筑波大学
University of Tsukuba

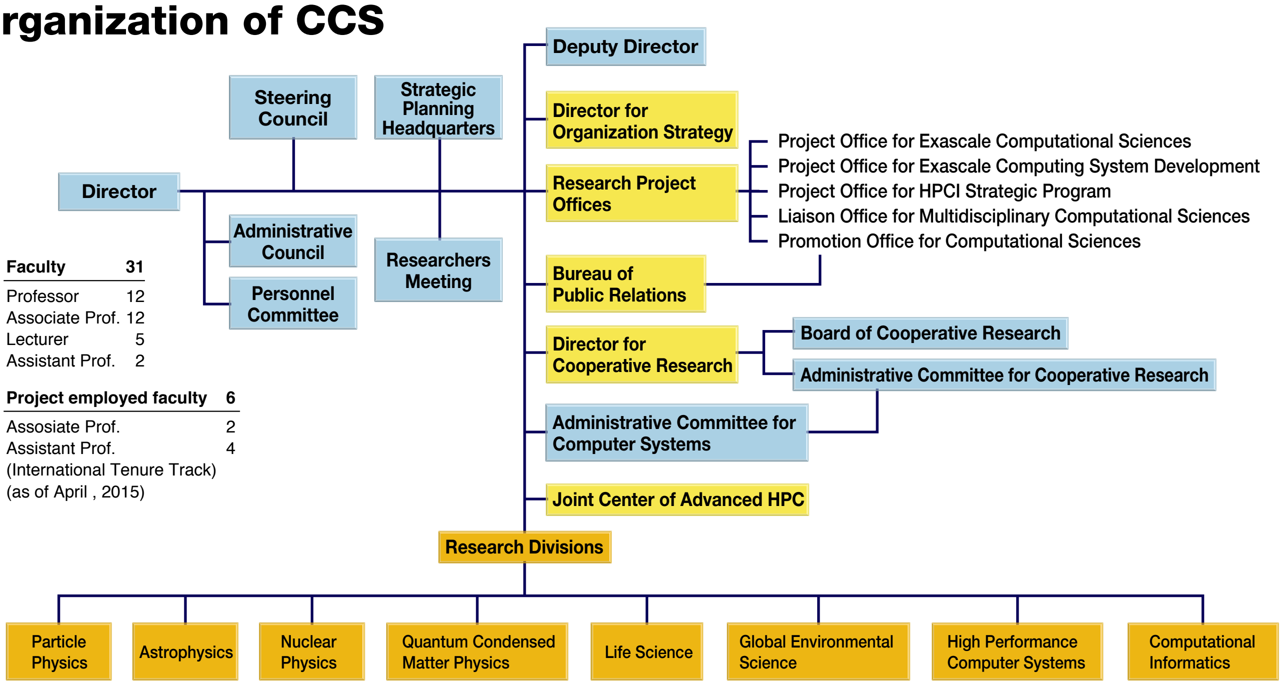
University of Tsukuba
Center for Computational Sciences
2015

C enter for Computational Sciences (CCS)

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. To realize the high-speed, large-scale simulations required in these research areas, the CCS works continuously to develop new state-of-the-art computing systems and networks, while also striving to advance cutting-edge knowledge in computational intelligence, computational media, and database technology.
Originally formed as the Center for Computational Physics (CCP) in 1992, the CCS was reorganized and relaunched under its current name in April 2004. Currently, the CCS is known as one of the world' s leading research institutes engaged in the pursuit of the above-mentioned fields, and is also a notable joint-use facility for outside researchers. In all of these areas, the CCS plays a significant role in the development of the Multidisciplinary Computational Science. 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.

Organization of CCS



Message from the Director

Masayukia 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. The mission of the CCS is promoting multidisciplinary computational science based on the fusion of computational and computer sciences, while nurturing the efforts of multidisciplinary and international researchers who play active roles in merging the fields of science and technology. The CCS is also proud to support various other programs aimed at improving collaboration between different research fields.
In 2010, the CCS was recognized under the Advanced Interdisciplinary Computational Science Collaboration Initiative (AISCI), and has since provided the use of its computational facilities to researchers nationwide as part of the Multidisciplinary Joint-use Program. Furthermore, as part of efforts aimed at supporting collaboration in multidisciplinary computational science, the CCS welcomes applications for scientific meetings, hosts talented researchers from overseas, and strives to locate and retain short-term auxiliary supporters. All these efforts combine to create a strong bridge between domestic and international collaborations, while promoting the interchange of researchers and students.
Also in 2010, the CCS was recognized as an affiliated institute of the High Performance Computing Infrastructure (HPCI) Strategic Program Field 5 "Origin of Matter and the Universe", which aims to further advance the computational sciences using the K computer. Furthermore, the CCS is active in the HPCI "Study on Exascale Heterogeneous Systems with Accelerators", which is being conducted to realize exascale computers. In this project, being conducted through collaboration between computational and computer scientists, the hardware and software best suited for advanced scientific research are being explored.
To date, the computational science field has achieved significant results in a wide variety of scientific fields that are complementary to experimental/observational and analytic approaches. Moreover, computational science has pioneered a novel methodology based on the first principles that has allowed us to make collaborations between different fields especially fruitful. By stimulating international collaborations, the CCS aims to become a hub institute for multidisciplinary computational science through enhanced cooperation between computational and computer sciences.

CCS Vision of "Multidisciplinary Computational Science"

The mission of the CCS centers on developing computers best suited for scientific exploration based on cooperation between computational and computer scientists, not solely providing computational facilities to such scientists. We define this approach as "Multidisciplinary Computational Science" and use it to promote research in a wide variety of fields related to computational sciences, while supporting researchers nationwide by providing computational resources and technical advice from computer scientists in joint-use programs.

While high-performance computing systems are essential tools for carrying out successful computational science research, the development of computational science cannot be satisfactorily achieved solely by scientists using computers. Instead, close collaboration and synergy is required between computer scientists (with expertise in computer hardware, software, algorithms and programming) and information scientists (with expertise in data and media engineering and various technologies). Therefore, in order to establish a solid foundation for the development of computational science, it was necessary to develop a system that integrates the activities at the forefront of scientific research with those of computer and information science.

The CCS has been striving to carry out collaborative research in a number of ways. For example, we have developed the massively parallel supercomputer named the Computational Physics by Parallel Array Computer System (CP-PACS), which was ranked as the No. 1 system on the Top 500 List of November 1996, through collaboration between physicists and computer scientists. 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 through interdisciplinary collaboration. The T2K-Tsukuba system (2008) is a large-scale general-purpose cluster system designed by the University of Tokyo and Kyoto University researchers through the T2K open supercomputer alliance. The "T2K" acronym itself refers to the alliance between the University of Tsukuba, the University of Tokyo, and Kyoto University. We are now moving forward with a project aimed at post-petascale computing using accelerators, which is known as Highly Accelerated Parallel Advanced system for Computational Sciences [HA-PACS (2011)].

Our vision of "Multidisciplinary Computational Science" aims at developing and enhancing close collaboration among various scientific disciplines by applying the activities undertaken in the computer sciences pursued at the CCS, which are unique worldwide. This approach has capitalized on "Study on Exascale Heterogeneous Systems with Accelerators" to realize exascale computing beyond current petaflop computing levels.

Collaborations and Alliances

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. 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 chromodynamic (QCD) configurations worldwide. An XML-based markup language, QCDml, which describes metadata for QCD configurations and ensembles (sets of configurations with common physics parameters), has been developed. 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)].

Regional grid interoperability has been achieved for download operations, and valuable configurations have already been archived in the grid. 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.

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, which resulted in the construction of an unprecedentedly large-scale computational facility.

Furthermore, 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).

