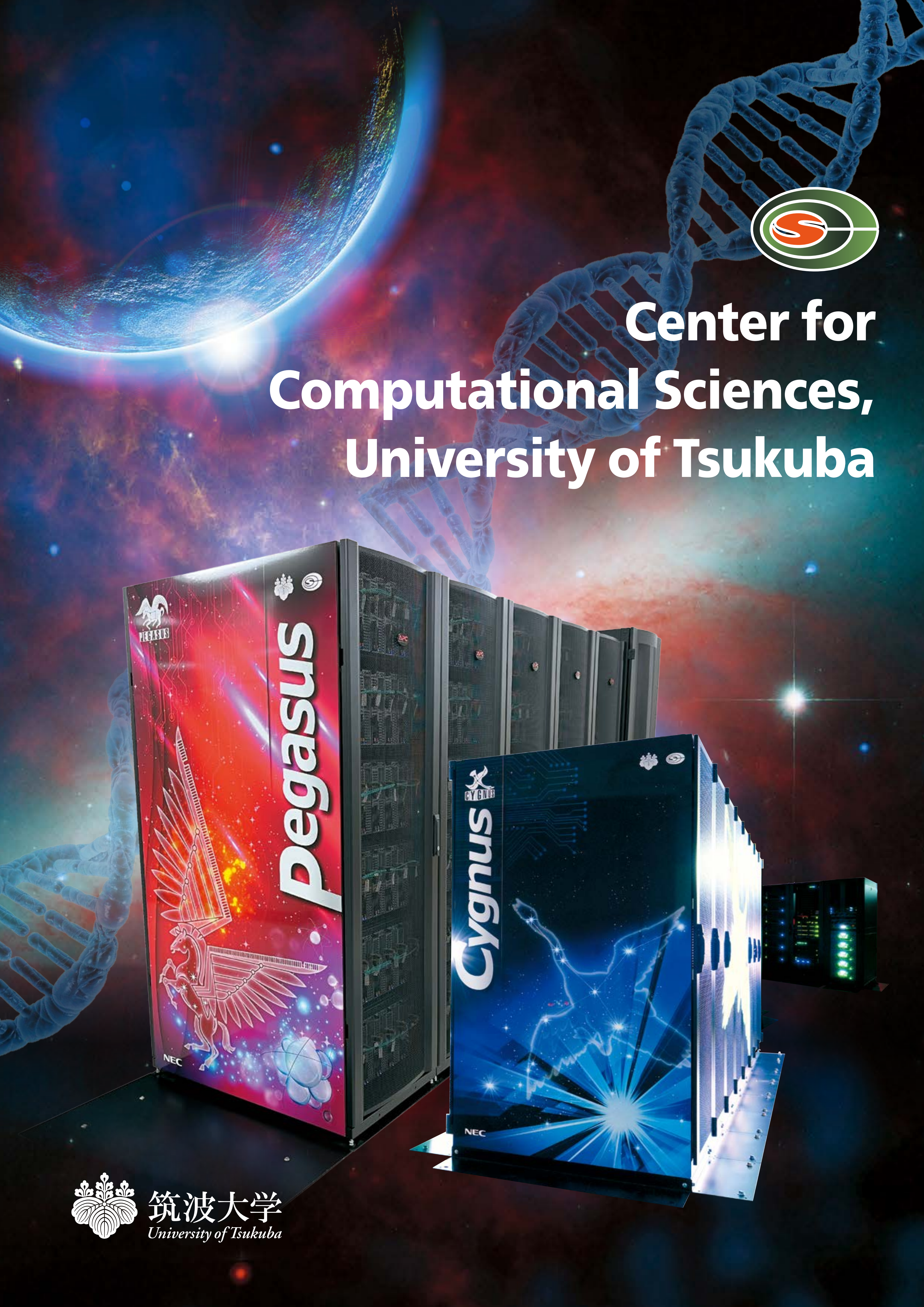
Center for Computational Sciences, University of Tsukuba



筑波大学
University of Tsukuba

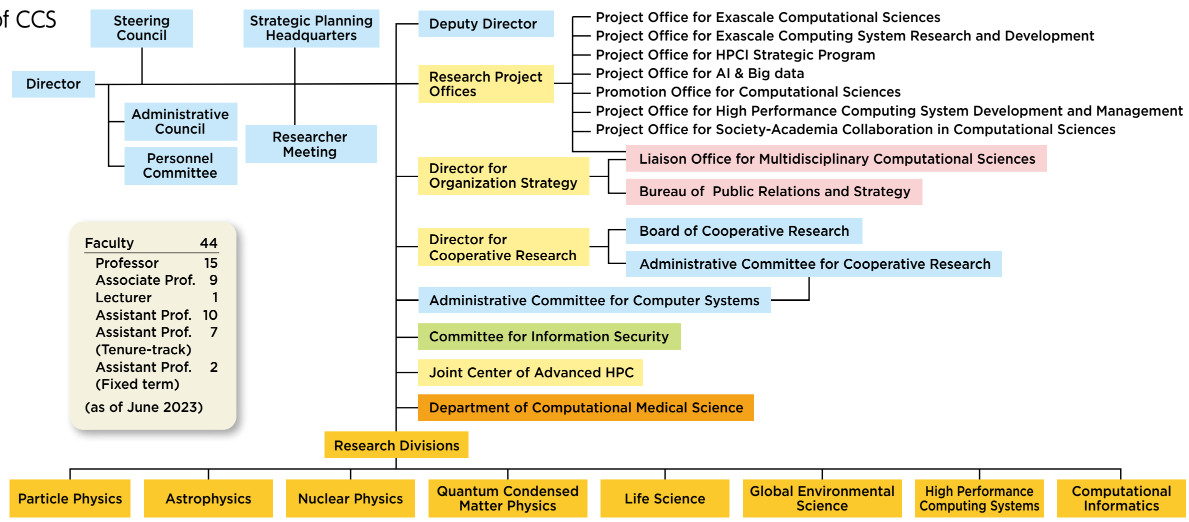
Overview

The University of Tsukuba's Center for Computational Sciences (CCS) promotes "multidisciplinary computational sciences" through the collaboration and fusion of different scientific and computer science fields and conducts research on cutting-edge applications of information science, ultrafast simulation, and large-scale data analysis through the development of ultrafast computer systems and network technologies. Areas of science that we deal with include particle physics, astrophysics, nuclear physics, nano-science, life sciences, earth and environmental sciences, and big data.

