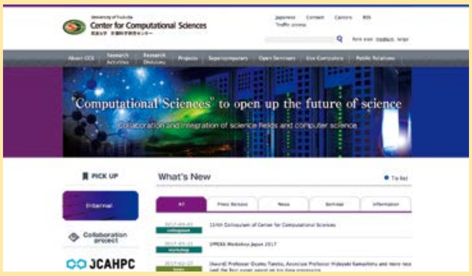
Press release

Results of research and activities in the CCS are announced to the media and the public through press release and a press conference.

You can find a lot of contents;
movies, brochures, interviews and so on.

Contents

CCS publish various information via our website.
(http://www.ccs.tsukuba.ac.jp/eng/)



CCS Tour / Open day

At the CCS tour for high school students, we show our research activity and the supercomputer of the center. About 2000 people a year visit the CCS.

Projects, symposiums, and conferencing support

- Public relations activities on the Mt. Tsukuba project
- Support to Joint Center for Advanced HPC (JCAHPC)
- Booth design and management support at SC

etc.

Leaflet of Mt. Tsukuba Project

Article about Oakforest-PACS, HPCWIRE Japan

SC16

ACCESS

Airport Bus

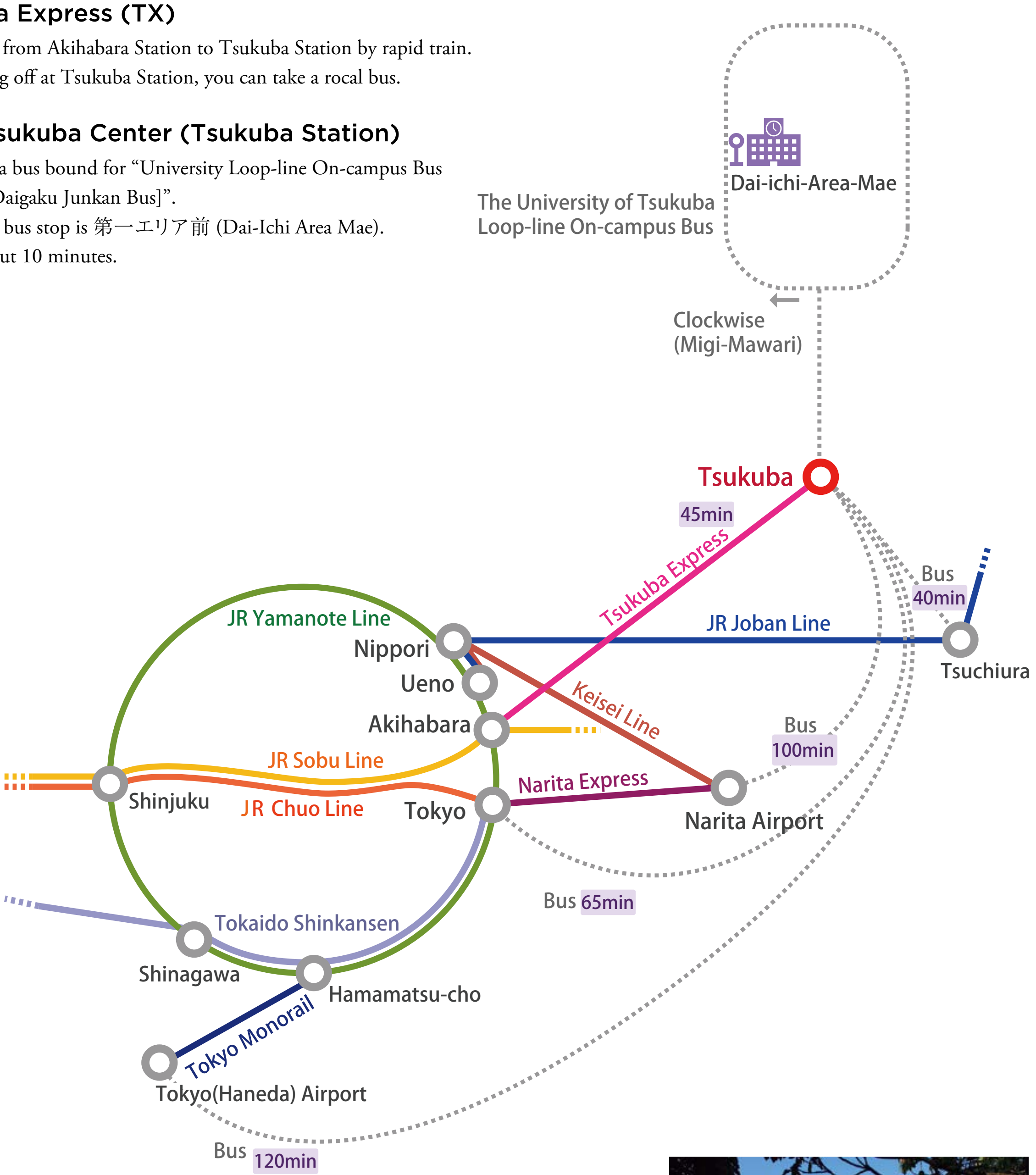
Narita Airport: About 60 minutes from Narita Airport by bus bound for "Tsukuba Center".
Take a bus at the bus stop at the Terminal 1, the Terminal 2, or the Terminal 3.
Haneda Airport: About 120 minutes from Haneda Airport by bus bound for "Tsukuba Center".
Take a bus at the bus stop No.6 in the International Terminal or at the bus stop No.13 in the Terminal 1 or 2.
After getting off at Tsukuba Center, you can take a rocal bus.

Tsukuba Express (TX)

45 minutes from Akihabara Station to Tsukuba Station by rapid train.
After getting off at Tsukuba Station, you can take a rocal bus.

From Tsukuba Center (Tsukuba Station)

Please take a bus bound for "University Loop-line On-campus Bus [Tsukuba Daigaku Junkan Bus]".
The nearest bus stop is 第一エリア前 (Dai-Ichi Area Mae).
It takes about 10 minutes.



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