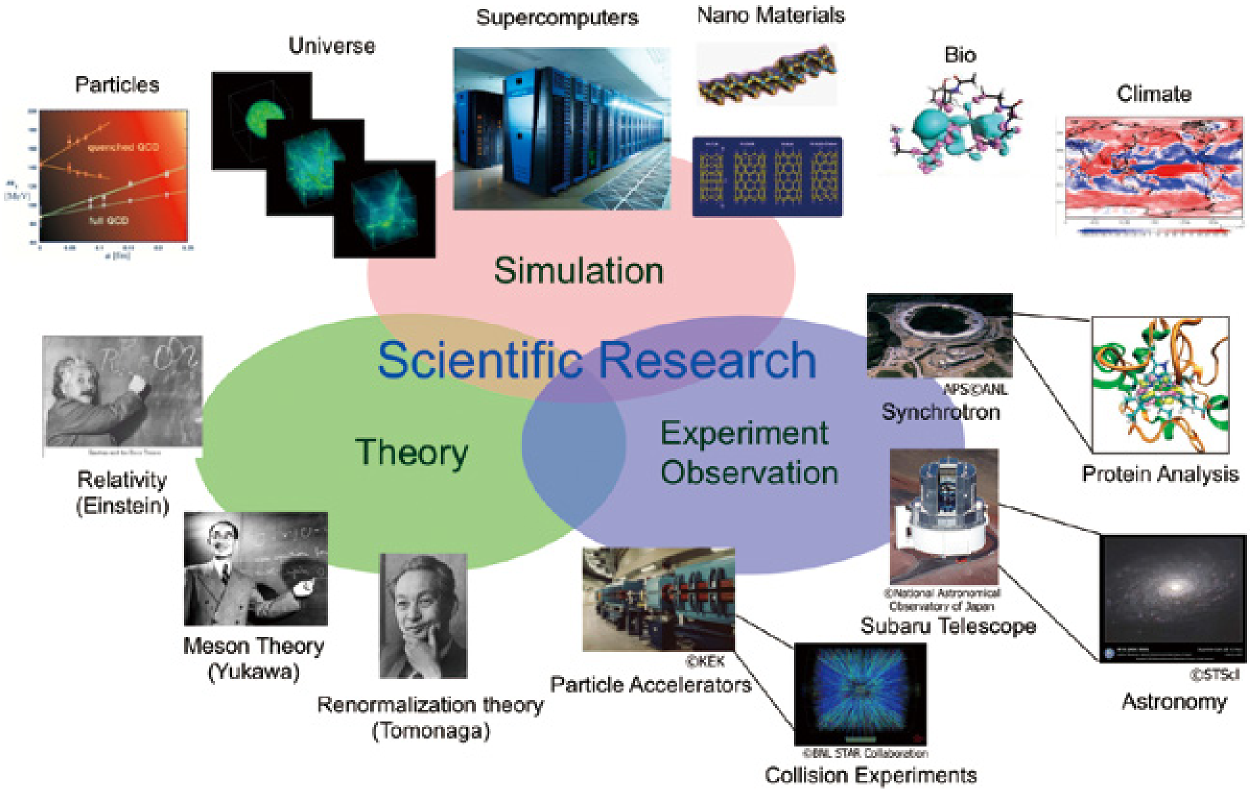
Chronology of CCS

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 established in alliance with the University of Tokyo
2014	April	COMA installed and started operation

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.

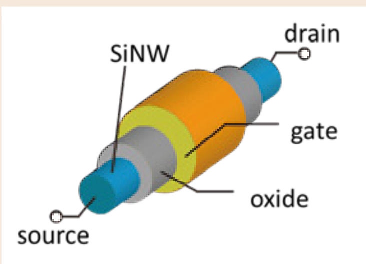
Computational science has shifted the scientific research paradigm to include simulation – along with experiment and theory – as fundamental methods of science. Computer simulation allows us to acquire scientific insights into problems that are too complex or difficult to study analytically using just “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.



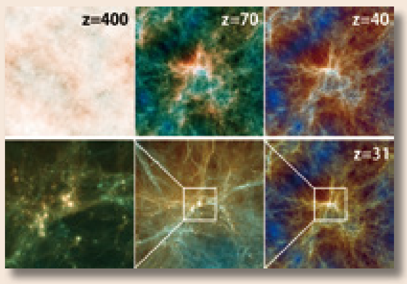
◆Awarded Gordon Bell Prize Two Years in a Row

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

The Highly Accelerated Parallel Advanced system for Computational Sciences (HA-PACS) Base Cluster System is a GPU(Graphic Processing Unit) cluster that incorporates the latest CPU and GPU technologies. Capable of providing 802 Tflops of peak performance with just 268 computation nodes, the system was ranked at number 41 on the June 2012 Top 500 List. Each node of the system is based on the GreenBlade 8200 series produced by Appro International Co., and consists of two Intel E5-2680 (8 core, SandyBridge-EP) processors operating at 2.6 GHz as the CPU, and four NVIDIA M2090 processors as the GPU.

The theoretical peak performance of one node is approximately 3 Tflops. All nodes are joined via the interconnection network with dual-rail InfiniBand QDR × 4 in a Fat-Tree configuration to provide 2.14 TByte/s of bisection bandwidth.

The full system, which entered service in February 2012, is dedicated to the development of application on state-of-the-art computational sciences that require the accelerated computing performance provided by such large scale GPU clusters. This Base Cluster system is finally extended with additional nodes that include a special feature named Tightly Coupled Accelerators (TCA) architecture, which enables direct communication between GPUs over computation nodes by the external link PCI Express.

This TCA system, which is currently under development at CCS is based on field programmable gate array (FPGA) technology and is the main focus of the HA-PACS Project, which is supported by the Ministry of Education, Culture, Science, Sport and Technology (MEXT). The extended system, named HA-PACS/TCA, was completed on October 2013 with 364 Tflops of peak performance, and the entire system performance reached to 1.166 Pflops.

HA-PACS

COMA (PACS-IX)

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 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 systen.

CCS and Information Technology Center at the University of Tokyo plan to introduce a massively parallel supercomputer based on many-core architecture processor at JCAHPC (Joint Center for Advanced HPC) which is a joint organization by two centers. We will develop various large scale computational science applications based on our experience on COMA, especially focusing on particle physics, astrophysics and biological science.

COMA

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.

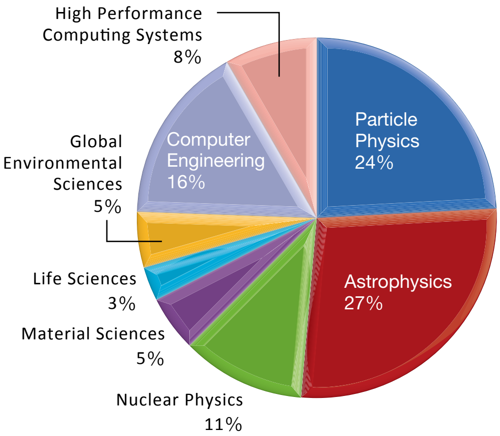
The MCRP consists of the following programs:
(1)Multidisciplinary Pioneering Program (MPP) (2)Priority Subjects Promoting Program (PSPP) (3)Cooperative Research Promoting Program (CRPP)

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, 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-)], and COMA(PACS-IX)(2014-).
The number of MCRP-approved projects conducted over the last seven years is shown in the table. Approximately 30 to 60 projects are approved each year. A breakdown of the 2013 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

A breakdown of the 2013 projects by research fields



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

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

Joint Center for Advanced High Performance Computing (JCAHPC)

Center Director: Hiroshi Nakamura, Professor, Director of Information Technology Center, University of Tokyo
Deputy Center Director: Masayuki Umemura, Professor, Director of Center for Computational Sciences, University of Tsukuba

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 installation of a supercomputer system, designed (for the most part) by the faculties of both organizations, at the ITC at the Kashiwa Campus of the University of Tokyo, and to fabricate and operate an advanced, large-scale, high-performance computing platform. 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.

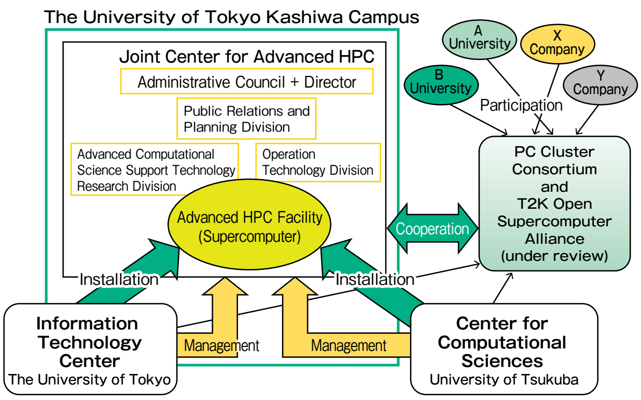
Background and History

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

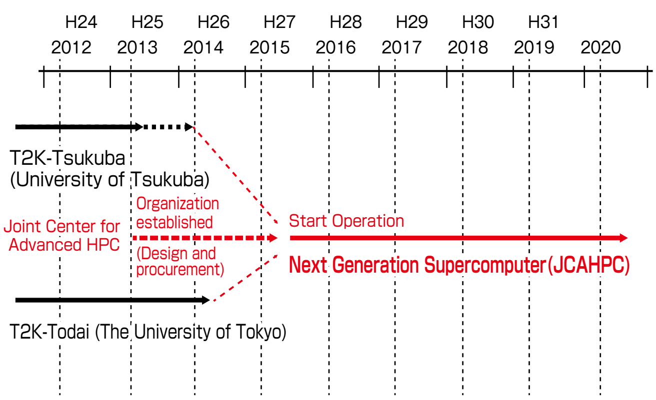
The objective of the JCAHPC mission is to design and develop of a large-scale HPC system worthy of becoming the hub of Japan's computational sciences, and to architect an advanced system that exploits many-core technology, which is believed to be the key to future HPC systems. Furthermore, such research 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.
This system is scheduled to be installed for operation and management after April 2015.
After the system is operational, both institutions will distribute the system proportionally based on computation volume, operate their portions separately, and offer services to each user based on the programming used. This arrangement not only reduces administrative costs and the like, but also enables computing at a larger-scale than the case where each institution independently owns a supercomputer system. This effort represents the first attempt to create such a facility in Japan, as well as the first attempt in Japan to jointly operate and administer a supercomputer.