The CCS was founded in April 2004, having been reorganized and expanded from the Center for Computational Physics (CCP), which was established in 1992. It achieved worldwide recognition owing to its massively parallel supercomputer CP-PACS, which was developed in 1996 and has been ranked as the fastest supercomputer in the world in TOP500 List of November 1996. The CCS is currently undergoing intensive enhancement of its functions as an "Advanced Key Research Center" within the university. In 2013, according to an agreement with the Information Technology Center of the University of Tokyo, we established the "Joint Center for Advanced HPC (JCAHPC)" as the first inter-university joint computer development facility in Japan, and in 2016, we deployed a new supercomputer Oakforest-PACS as the fastest supercomputer in Japan at that time. The CCS has eight research divisions with 46 full-time faculty members. Additionally, we have established eight Research Project Offices, a Liaison Office for Multidisciplinary Computational Sciences, and a Bureau of Public Relations and Strategy for strategic promotion and dissemination of multidisciplinary computational sciences. These offices are responsible for overseeing multidisciplinary collaboration in the field of computational science, development of fundamental technologies for the next generation of systems, domestic and international collaboration, dissemination and promotion of computational science, and operation and development of the CCS's computational resources. Additionally, Joint Institute for Computational Fundamental Science, Organization for Collaborative Research on Computational Astrobiology, and Department of Computational Medical Science work to accelerate multidisciplinary collaboration among various fields.

In addition to being an organization that conducts research and development, the CCS serves as a national collaborative use facility that provides computing resources to outside researchers to support a wide range of research. In 2010, the CCS was designated as a "Joint Research Center for Advanced Multidisciplinary Computational Sciences" by the Ministry of Education, Culture, Sports, Science and Technology (MEXT), and this certification was renewed in 2015. We share the CCS's supercomputer resources with the rest of the country under the Multidisciplinary Collaborative Research Program and also provide support for researcher–student exchange with the goal of promoting joint research. Such support is provided for research meetings, researcher invitationals, research travel expenses, short-term employment, etc.

Organization of CCS



Message from the Director

BOKU Taisuke

Director of Center for Computational Sciences, University of Tsukuba

Computational science, which involves the use of computers to solve scientific problems, has become indispensable in scientific research, including its fundamental, theoretical, and applied fields. It has contributed to scientific development in numerous fields.

Advanced computational science is no longer achieved simply by the use of high-speed supercomputers and programs for each application. While necessary for computational science, their mere existence is no longer sufficient. This is because today's state-of-the-art high-speed computer systems are reaching their limits in terms of semiconductor technology, system size, power consumption, and other hardware constraints, and the performance limits will soon be reached if computers simply continue to get faster and users continue to use them as freely as they have in the past. To overcome these barriers, "co-design" based on mutual understanding of two parties is essential: the computer system must be optimized according to the requirements of the application, and the application must be modified with consideration of the limitations and capability of the computer system. Since its inception, the CCS has been developing systems and applications based on the co-design concept. This framework has evolved to include collaboration between applied fields, sharing of knowledge for system use, and mutual use of libraries. This is the definition of "multidisciplinary computational science" under which we operate. Multidisciplinary computational science is a powerful means of exploring the increasingly sophisticated and diverse science of the future, and its potential is unlimited. The CCS has been able to apply this concept to important scientific achievements across many scientific fields and endeavors to further strengthen multidisciplinary collaboration across applied fields.

We hope to continue to advance such multidisciplinary computational science and act as a hub for it with strengthened collaborative efforts both domestically and internationally.

CCS Vision of "Multidisciplinary Computational Science"

Computational science is explored by large-scale simulations with high performance computing resources as well as the high-bandwidth networks. The pivot for computational science is the collaboration between wide field of computer hardware, software, algorism, and application coding. This collaboration allows us to develop computers vest suited for scientific exploration. We define such a "codesign" as "Multidisciplinary Computational Science".

Based on the codesign concept, the CCS developed the massively parallel supercomputer named the Computational Physics by Parallel Array Computer System (CP-PACS) in 1996, which was ranked as the No. 1 system on the TOP500 List of November 1996. Large-scale computations carried out on CP-PACS have resulted in significant progress in particle physics and astrophysics. Since then, a large-scale cluster system named the Parallel Array Computer System for Computational Sciences (PACS-CS, 2006), and a special-purpose parallel system for astrophysics, the Cosmo-simulator FIRST (2007), have been developed. After that, a series of codesigned supercomputers for HA-PACS (2011), COMA (2014), Cygnus (2019) and Pegasus (2022) were launched.

The CCS has been striving to carry out collaborative research with computer scientists in a field of fundamental science for more than 30 years. Currently, in addition to fundamental science (particle physics, astrophysics, and nuclear physics), applied field are spread to materials science, life science, and global environment. As a result, a wide variety of collaborations among different fields have been initiated. This is a significant potentiality of "Multidisciplinary Computational Science".