JCAHPC Organization Chart



(JCAHPC: Joint Center for Advanced HPC)

Plan



Division of Particle Physics

Particle Physics Group

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

Overview of the Field

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 particles), 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)

Recent accomplishments

Since the physical point simulations with the quark masses in nature have been made possible thanks to algorithmic improvemens 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 recent studies, the results for the hadron masses obtained by our lattice QCD simulation had almost reproduced the experimental values (Fig.1). Furthermore, we have embarked on a direct construction of helium nuclei and deuteron from quarks with a successful extraction of their binding energies, though the quark masses are still heavier than the physical values. In addition, as a different approach, an attempt to determine the effective baryon interactions is pursued by measuring the potential between baryons with lattice QCD (Fig.2).

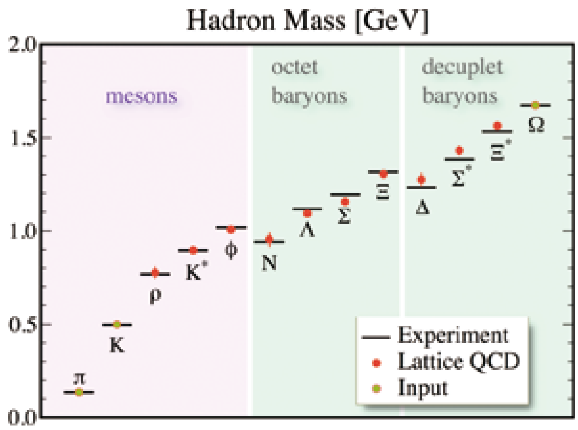


Fig.1 Hadron masses with lattice QCD in comparison with experimental values

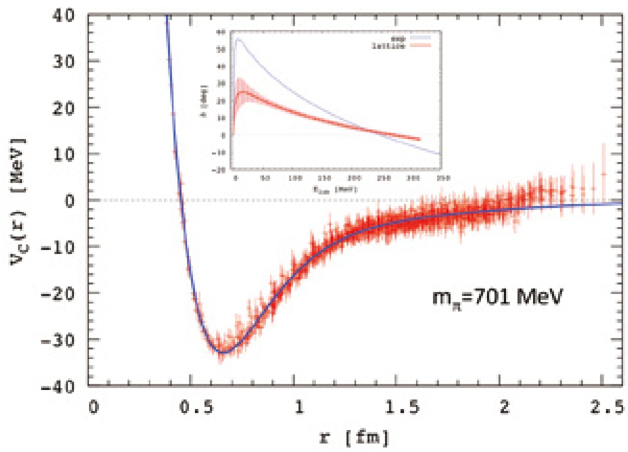
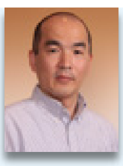


Fig.2 Measured potential between two nucleons and corresponding scattering phase shift



Chief : Yoshinobu Kuramashi

Professor, University of Tsukuba Faculty of Pure and Applied Sciences/Center for Computational Sciences (CCS)

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:** Yuri Aikawa, Professor, Ph. D. / Masao Mori, Associate Professor, Ph. D. / Kohji Yoshikawa, Lecturer, Ph. D. / Wagner Alexander Takeshi, Assistant Professor, Ph. D. / Naohito Nakasato, Visiting Associate Professor, Ph. D.

Outline

The Universe is thought to have been born 13.7 billion years ago with the occurrence of the Big Bang, but it wasn' t until approximately 0.38 million years later that hydrogen atoms formed. Of course, this means that there were neither stars nor galaxies at that time (known as the recombination epoch), but there were density fluctuations with contrasts of 1/100,000. Moving ahead to 0.1 gigayears after the Big Bang, research shows that a number of newly born galaxies had formed. Yet the era from 0.38 million years to 0.1 gigayear is often referred to as the "Dark Age of the Universe", and is shrouded in mystery.

It is believed that, in this Dark Age, the first generation stars were born and the primordial galaxies formed (Fig.1). 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. To perform these intensive numerical simulations, a dedicated high-performance parallel computer named "Astrophysics Simulator FIRST" has been developed through collaboration with computer scientists.

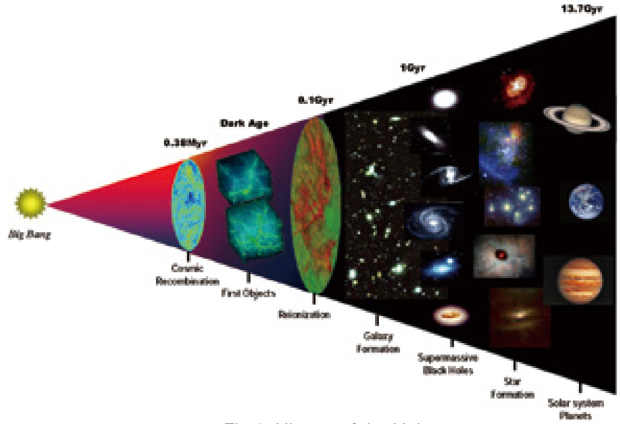


Fig.1 History of the Universe

Research topics

- **Formation of first generation stars**
  Our research efforts involve three-dimensional (3D) radiation hydrodynamic simulations of secondary star formations in the early universe. Using such simulations, we explore the formation of secondary Population III stars through radiation hydrodynamic feedback from a preformed massive star of the early universe. Each panel of this figure shows the evolution of a collapsing cloud near a first luminous star, as a function of time.(Fig.2)
- **Formation of primordial galaxies**
- **Formation of clusters of galaxies and a large-scale structure**
- **Formation of massive black holes and the evolution of active galactic nuclei**
- **Galaxy collision and merger**
  N-body simulations of the interaction between an accreting small galaxy and the Andromeda galaxy are shown in this figure. Large galaxies such as the Andromeda galaxy are believed to have formed, in part, from the merger of many less massive galaxies. Here, we examine the interaction between an accreting small galaxy and the Andromeda galaxy using N-body simulations. Each track along an arrow corresponds to the evolution of the projected stellar mass density of the merging small galaxies with the different binding energy.(Fig.3)
- **Intensive numerical simulations of radiation hydrodynamics**
- **Development of dedicated computers and exploitation of computational technique**

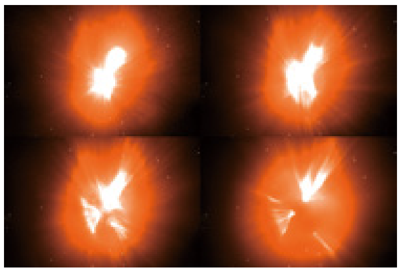


Fig.2 Secondary star formation in the early universe

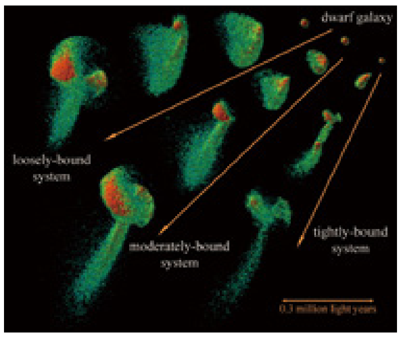


Fig.3 An accreting small galaxy and the Andromeda galaxy

Websites

http://www.rccp.tsukuba.ac.jp/Astro/index.html
http://www.ccs.tsukuba.ac.jp/people/umemura/FIRST/index-j.html

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 1998, Dr. 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. Umemura became a full professor at the university in 2002, and is serving as the director of CCS since 2013.

Division of Nuclear Physics

Nuclear Physics Group

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

Overview of the field

An atomic nucleus is an extremely high-density particle of matter located in the center of an atom. It is a finite quantum many-body system composed of two kinds of fermions, protons and neutrons, bound by nuclear force. The complex nature of the nuclear force brings unique and diverse properties to atomic nuclei. One of current concerns in nuclear physics is the problem of the origin of elements: where and how nuclei are created in the Universe. To answer this question, it will first be necessary to understand the structure and reactions of extremely unstable nuclei. Describing and comprehending atomic nuclei, while starting solely from investigations into underlying nuclear force, is a long-standing goal of theoretical nuclear physics. Since an atomic nucleus is a quantum system composed of many-fermions, theoretical nuclear physics is also intimately related to other fields, such as the quantum exploration of many-body systems like atomic and molecular physics, condensed matter physics, and quantum chemistry.

Structure, synthesis, and decay dynamics of atomic nucleus

Our group has been developing computational approaches for excitations and dynamics of many-fermion systems, in particular those based on energy-density functional theory. Figure 1 shows structure calculation for a ^{12}C nucleus using a newly developed computational approach that superposes many Slater determinants with parity and angular momentum projections. The figure reveals a drastic structural change in the atomic nucleus as the excitation energy increases. More specifically, while the ^{12}C nucleus shows a mostly spherical shape in the ground state, a dilute three alpha-particle structure appears in the first excited state, and an alpha-chain structure appears in the second excited state. The ^{12}C nucleus is produced by the triple-alpha reaction, which is a key reaction in the synthesis of heavy elements. We have recently developed a new formalism for the thermonuclear reaction rate solving the Schrödinger Equation along an imaginary-time axis. By applying this formalism to the triple-alpha reaction, we expect to obtain a reliable reaction rate for this important process.

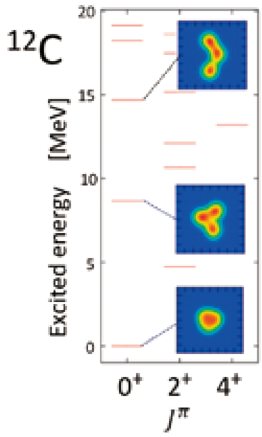


Fig.1 Energy spectrum and density profiles of ^{12}C nucleus

Nuclear methodology in other fields — First-principles electron dynamics simulation

We have been working actively to apply nuclear methodology to the material and optical sciences, since we achieved pioneering electron dynamics simulations through the application of computational methods developed in nuclear physics. The center of our methodology is the real-time and real-space method used to solve the time-dependent Kohn-Sham Equation, which is the basic equation of time-dependent density functional theory. We are currently applying this method to describe electron dynamics in crystalline solids induced by optical electric fields. This method provides unified descriptions of optical phenomena in linear and nonlinear regimes, including the dielectric function, coherent phonon generation, and optical breakdown. Recently, we successfully extended our methodology to the coupled dynamics of microscopic electron motion and macroscopic electromagnetic fields. This powerful simulation is expected to be extremely useful in investigations of femto- and attosecond electron dynamics in crystalline solids induced by strong and ultra short laser pulses.

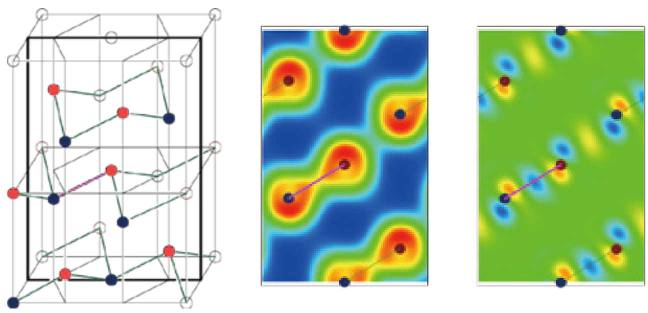


Fig.2 Electron dynamics in Sb. (Left) Crystalline structure, (Middle) Electron density in the ground state, (Right) Density change under laser pulse irradiation.

Chief : Takashi Nakatsukasa

Dr. Takashi Nakatsukasa graduated from the Department of Physics, Kyoto University, with a doctorate in theoretical nuclear physics in 1994. He has been appointed as Professor in University of Tsukuba Faculty of Pure and Applied Sciences/Center for Computational Sciences (CCS) in 2014, after postdoctoral and academic posts in Osaka University, Chalk River National Laboratory (Canada), University of Manchester Institute of Science and Technology (UK), Tohoku University, and RIKEN. His current main interests are quantum dynamics of nuclear many-body systems.

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.

About our group

The Quantum Condensed Matter Physics Group is dedicated to the study of nanometer-scale material sciences such as semiconductor device physics, high temperature superconductivity, and the physics of light-matter interactions by means of computer simulations based on quantum mechanics. Despite the progress made to date, the downsizing of semiconductor devices is still the most important and effective way to improve their performance levels. Today' s device sizes are often measured on the nanometer scale, and further progress has required the utilization of new structure types and/or novel nano-materials instead of conventional planar-type silicon-based devices. Since, in the nanometer size region, it is essential to describe the behavior of electrons in terms of quantum mechanics, computer simulations based on quantum mechanics are especially important for clarifying the physics of nano materials and devices.

Research topics

Multiple exciton generation in single-walled carbon nanotubes

Currently, the multiple exciton generation (MEG) in single-walled carbon nanotubes (SWNTs) is under theoretical investigattion. We perform MEG rate calculations by considering the direct photogeneration of multiple excitons. Specifically, we consider the generation of two-exciton states. While a single photon is unable to excite two excitons due to the selection rule, it is possible to consider situations where superposed multiexciton states can result because Coulomb interaction resonantly couples among multiexciton states. This process was originally proposed for the MEG in nanocrystal. The resulting direct photogeneration produces many excitons by a single photon absorption and is thus a simultaneous process (Fig. 1).

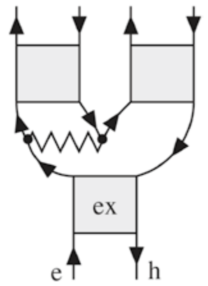


Fig.1
Feynman MEG process diagram. The solid lines indicate the Green's function of the electron and hole, the wavy lines indicate Coulomb interaction, and the squares mark the exciton states.

Mechanism of superconductivity in the Cuprate

The mechanism of the high transition temperature superconductivity in the cuprate has been studied by Koizumi and collaborators. They have found that many anomalous properties of the cuprate are explained by the existence of nano-sized spin-vortices, and nano-sized loop currents that are induced by the spin-vortices (Fig. 2). They also investigate the possible application of the nano-sized spin-vortex-induce loop currents as qubits of quantum computers.

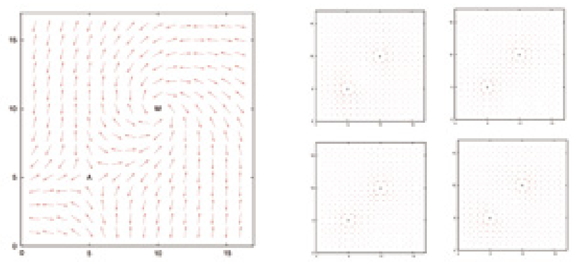


Fig.2 Two spin-vortices in the CuO_2 plane in the cuprate (left) and four patterns of the spin-vortex induced loop currents around them (right)

Laser-material interaction

We are investigating the mechanism of intense laser-material (atoms, molecules and clusters) interactions and searching effective ways to control the dynamics or material properties in a femtosecond (10^{-15} s) or attosecond (10^{-18} s) time scale by computer simulation. For example, by solving the time-dependent Schrodinger equation, we found that the transparency of a material can be controlled by tuning the time delay between an attosecond XUV pulse and infrared laser in a few femtoseconds. The proposal has been realized in a recent experiment as shown in Fig. 3. The mechanism can be used to produce an ultrafast optical switcher in a femtosecond time scale.

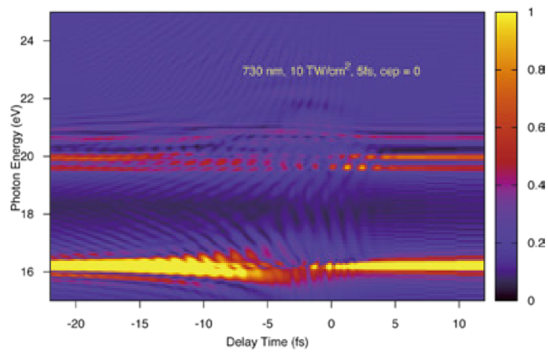


Fig.3 Controlling the XUV transparency by a pulsed infrared laser.

Quantum control of electronic states by intense laser

Interactions between materials and lasers are also important issues from both fundamental physics and technological application points of views. Since light-matter interactions are essentially quantum phenomena, computer simulations based on quantum mechanics are also useful for theoretical investigations into the physics of such interactions. By employing large-scale quantum simulations, we study the Floquet states of electrons and holes confined in semiconductor nano structures as well as photo-induced phase transitions in organic and inorganic strongly correlated systems.

Chief : Kazuhiro Yabana

Dr. Kazuhiro Yabana graduated from Kyoto University with a doctorate in theoretical nuclear physics in 1987. He then joined the nuclear theory group at Niigata University and moved to University of Tsukuba in 1999. His research interests range from theoretical nuclear physics to atomic, molecular, optical, and condensed matter physics. Dr. Kazuhiro Yabana has been enthusiastic in developing computational approaches for quantum dynamics of many-fermion systems.

Division of Life Science

Biological Function and Information Group

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

Outline

The life systems of living organisms are full of surprises. Biological functions such as metabolism, photosynthesis, self-replication, and cognition are all sophisticated and highly efficient. Even now, there remain a great number of unresolved mysteries in various fields of biology, where the functions and/or geometric structures of numerous biomolecules have yet to be determined, and where the working mechanisms of most of biological systems have yet to be fully resolved. Understanding such biological systems is quite important in many areas, including the chemical, pharmaceutical, and medical fields.