Collaborations and Alliances

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

International collaborations and alliances in computational science research are important factors for promoting and accelerating multidisciplinary computational science. To that end, we have strengthened international collaborations through alliance with the University of Edinburgh in the UK and Lawrence Berkeley National Laboratory (LBNL) in the USA. With Korea Institute of Science and Technology Information (KISTI), we organize a winter school and workshop for advanced computational science every year. The International Lattice Data Grid (ILDG) is an international project aimed at the development of data grids for sharing lattice quantum chromodynamics (QCD) configurations worldwide. The construction of regional ILDG grids has been finalized Japan Lattice Data Grid (JLDG). The JLDG is supported by the "Cyber Science Infrastructure Project" carried out by the National Institute of Informatics as a part of grid infrastructure developments for academic research between the universities and research institutions.

Chronology of CCS

1992	April	CP-PACS Project begins (5-year project). Center for Computational Physics (CCP) founded (10-year term).
1993	August	Computer building is completed.
1995	March	First research building is completed.
1996	September	CP-PACS (2048 PU) is completed and installed.
	November	Ranks as No. 1 on the TOP500 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 is completed.
	April	Cosmo-Simulator FIRST is completed and installed.
2008	June	Operation of T2K-Tsukuba begins.
2010	April	Approved under the Advanced Interdisciplinary Computational Science Collaboration Initiative (AISCI). CCS is reorganized from five to seven divisions.
2012	February	HA-PACS starts operation.
2013	March	Joint Center for Advanced HPC (JCAHPC) is established in alliance with the University of Tokyo.
2014	April	COMA (PACS-IX) is installed and starts operations.
2015	April	CCS is reorganized from seven to eight divisions.
2016	December	Oakforest-PACS is installed and starts operations in JCAHPC.
2017	March	CCS building is extended to hold all faculty members in the center.
2019	April	Cygnus is installed and starts operations.
2022	December	Pegasus is installed and starts operations.

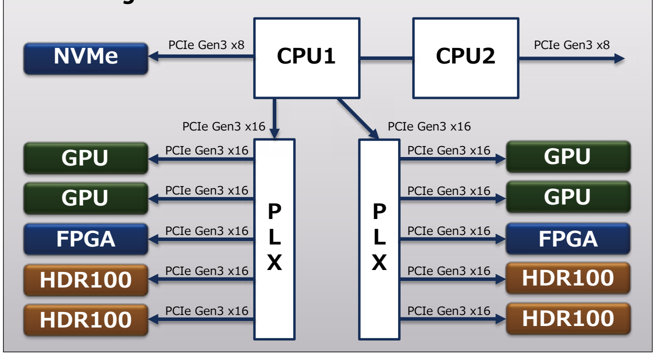
Cygnus

Cygnus supercomputer system demonstrates the 10th generation of PACS series supercomputer developed at the Center for Computational Sciences, University of Tsukuba. It has been operated from April, 2019. It is a large-scale parallel GPU/FPGA cluster system, which consists of 81 compute nodes, each node has GPU and FPGA. The peak performance is 2.43 PFLOPS without FPGA. Each compute node has 2 sockets of 2.6GHz 12core Intel Xeon Gold 6126 processors, 4 NVIDIA Tesla V100 GPUs. 32 nodes within the 81 nodes consists of FPGA nodes, each node has additionally 2 Intel Stratix 10 FPGAs. Compute nodes are connected by 4 ports of InfiniBand HDR100 (400 Gbps). 78 nodes are connected by a fat-tree network with the full bisection bandwidth. Additionally, among FPGA nodes, 64 FPGA cards are connected by 100 Gbps Ethernet in the two-dimensional 8 × 8 torus network. FPGA nodes are supposed to accelerate irregular computation that cannot be accelerated by GPU. Cygnus is named after a northern constellation in the summer. GPU nodes of Cygnus are called the bright first-magnitude star Deneb, and FPGA nodes are called the beautiful binary star Albireo.

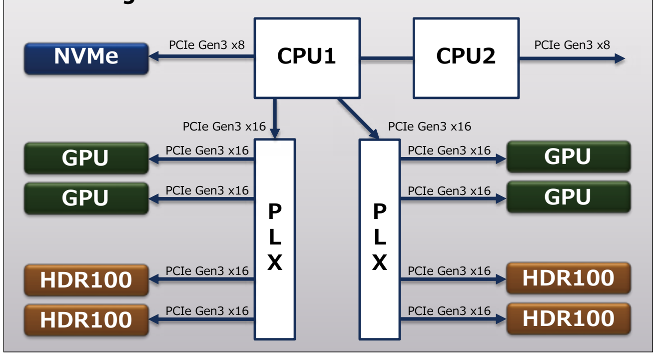
Cygnus

All compute nodes have 3.2 TB of node-local NVMe SSD (Intel SSD DC P4160), which can support for better storage I/O performance in not only HPC applications but also big-data and AI applications strongly.