In our division, we focus our theoretical investigations into key biological systems and their attendant molecular mechanisms in collaboration with experimental groups. Biological systems are composed of vast numbers of macromolecules and huge computational costs are incurred when creating realistic theoretical models.

Utilizing the HA-PACS and COMA at Tsukuba University, we have performed various simulations involving molecular dynamics and quantum mechanical calculations as we continue efforts to penetrate the molecular mechanisms of biomolecules operating in living systems.

Research topics

Reaction mechanisms of enzymes (NOR, Topo)

In our investigations quantum mechanical/molecular mechanical (QM/MM) methods have been used to elucidate the reaction mechanisms of two enzymes (Fig. 1). These are outlined below:

(1)Nitric oxide reductase (NOR) is a transmembrane protein that catalyzes a reduction of nitric oxide (NO) to nitrous oxide (N2O). The reaction is critical for the denitrification process in the anaerobic respiration. The reaction energy profile and intermediate states were determined for NOR.

(2)DNA topoisomerase (Topo) is a DNA-binding enzyme that catalyzes the interconversions of different topological forms of DNA. Through these efforts, a novel reaction mechanism for the religation reaction step has been found, which will be helpful when designing new enzyme-related pharmaceuticals.

Development of GPU accelerated supercomputing programs

The graphical processing unit (GPU) accelerated Fock matrix preparation of a Hartree-Fock (HF) calculation routine, which is a basic and common process in various *ab initio* molecular orbital (MO) calculations, has been implemented into the OpenFMO program. By implementing overlapping mixed CPU and GPU calculations, total elapsed time was remarkably reduced (Fig. 2).

Origin of Life (Photo-induced chirality formation of amino acids)

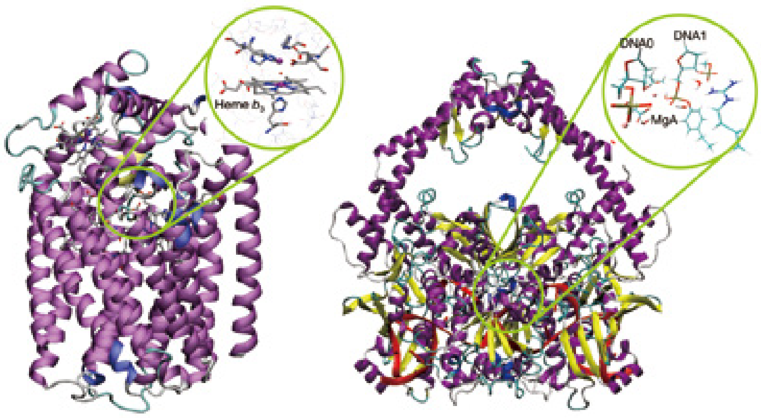


Fig.1 Enzymes (NOR, Topo)

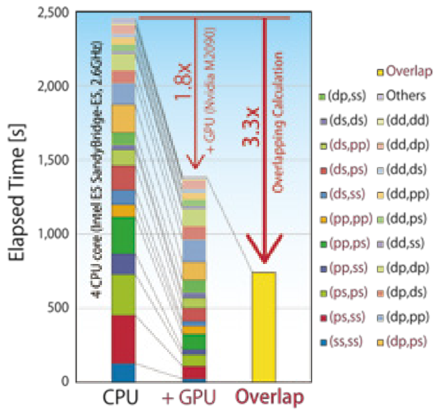


Fig.2 Performance of a GPU-accelerated MO calculation

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.

Biological Science Group

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

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.

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.

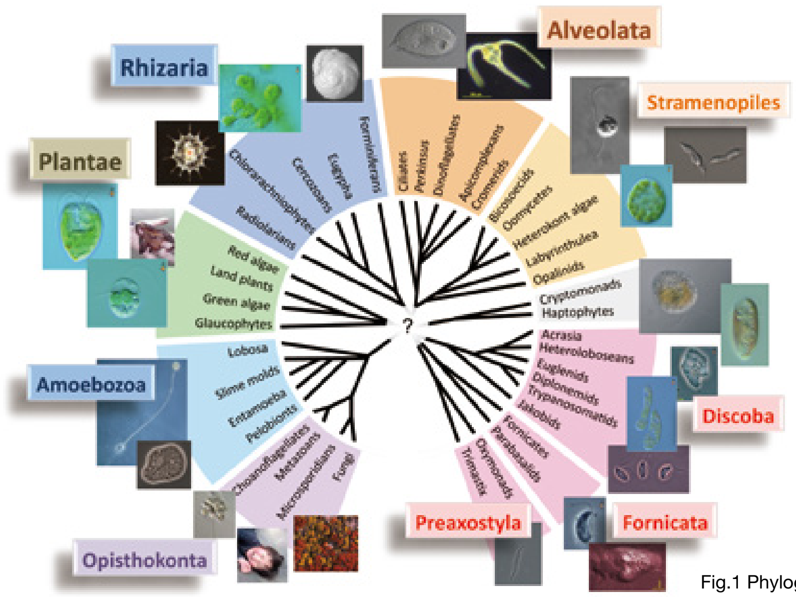


Fig.1 Phylogenetic tree

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 Tsukuba University 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.

Division of Global Environmental Science

Global Environmental Science Group

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

About our group

The Global Environmental Science Group pursues the study of global-, synoptic-, and local-scale weather and climate using the Nonhydrostatic ICosahedral Atmospheric Model (NICAM) for general circulation and the Weather Research and Forecasting model for regional studies. Advanced supercomputer technology is used to enhance the accuracy of the group' s predictions. The group operates two faculties. One is led by Prof. Hiroshi L. Tanaka and Associate Prof. Hiroyuki Kusaka with the assistance of Prof. Hiroyuki Ueda (Faculty of Life and Environmental Sciences) , Senior Researcher Akio Kitoh (Faculty of Life and Environmental Sciences), and Assistant Prof. Yasutaka Wakazuki(Faculty of Life and Environmental Sciences). At the other Agency, leadership is provided Prof. Fujio Kimura (Japan Agency for Marine Earth Science and Technology).

Research topics

NICAM (Non-hydrostatic ICosahedral Atmospheric Model):
NICAM, which is the most promising cloud resolving general circulation model today, was originally developed by the Center for Climate System Research (CCSR), the University of Tokyo, and by the Frontier Research Center for Global Change (FRCGC) of the Japan Agency for Marine-Earth Science and Technology (JAMSTEC), and has recently been installed in the Center for Computational Sciences (CCS) T2K-Tsukuba supercomputer systems. Using NICAM, we investigate tropical cyclones, extra-tropical cyclones, arctic cyclones, and work to predict blocking anticyclones, stratospheric sudden warming, and Arctic Oscillation in the global atmosphere.

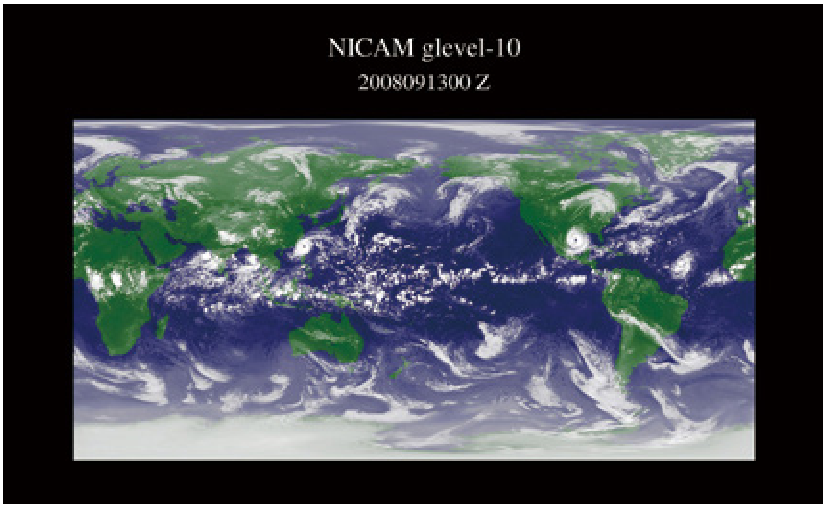


Fig.1 Numerical simulation of the general circulation of the atmosphere produced by 7-km resolution NICAM. NICAM-based modeling accurately predicted the evolution and movements of Typhoon Sinlaku and Hurricane Ike in 2008.

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.

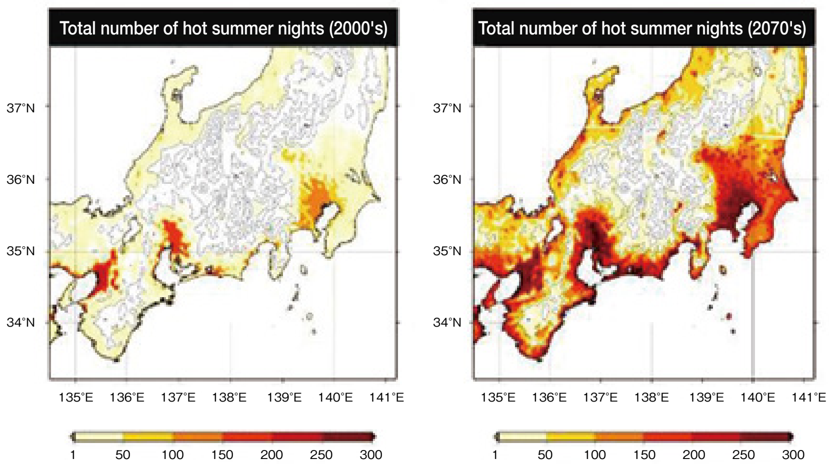


Fig.2 Regional climate projection by 3-km resolution WRF. In this figure, the total numbers of hot summer nights for the 2000' s are compared with predictions for the 2070' s.

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.

Division of High Performance Computing Systems

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, Lecturer, Ph.D. / Hiroto Tadano, Assistant Professor, Ph. D. / Toshihiro Hanawa, Visiting Associate Professor, Ph. D.

About our group

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, Graphics Processing Unit (GPU)-accelerated computing systems, large scale distributed storage systems, and grid/cloud technology. The following are among our more recent research topics.

Research topics

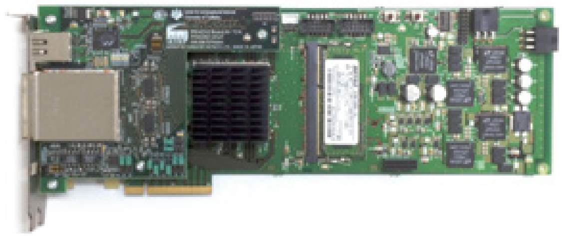


Fig.1 Prototype PEACH2 chip test board for TCA environment use

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) is under development 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.

XcalableMP: 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 XMP-dev in order to cover, for example, large-scale GPU clusters.

Gfarm: 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 now officially adopted as the High Performance Computing Infrastructure (HPCI) shared file system and already 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.

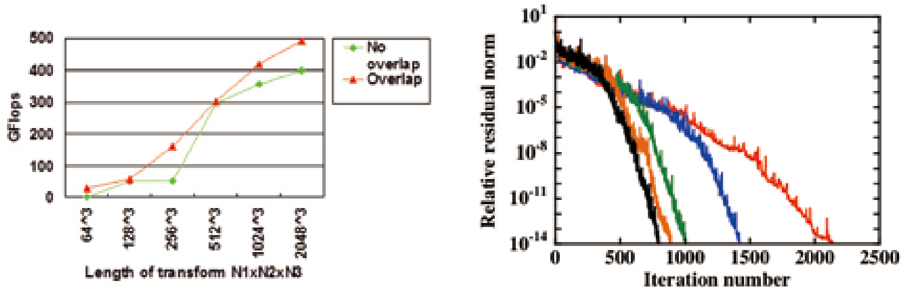


Fig.2
Three-dimensional (3D) FFT performance on the T2K-Tsukuba supercomputer (left), and residual reduction via the Block Krylov subspace method with Jacobi preconditioning (right).

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 more than 20 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-accelerated computing.

Database Group

Chief: Hiroyuki Kitagawa, Professor, Dr. Sc. **Member:** Toshiyuki Amagasa, Associate Professor, Ph. D.

Introduction

In the field of computational sciences, management and utilization of massive data are extremely important issues. The Database Group is in charge of research and development in the field of data engineering. In particular, we have been engaging in the following research topics: infrastructure for integrating heterogeneous databases and various information sources, data mining and knowledge discovery technologies to discover knowledge and outliers from massive data, and scientific data management. Additionally, we also have engaged in application studies, such as the development of Grid Point Value/Japan Meteorological Agency (GPV/JMA) meteorological databases, along with knowledge discovery from those databases in cooperation with the Division of Global Environmental Science, as well as management of the Japan Lattice Data Grid (JLDG), in cooperation with the Division of Particle Physics.

Research topics

Infrastructure for Information Integration: A recent project has been the development of JsSpinner, which allows us to integrate not only conventional data sources, such as relational databases and Web data, but also stream data, such as network packets, sensor data and location information. Based on JsSpinner, we are studying (1) information integration over semi-structured data streams, and (2) data mining from data streams.
Data Mining and Knowledge Discovery: We have also been studying various data mining and knowledge discovery techniques, such as (1) outlier detection on uncertain datasets, (2) graphical processing unit (GPU) acceleration of data mining algorithms, and (3) social data analysis and mining.
Scientific Data Management: To deal with rapidly increasing big scientific data, research has been conducted on the following topics: (1) hot spot detection from satellite data, (2) application of data engineering techniques for better management and utilization of scientific data, and (3) development and operation of scientific data bases, such as the GPV/JMA, Archive, the Japanese 25-year ReAnalysis (JRA-25) Archive, and the JLDG.

Recent results

1) Infrastructure for Information Integration
   We have demonstrated StreamSpinner and SS* with applications in many exhibitions, such as Innovation Japan every year from 2005 to 2011, and have proposed a query optimization technique (Y. Watanabe and H. Kitagawa 2010).
2) Data Mining and Knowledge Discovery
   We proposed a method for probabilistic frequent itemset mining using general purpose computing on graphical processing unit (GPGPU) technology that is based on the Apriori algorithm, with the idea of accelerating probabilistic computations by employing a filter primitive and tree-based approach with low-latency memory on the GPU. The results show that our method outperforms the Apriori algorithm running on a CPU by a factor of two orders of magnitude (Y. Kozawa, T. Amagasa, and H. Kitagawa CIKM 2012). Data representation by GPU is shown in Fig. 1.
3) Scientific Data Management
   We have developed and have been operating GPV/JMA and JRA-25 meteorological numerical database achieves in cooperation with the JMA (http://gpvjma.ccs.hpcc.jp/~gpvjma/index.html). These databases can be mapped to Google Earth (Fig. 2). As of September 2012, the amount of stored data is 10 TB and there are 539 registered users.
4) Numbers of Refereed Papers
   2012: 19 (7 Journal papers 12 Refereed conference papers 2 Demos/Posters)
   2011: 13 (4 Journal papers 9 Refereed conference papers 3 Demos/Posters)
   2010: 20 (6 Journal papers 14 Refereed conference papers 0 Demos/Posters)
   (As of September 2012)
5) Relating to the above research activities, we have received two paper awards and seven awards for students.

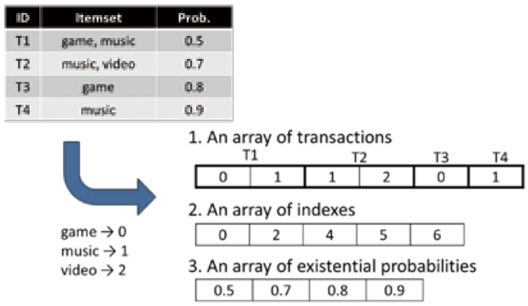


Fig.1 Data representation by GPU

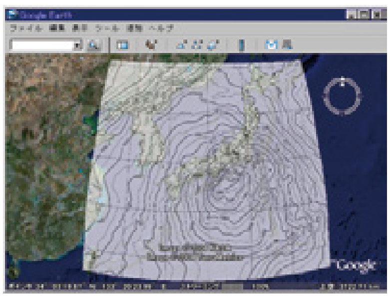


Fig.2 Mapping GPV/JMA/JRA-25 data to Google Earth

Chief : Hiroyuki Kitagawa

Dr. Hiroyuki Kitagawa received his Bachelor of Science degree in physics, and later his Masters and Doctorates in computer science, all from the University of Tokyo. He is currently a full professor at Graduate School of Systems and Information Engineering and at Center for Computational Sciences, University of Tsukuba. Dr. Kitagawa' s research interests include integration of information sources, data mining, stream-based ubiquitous data management, Web data management, XML, and scientific databases. He is a fellow of IPSJ and IEICE, as well as a Vice-Chair of DBSJ.

Computational Media Group

Group Leader: Yoshinari Kameda, Associate Professor, Ph. D.
Member: Itaru Kitahara, Associate Professor, Ph. D.

About our group

Computational media are advanced information media on which high sensing functionality and huge computing resources are elegantly unified over computer networks. We can 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.

While many surveillance cameras have been installed in public spaces, some people may feel uncomfortable with such observations, even though they play important role in keeping us safe and secure in our daily lives. However, computational media will also give a new role to such cameras, with which people can more thoroughly enjoy the advantages provided by information technology. For example, users can effectively utilize the video information provided by our "see-through vision" method and our "visual support system for car drivers in intelligent transportation system".