Block diagram of Albireo node

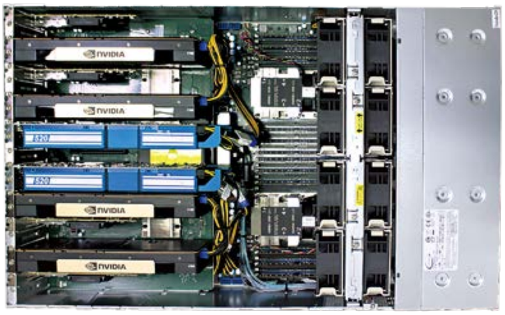


Block diagram of Deneb node



Specification of Cygnus

Item	Specification
Peak performance	**2.43 PFLOPS Double Precision** (GPU: 2.27 PFLOPS, CPU 0.16 PFLOPS) FPGA: 0.64 PFLOPS Single Precision
Number of nodes	81 (Albireo nodes 32, Deneb nodes 49)
Memory	CPU: 192 GB DDR4-2666 /node (255.9 GB/s) GPU: 32GB × 4 (3.6TB/s)
CPU / node	Intel Xeon Gold 6126 (2.6 GHz 12 cores) × 2 sockets
GPU / node	NVIDIA Tesla V100 × 4 (PCIe 3.0 × 16)
FPGA / node	Nallatech 520N with Intel Stratix10 × 2 (each with 1 OOGbps interconnect × 4 links/FPGA)
Global File System	DON Lustre, RAID6, 2.5 PB
Interconnection Network	Mellanox InfiniB and HDR100 × 4 (two cables of HDR200 / node), 48 GB/s
Programming Language	CPU: C, C++, Fortran, OpenMP, GPU: OpenACC, CUDA FPGA: OpenCL, Verilog HDL
System Vendor	NEC



Cygnus node

CYGNUS

Pegasus

The new supercomputer, Pegasus is one of the first systems in the world to introduce 4th Gen Intel Xeon Scalable processors (formerly codenamed Sapphire Rapids), Intel Optane persistent memory (codenamed Crow Pass), and the NVIDIA H100 Tensor Core GPU with 51TFlops of breakthrough acceleration. Pegasus consists of 120 compute nodes, and the overall theoretical peak performance is 6.5 PFlops. The system started operation in December 2022 and will start providing computing resources to general users in April 2023.

To drive big data analytics and ultra-large scale AI, not only high computing performance is required, but also high-bandwidth large memory and ultra-fast storage systems; Pegasus has introduced H100 GPUs, DDR5 memory, and persistent memory to solve this problem. The H100 GPU is 2.7 times faster in computing performance than the current A100 GPU, and DDR5 memory provides twice the memory bandwidth of conventional DDR4 memory. The CCS has been offering solutions with Intel Xeon processors and Intel Optane persistent memory since 2020 to research partners. Based on previous generations of Intel Optane persistent memory, allowing direct access to persistent data structures has potential to significantly improve application performance. In addition, unlike DRAM, persistent memory does not require refresh to retain data, thus dramatically reducing power consumption compared to DRAM of the same capacity. Moreover, memory expansion with persistent memory enables calculations with memory sizes that exceed DRAM capacity, and the performance of computational science applications remains largely unchanged. The effectiveness of compute accelerators (GPUs) in HPC, data-driven science, and AI-driven science has already been demonstrated, and Pegasus has been designed to incorporate state-of-the-art CPUs, GPUs, memory, and persistent memory, connected via a state-of-the-art network.

The CCS makes Pegasus available to users around the world through various usage programs such as Interdisciplinary Collaborative Use, HPCI Collaborative Use, and General Use, thereby contributing to the further development of computational science.

Pegasus

Specification of Pegasus

Computation node	CPU	Intel Xeon Platinum 8468 (codenamed Sapphire Rapids) 2.1GHz/48c (3.2256 TFlops)
	GPU	NVIDIA H100 Tensor Core GPU with PCle (51 Tflops in FP64 Tensor Core)
	Memory	128GiB DDR5-4800 (282 GB/s)
	Persistent memory	2TiB Intel Optane persistent memory 300 series
	SSD	2 × 3.2TB NVMe SSD (7 GB/s)
	Networking	NVIDIA Quantum-2 InfiniBand platform (200 Gbps)
Number of nodes		120
Peak performance		6.5 PFlops
Parallel file system		7.1PB DDN EXAScaler (40 GB/s)
System vendor		NEC

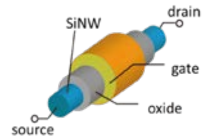
Awarded Gordon Bell Prize

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. 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)

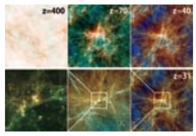
Atomic state simulation at actual semiconductor device scale. The electronic state of silicon nanowire materials, which are attracting attention as base materials of next-generation semiconductors, was calculated and quantum mechanical calculations were made for the electronic state of the nanowire at 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)

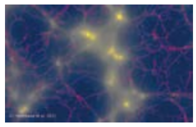
World's largest scale of a dark matter simulation. The "K computer" was employed to perform calculations related to the evolution of gravity for the early period of space consisting of about 2 trillion dark matter particles.



selected as a finalist of 2021 Gordon Bell Prize

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

The paper "A 400 trillion-grid Vlasov Simulation on Fugaku Supercomputer: Large-scale Distribution of Cosmic Relic Neutrinos in a Six-dimensional Phase Space," was selected as a finalist of the Gordon Bell Prize, 2021.



2022 Gordon Bell Prize

(CEA / LBNL / ARM / ATOS / CNRS / GENCI / RIKEN)

The paper "Pushing the Frontier in the Design of Laser-Based Electron Accelerators with Groundbreaking Mesh-Refined Particle-In-Cell Simulations on Exascale-Class Supercomputers," presented by an international collaborative research group has won a Gordon Bell Prize. One of the members of the group includes CCS fellow.

Joint Center for Advanced High Performance Computing (JCAHPC)

Overview

JCAHPC

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

Background and History

The advancement of computational sciences through cutting-edge high performance computing (HPC) platforms is vital to maintaining a world-leading position in science and technology in the 21st century. Although the K computer, operated at the RIKEN R-CCS, set a new world record in terms of speed since entering shared use in 20112, 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 two 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 largescale 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 system software. Based on this design and development, the institutions will jointly procure, operate, and administer the supercomputer. As the result of its first primary mission, we successfully procured and installed Oakforest-PACS as the fastest supercomputer in Japan at the installation time, November 2016. The establishment of such an interuniversity joint organization and joint operation of a supercomputer is the first challenge in Japan in the history of HPC. Although the Oakforest-PACS shutdown was done in 2022, JCAHPC continues to work toward joint organization and joint operation of the next supercomputer.

Multidisciplinary Cooperative Research Program (MCRP)

Provision of Computing Resources

In addition to utilization of computational resources in various fields of science, the CCS has been developing computers specifically suited for scientific researches in collaboration among researchers in computational and computer sciences. Those computers have been provided for public use since 2002 to contribute to the nationwide development of computational science. Based on these developments, we have been promoting the "Multidisciplinary Cooperative Research Program" (MCRP) since 2007, which has strengthened collaborative links with the field of computer science. In 2010, we were recognized as a "Joint Research Center for Advanced Multidisciplinary Computational Sciences" by the MEXT, in which the MCRP has been performed. To further promote multidisciplinary computational science, we provide joint research support for research meetings, researcher invitations, travel expenses for joint research, and short-term employment.

The online application system was first introduced in the 2018 academic year, and in 2019, to cope with the significant increase in application computational resources, an upper limit was set on such resources, and classifications were introduced according to application size. Furthermore, to promote internationalization, the application form and online application system were translated into English to allow for direct applications from abroad, which significantly increased the number of international users.

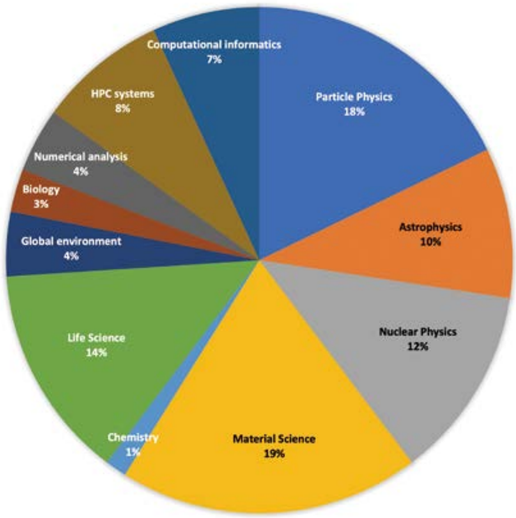
We have invited research projects in the following scientific fields: elementary particle physics, astrophysics, nuclear physics, material science, life sciences, chemistry, earth and environmental sciences, and biology, as well as computer engineering fields such as ultrahigh-speed computing systems, computational informatics, and numerical analysis. The MCRP has offered free computing resources such as PACS-CS (2007-2011), FIRST (2009-2011), T2K-Tsukuba (2008-2013), HA-PACS (2012-2017), and COMA (PACS-IX) (2014-2018), Oakforest-PACS (2017-2021) operated by JCAHPC, Cygnus (since 2019), Wisteria/BDEC-01(Odyssey) (since 2022) operated by Information technology center at the University of Tokyo, and Pegasus (since 2023).

The table presents the number of approved proposals in the MCRP since the 2010 academic year. Recently, more than 70 proposals have been approved by the review process. The graph shows the percentage of the number of submitted proposals in each field for 2022. We have a number of projects across a wide variety of fields in the natural sciences and engineering.

Number of approved projects

Year	# of projects	Computers
FY2010	24	PACS-CS, T2K-Tsukuba, FIRST
FY2011	31	PACS-CS, T2K-Tsukuba, FIRST
FY2012	48	T2K-Tsukuba, HA-PACS
FY2013	59	T2K-Tsukuba, HA-PACS
FY2014	41	HA-PACS, COMA
FY2015	51	HA-PACS, COMA
FY2016	62	HA-PACS, COMA
FY2017	61	HA-PACS, COMA, Oakforest-PACS
FY2018	67	COMA, Oakforest-PACS
FY2019	78	Oakforest-PACS, Cygnus
FY2020	83	Oakforest-PACS, Cygnus
FY2021	75	Oakforest-PACS, Cygnus
FY2022	73	Cygnus, Wisteria/BDEC-01(Odyssey)

Ratio of each field in the proposed projects for 2022



● CCS symposiums with MCRP annual reports ●

Since the first symposium on "Discovery, Integration, and Creation of New Knowledge through Multidisciplinary Computational Science" was held in May 2010, it has been held every year, together with annual progress reports of MCRP projects. Since 2018, it has been international with overseas speakers and English as the official language. In 2022, we celebrate the 30th anniversary of the CCS and the symposium was held in person first time since 2019.

The 30th Anniversary Symposium of the Center for Computational Sciences, University of Tsukuba (October 2022)

Particle Physics Group

Chief: KURAMASHI Yoshinobu, Professor, Ph.D.
Members: ISHIZUKA Naruhito, Associate Professor, Ph.D. / AKIYAMA Shinichiro, Assistant Professor, Ph.D. / OHNO Hiroshi, Assistant Professor, Ph.D.

Overview

In nature, there are four basic forces: gravity, electromagnetism, the weak force, and the strong force. The strong force makes stars shine and holds together the nuclei in the various molecules that form our bodies. It acts on quarks, which are the smallest constituent particles (elementary particles) of matter, causing a characteristic phenomenon called "confinement" due to non-perturbative effects. In experiments, only the bound state of multiple quarks (called "hadrons") is observed—not individual quarks. Therefore, a non-perturbative method is needed to study the strong force. Lattice quantum chromodynamics (QCD) involves the application of the theory of QCD to a discretized lattice of four-dimensional space–time—consisting of the three dimensions of space and one dimension of time—and can be used to quantitatively examine the 10^{-15} m world of strong forces on the basis of first principles using supercomputers.