Research topics

- **Three-dimensional (3D) Live Video of Soccer Games :** Free-viewpoint video for multiple online viewers over computer networks. Viewers can freely fly through the soccer field and see the game from arbitrary viewpoints.
- **See-Through Vision :** A framework that can enable people to see through objects by processing video from surveillance cameras. It also covers privacy-safe visualization for cases where other people may be present.
- **Collaborative Mixed Reality :** This is an augmented communication system designed to fuse both of real and virtual visual information.
- **Massive Sensing :** This system involves intelligent video processing and understanding human behavior via networked sensors.
- **Visual Support in Intelligent Transportation Systems :** Here, we provide enhanced vision support for vehicle drivers based on augmented reality technology. This system utilizes online videos from road surveillance cameras.
- **Video Surveillance by mutual utilization of fixed surveillance camera and mobile camera :** In this system, we work to enhance area surveillance by integrating the advantages of fixed surveillance cameras and mobile cameras.
- **Hostile Intent Analysis :** This is an advanced face analysis system that operates by way of extraordinary image sensing data, along with intelligent media processing inspired by psychological analysis.

Research results

Free-viewpoint video is a visual information medium that freely reproduces scene views from arbitrary viewpoints. The Computational Media Group is engaged in research that aims at applying free-viewpoint video technologies to large-scale spaces such as soccer stadiums, which will realize the world' s first live free-viewpoint video system by developing a real-time 3D modeling method. We are currently actively developing a user-friendly video-browsing method that will allow anybody to enjoy free-viewpoint video.

One of the approaches is generating a player' s view video of an actual soccer match (Fig. 1). With this technology, users can enjoy 3D video simply by choosing a target player and concentrating on a soccer match from that player' s point of view. The generated video provides an immersive sight as if the user is actually running on the pitch. We have also developed a novel computer vision technique for player tracking in 3D space that robustly works in an actual soccer stadium.

We have also proposed a 3D free-viewpoint video-browsing interface that applies multi-touch manipulation to virtual camera control (Fig. 2). It is difficult for general users to browse 3D free-viewpoint video because they are not accustomed to controlling a virtual camera from a free-viewpoint perspective. To deal with this issue, we utilize the multi-touch interface installed in tablet personal computers (PCs), which has become a popular interface thanks to its easy and intuitive manipulation. We are currently conducting subjective evaluations to define suitable gestures for virtual camera control. The results so far have revealed which multi-touch gestures users tend to prefer for controlling a virtual camera.

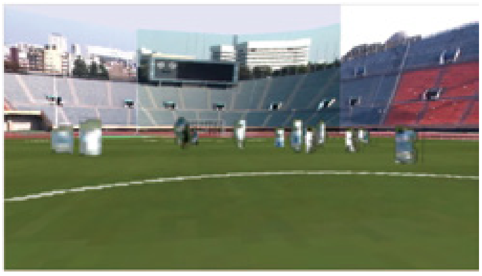


Fig.1 Player' s View Video

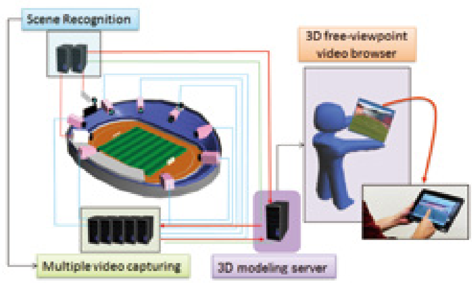


Fig.2

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. After holding a faculty position in the Department of Information Science at Kyoto University until 2003. He was a visiting scholar in AI Laboratory at MIT in 2001-2002. In 2003, he joined the University of Tsukuba and is now an associate professor. Dr. Kameda's research interests includes the vision enhancement of human vision, augmented reality, video media processing, computer vision, and sensor fusion.

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 under close cooperation with the Project Office for Exascale Computing System Development, which is the organization promoting the development of new computers.

The Center' s future plans include tackling innovative technologies such as the Tightly Coupled Accelerator (TCA) technology that will be incorporated in the extended HA-PACS system and a massively-parallel computer equipped with processors of Many Integrated Core architecture, which will be introduced in Joint Center for Advanced High Performance Computing (JCAHPC).

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

	Scientific Target	Numerical calculations employing GPU
Particle Physics	Multiscale physics Physics at finite temperature and/or finite density	Solution of large-scale sparse linear equations Matrix-matrix product calculation of dense matrices
Astrophysics	Realization of computational astrophysics in six dimensions Simulations of collisional self-gravitating systems	Ray-tracing calculations of light-intensity and chemical reactions Calculations of gravitational acceleration and its derivatives
Nuclear Physics	Research on nuclear response and reaction dynamics First-principles calculations for light-matter interaction	Real-time and real-space finite difference calculations 3D Fast Fourier Transformations
Material Science	Investigations on structure and dynamical processes of matter, and control of quantum processes	Real-time and real-space finite difference calculation of time-dependent Schrödinger Equations
Life Science	Enzymatic reaction mechanisms Dynamical structures of biomolecules	Quantum mechanical calculations Molecular dynamics simulations
Global Environmental Science	Next-generation atmospheric circulation model (NICAM) Calculation of urban climate	3D normal-modes expansion LES
Computational Informatics	Knowledge discovery from large-scale database	Association rule mining Time-series data retrieval Clustering

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 Highly Accelerated Parallel Advanced System for Computational Sciences (HA-PACS) is an experimental testbed for TCA architecture, as well as the application development platform with the latest graphics processing unit (GPU) computing technology. The system consists of two parts, a base cluster part with commodity GPU technology, and a TCA part that incorporates our original GPU-direct communication technology.
The HA-PACS base cluster part has been operating since February 2012 using 268 nodes, each of which consists of two Intel E5 SandyBridge CPU sockets and four NVIDIA M2090 (Fermi) GPUs. From November 2013, the additional TCA part, equipped with 64 nodes each consisting of two Intel E5 IvyBridge CPUs sockets and four NVIDIA K20X (Kepler) GPUs, connected by our original named PCI-Express Adaptive Communication Hub ver.2 (PEACH2) technology is added to facilitate the development of TCA system software and its applications.

■ Base Cluster part

GPGPU (General Purpose GPU) is a computing method that applies GPUs to general purpose scientific computing as the computation-accelerating device. The latest GPUs provide extremely high theoretical performance in floating point operations, which can then be applied to a wide variety of high performance computing (HPC) problems.

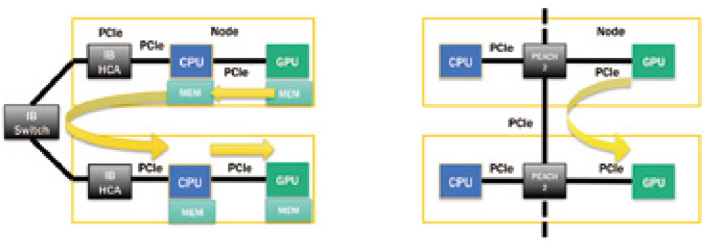
■ HA-PACS/TCA part

Current GPU clusters often encounter performance bottlenecks caused by poor communication performance during inter-node GPU to GPU communication on parallel processing systems. TCA architecture provides a fundamental solution to this problem by using hardware that enables true GPU-direct communication over nodes by achieving strong scaling on various HPC problems that are often subject to communication latency bottlenecks.

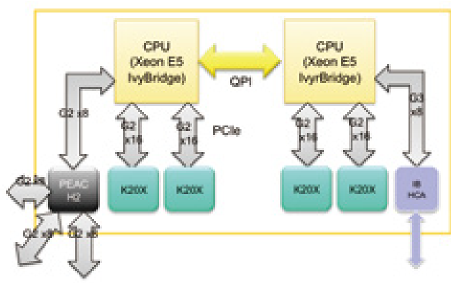
■ PEACH2

As the experimental TCA concept testbed for developing a communication system to enable GPU to GPU direct communication over nodes, this system consists of a field programmable gate array (FPGA) PEACH2 chip and its PCI Express attachable board. Since it is constructed with FPGA technology, it is easy to enhance the performance and function of PEACH2 as the TCA concept evolves. PEACH2 realizes the following functions:

- Autonomous communication by GPUs without depending on host CPUs → high performance parallel processing of general purpose code and accelerated code
- Direct data copy between GPUs on different nodes → processing by GPUs only
- Direct I/O between GPU and other peripheral I/O devices → fault tolerant I/O system in the event of CPU failure



Inter-GPU communication on general GPU clusters (left) and true GPU-direct communication by TCA (right)



Block diagram of a computation node of HA-PACS/TCA

Project Office for HPCI Strategic Program

Innovative Research Using the K Computer 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 a framework to advance computational science and technology in major fields (HPCI Strategic Program), and producing revolutionary results through the exploitation of HPCI are cited.