Research Topics

- Precise calculation of the hadron mass spectrum
- Precise determination of the fundamental parameters of QCD (coupling constants and quark masses)
- Search for new physics beyond the standard model of particle physics
- Understanding the internal structure of hadrons
- Composition of light nuclei with quarks as degrees of freedom
- Understanding the phase structure of QCD, including the ultrahigh-temperature state (early universe) and high-density state (inside the neutron star)
- Application of tensor network method to relativistic quantum field theory

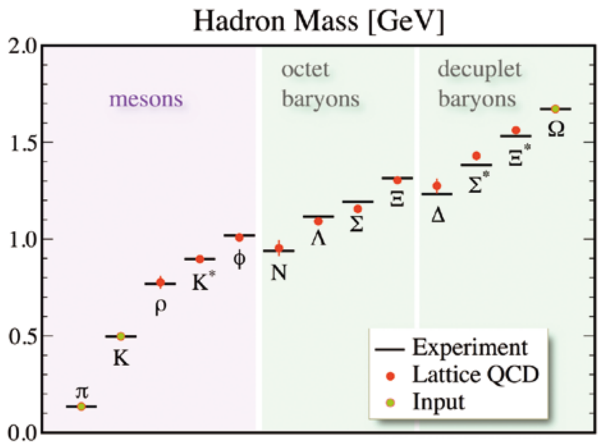


Fig.1 Hadron masses with lattice QCD in comparison with experimental values

Latest Accomplishments

Recent improvements in algorithms and computer performance have made it possible to perform physical point calculations (calculations using the quark masses in nature), which has been a goal for many years. Thus, lattice QD calculations are entering an era where precision calculation error levels are improving from 10% to 1%. Figure 1 shows the hadronic mass calculated via lattice QCD. Although this report was published in 2009, the calculation nearly reproduces the experimental value. Since then, lattice QCD calculations have made progress, and we now approach an era in which we can strive for a new type of physics based on small deviations between experimental values and theoretical calculations. For example, in Figure 2, we compare the theoretical calculation (with error symbols) and experimental values (light blue vertical band) of a physical parameter called $|V_{us}|$ using lattice QCD. Because the discrepancy between the two is evidence of an unknown physical phenomenon, it is important to evaluate this discrepancy through further precise calculations in the future.

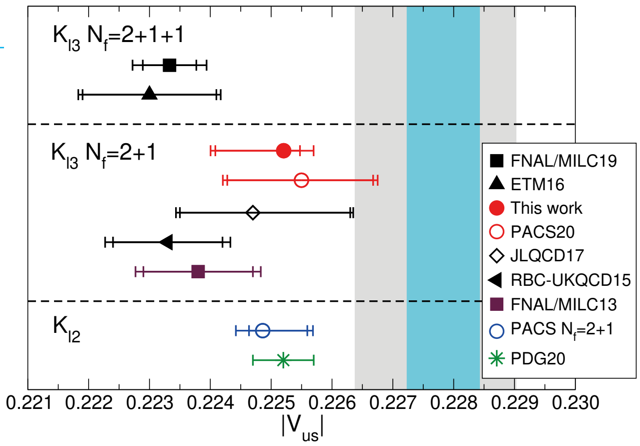


Fig.2 Comparison between lattice QCD calculation and experimental data (light blue vertical band). The red and blue circles represent the results of our group's calculations.

Chief: KURAMASHI Yoshinobu, Professor, Ph.D.

He 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. His major research themes are large scale lattice QCD simulations and application of the tensor network method to particle physics.

Astrophysics Group

Chief: OHSUGA Ken, Professor, Ph.D.
Members: MORI Masao, Associate Professor, Ph.D. / YAJIMA Hidenobu, Associate Professor, Ph.D. / YOSHIKAWA Kohji, Lecturer, Ph.D. / WAGNER Alexander, Assistant Professor, Ph.D. / FUKUSHIMA Hajime, Assistant Professor, Ph.D. / ASAHINA Yuta, Assistant Professor, Ph.D. / NAKASATO Naohito, Visiting Associate Professor, Ph.D.

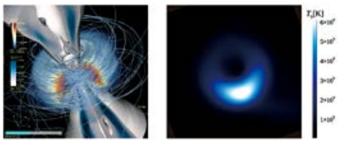
Overview

We aim to use fundamental physics to understand a wide variety of questions, such as the birth and evolution of the first stars and galaxies in the universe; the characteristics of the light they emit; the formation and evolution of galaxies, galaxy clusters, and other large-scale structures; the formation and evolution of black holes and their activity; the formation of planets; and the birth of life in the universe. We are also researching how technologies developed in this field may find applications in medicine.

Research Topics

● Black hole physics:

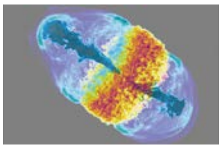
In the accretion disk where matter accumulates owing to the strong gravity of a black hole, strong radiation and jets are generated by the release of gravitational energy. We are investigating such high-energy astrophysical phenomena around black holes and the radiation characteristics of black hole objects through general relativistic radiation magnetohydrodynamic simulations.



(left) Black hole accretion disks and jets in general relativistic radiative magnetohydrodynamic simulations
(right) Black hole shadow reproduced by general relativistic radiative transfer calculations

● Supermassive black holes and galactic evolution

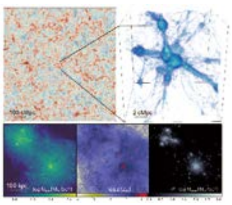
A supermassive black hole exists universally at the galaxy center and grows while swallowing the surrounding stars and interstellar medium. Simultaneously, its jets blow away the interstellar medium, strongly influencing the evolution of the galaxy. We are investigating this complex interdependence using relativistic magnetohydrodynamic simulations in an attempt to grapple with the mystery of galactic evolution.



Interaction between interstellar gas and jets

● Galaxy formation

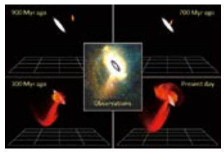
In the early universe, massive galaxies and supermassive black holes may have been formed by the frequent merging of galaxies and accretion in dense regions of galaxies called primordial clusters. We are studying the physical phenomena occurring in primordial clusters of galaxies through cosmological radiation hydrodynamic simulations.



(upper left) Large-scale mater distribution in the universe
(upper right) Structure of gas near the central galaxy in a proto-galaxy cluster
(under) From left: galactic gas, heavy elements, and stellar surface column density

● Galactic evolution and dark matter

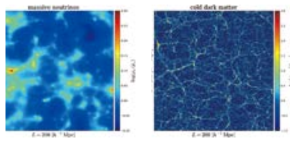
Dark matter is known to play an important role in the evolution of galaxies, but its nature remains shrouded in mystery, and many contradictions within existing theories have been pointed out. We are investigating the nature of dark matter haloes by studying galaxy collisions.



A galaxy collision that occurred in the Andromeda Galaxy approximately 1 billion years ago

● Neutrinos and formation of large-scale structures in the universe

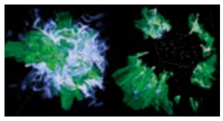
We are conducting theoretical research to investigate the mass of neutrinos, which is yet to be elucidated, in preparation for future observational projects of large-scale galaxy survey. To this end, for the first time, Vlasov simulations have been accomplished as a high-precision numerical simulation method instead of the conventional n-body simulation.



(left) Result with neutrino effect
(right) Result without neutrino effect

● Star cluster formation

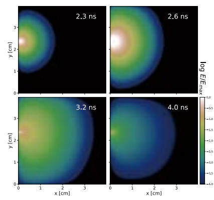
Most stars belong to star clusters initially. In the star cluster formation, radiation emitted from massive stars heats the surrounding gas, which impacts the subsequent star formation. We are studying the formation of stars and star clusters using radiation hydrodynamics simulations.



Gas and ionization front (green surface) structures in star cluster formation

● Applications in medicine

Diffuse optical tomography (DOT) using near-infrared light in the wavelength range of 700–1000 nm has been attracting attention as a new medical diagnostic method because it is a non-invasive procedure that does not expose the patient to radiation. We are studying light propagation in living organisms by applying the high-precision technique for radiative transfer calculation developed in astrophysics to DOT.



Radiative transfer simulation assuming pulsed light irradiation of a living body

Chief: OHSUGA Ken, Professor, Ph.D.

He graduated from the University of Tsukuba, in 2001 with a Ph.D. (Sciences). He was a JSPS Research Fellow (Kyoto University/Paris Observatory) in 2001, a Research Associate at Rikkyo University in 2004, a RIKEN Basic Science Fellow in 2007, and an Assistant Professor at NAOJ in 2008 before assuming his current position in 2018. He specializes in theoretical astrophysics. He studies black hole accretion flows, jets, and the formation process of supermassive black holes using radiation magnetohydrodynamics simulations.

Nuclear Physics Group

Chief: NAKATSUKASA Takashi, Professor, Ph.D.
Members: YABANA Kazuhiro, Professor, Ph.D. / SHIMIZU Noritaka, Associate Professor, Ph.D. / HINOHARA Nobuo, Assistant Professor, Ph.D.

Overview

The nucleus can be described as a collection of Fermi particles (protons and neutrons) called nucleons. The mechanics to rule over this microscopic world, such as the quantum mechanics of many-particle systems and quantum field theory, is essential. Three of the four fundamental forces of nature—the strong force, electromagnetic force, and weak force—play important roles in the atomic nucleus, leading to a variety of aspects of reactions and structure that are related to the existence of the matter around us. For example, the sun and the stars in the night sky shine with atomic nuclei as fuel, and they are the lights of the factories that produce the elements. The burning (nuclear reaction) process, which depends on the nature of the forces involved and the nuclear structure, controls the brightness and lifetime of the star, as well as the type and quantity of elements produced.

Nuclear physics has progressed through both experiments using accelerators and theoretical calculations using computers. Numerical calculations are indispensable for quantum many-body problems, such as nuclear problems. The Nuclear Physics division works on developing theories, models, and numerical methods based on quantum mechanics to clarify the nuclear structure, nuclear reactions, structure of stars, and quantum dynamics of matter.

Research Topics

Neutron stars, known as pulsars that emit regular periodic signals, remain shrouded in mystery even more than half a century after their discovery. In recent years, the study of neutron stars has entered a new stage with the observation of neutron star mergers using gravitational waves and the identification of neutron stars with masses that exceed twice the mass of the sun. The atomic nuclei on Earth are all microscopic, with radii of at most approximately 10^{-14} m; no larger atomic nuclei can exist. However, elsewhere in the universe, there are large nuclei with a radii of 10 km. These are the neutron stars. It is conjectured that protons and neutrons form a non-uniform structure near the surface of neutron stars, but existing studies have mainly used the quasi-classical approximation. We have been developing code for finite-temperature Hartree–Fock–Bogoliubov calculations in three-dimensional (3D) real space to describe the structure of neutron stars in a quantum and non-empirical manner using energy density functional theory, which can universally and quantitatively describe atomic nuclei. Figure 1 shows the structure of the inner crust of a neutron star calculated on this basis. In the inner crust, neutrons spread to fill the space while protons are localized and appear periodically in a manner that resembles a crystalline structure. It was confirmed that the neutrons are in a superfluid state because of the pair condensation. Extending the density functional theory to its time-dependent version, we are able to study response, reaction, and modes of excitation in nuclei and nuclear matter.