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

■ Strategic Objective of Field 5

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

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

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

(1)Determination of the baryon-baryon interactions using lattice QCD at the physical point
(2)Elucidation of nuclear properties using ultra large-scale simulations of quantum many-body systems and its applications
(3)Clarification of the processes underlying supernova explosions and the formation of black holes
(4)Investigation on the formation of first-generation stars in the Universe out of density fluctuations of dark matter

Research of these subjects is carried out using the K computer, which has a peak performance of 10.5 Pflops (calculations enabled at about 10 quadrillion times per second). Results have been yielded steadily. The dark matter simulation performed on the K computer won the Gordon Bell Prize, the most prestigious of its type in the field of high performance computing, in November 2012.

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

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 Processing Center (EPPC) 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.

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 summer school and other matters, 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 experience are necessary to advanced research in scientific fields such as physics, the 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 engaging in, concurrently and in parallel to, 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 13 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 summer school subjects, and are also 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
	Data Analysis
	Basic Computational Biology
	Special Lecture on Computational Science I～IV
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 877 m 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.

Build Better Relationships with Society and the Center for Computational Sciences

Tomoaki Yoshito, Senior Researcher

In fiscal year 2010, the Bureau initiated 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. To that end, three public relations concepts underlying the purposes behind the establishment of the Center have been set forth for use in guiding daily operations.

■ Public Relations Concepts

- We will conduct bilateral public relations to foster enhanced relations between the Center and society.
- We will aim at increasing the visibility of the Center and the computational sciences.
- We will enhance the level of understanding of the fundamental policies of the Center, and work to improve public confidence in its actions.

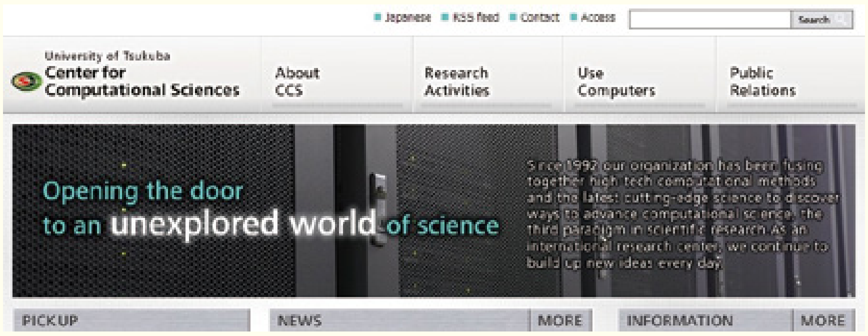
■ Activity Policy for the Bureau of Public Relations

- We will support public relations and public hearings for researchers associated with the Center.
- We will create content, including websites, in order to provide information to stakeholders.
- We will actively gather information and create feedback mechanisms for researchers within the Center.
- We will create a risk management organization.
- We will examine and implement methods to measure visibility, levels of understanding, and degrees of confidence.

■ Activity Results

- **Website: http://www.ccs.tsukuba.ac.jp/eng/**

Provides up to date information on researchers, projects, computer basics, database disclosures, symposiums/seminars, disaster preparedness and response, etc.



- **Brochures**

We prepare three types of brochures based on the intended readership: "Computational Sciences and Supercomputers" for the general public (this is aimed at high school readers and older); a Japanese text for professionals (aimed at graduate students and older); and an English text for professionals (for use by international graduate students and others).

- **Movies**

Productions of 12 movies (Japanese and English), including an introduction to the Center, the computing facility, and 10 research fields, have been produced to date.

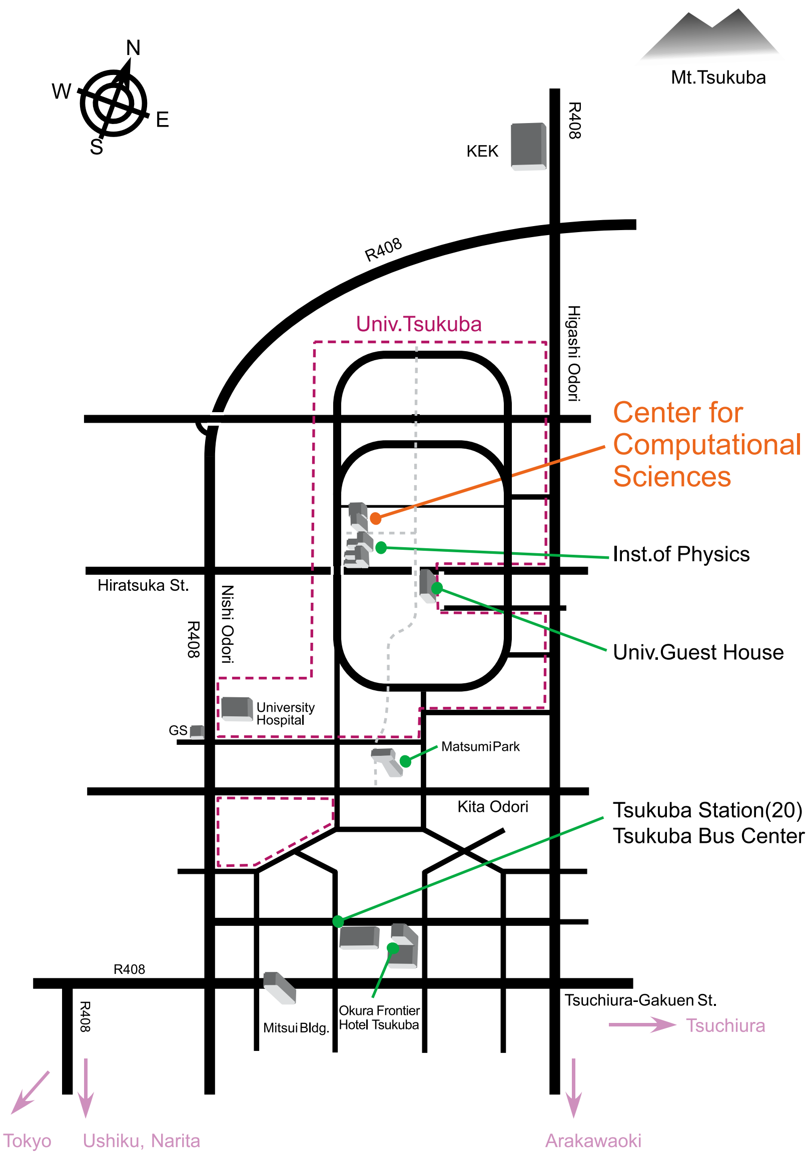
- **Tour and Open House**

The number of visitors was 351 in fiscal year 2010, 1,077 in fiscal year 2011, 972 in fiscal year 2012, 1571 in fiscal year 2013, and 1968 in fiscal year 2014. We created a FAQ section on the Center's website.

- **Media Promotions**

Seven press releases were disseminated to the mass media in fiscal year 2011, five were released in fiscal year 2012, seven were released in fiscal year 2013, and eight were released in fiscal year 2014. The Center is also active on the social media Twitter (@CCS_PR), where it has gathered 4,400 submissions and 1250 followers (as of May 2015)

Tsukuba City

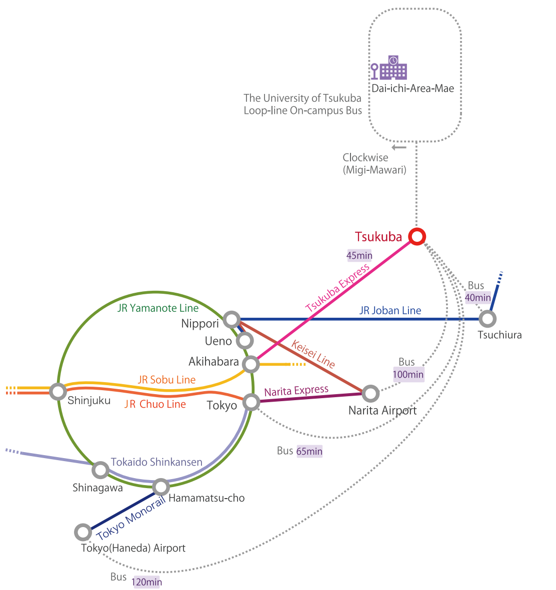


Access

■ The City of Tsukuba, the Science City, is located about 50km north-west of the New Tokyo International Airport (Narita Airport). About 100 minutes from Narita Airport by bus bound for "Tsukuba Center". Take a bus at the bus stop No.8 in the Terminal 1 or at the bus stop No.10 in the Terminal 2.

■ Taxi takes about 90 minutes to reach Tsukuba from Narita Airport and costs about 15,000 yen. Taxi stands outside the terminal buildings are separated depending on destinations. Locate the stand for Ibaraki prefecture area, and tell the driver to go to Tsukuba City.

■ 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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June 2015