Some unstable nuclei and light nuclei exhibit exotic phenomena, such as shape coexistence and cluster structure. We have succeeded for the first time to achieve structure of a resonance state called "Hoyle state" (Fig. 2) which plays a key role in heavy elements synthesis in the universe. Collaborating with many experimentalists at radioactive-ion beam accelerator facilities, we investigate the richness of the nuclear structures by performing large-scale quantum many-body calculations. For that purpose, we adopt the nuclear shell-model calculation, which requires solving the eigenvalue problem of a Hamiltonian matrix whose dimension is huge, e.g., over 10^{11}. To solve this problem efficiently, we also perform code developments for massively parallel computers.

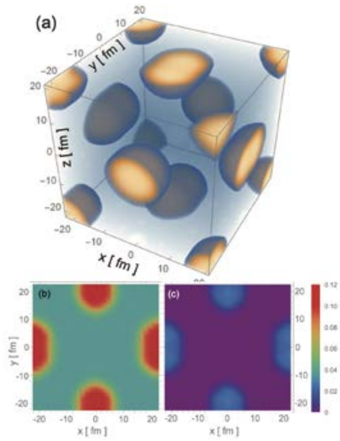


Fig.1 (a) Structure of the neutron star inner crust predicted to appear at a certain temperature and density, assuming a face-centered cubic lattice structure. Within the region indicated by the figure, there exist 136 protons and approximately 4,000 neutrons. The density distributions of (b) neutrons and (c) protons in the xy cross-section.

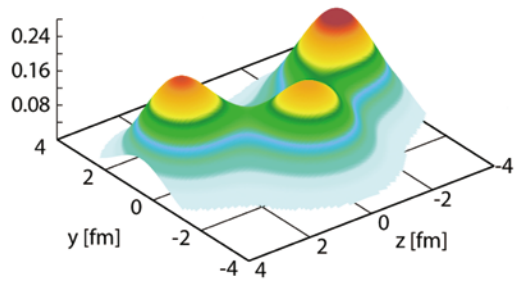


Fig. 2 Density profile of the Hoyle (second 0^+) state of the Carbon-12 nucleus produced by the large-scale quantum many-body calculations. The state consists of three alpha clusters.

Chief: NAKATSUKASA Takashi, Professor, Ph.D.

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

Quantum Condensed Matter Physics Group

Chief: OTANI Minoru, Professor, Ph.D.
Members: YABANA Kazuhiro, Professor, Ph.D., Deputy Director of CCS / KOIZUMI Hiroyasu, Associate Professor, Ph.D. / TONG Xiao-Min, Associate Professor, Ph.D. / MAESHIMA Nobuya, Lecturer, Ph.D. / SATO Shunsuke A., Assistant Professor, Ph.D. / HAGIWARA Satoshi, Assistant Professor, Ph.D. / ONO Tomoya, Visiting Professor, Ph.D.

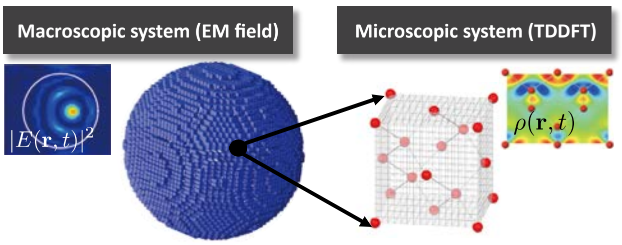
Overview

The matter that exists around us is made up of atoms, which are composed of nuclei and electrons. This matter exhibits a variety of properties depending on its composition and structure, and their use supports much of science and technology today. In our division, we consider diverse types of matter, such as quantum many-body systems coupled by Coulomb interactions, and use computers to solve quantum mechanics equations. We aim to obtain the knowledge that will become the basis for the next generation of technology by understanding the various properties of matter, utilizing the quantum information of matter, and searching for matter with new functions.

Research Topics

Interaction of light and matter

Light has given us the means to precisely measure the properties of matter. In recent years, the use of intense and very short pulses of light in optical science has led to real-time measurements of ultrafast electron motion and manipulation of electron motion by light. In collaboration with computer scientists and researchers from other institutions, we are investigating the interaction between light and matter using first-principles computational methods such as time-dependent density functional theory and developing the first-principles code SALMON (Scalable Ab initio Light-Matter simulator for Optics and Nanoscience), which works on massively parallel computations. SALMON was developed as an open-source software and can be downloaded at https://salmon-tddft.jp.

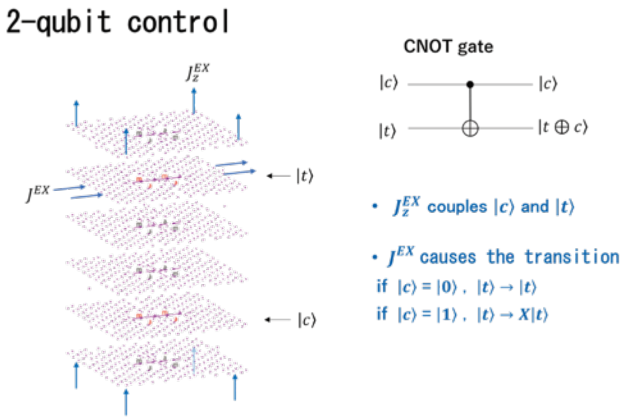


First-principles simulation of chemical reactions at the solid-liquid interface

With the growing concern for environmental issues, there is a need to significantly improve the performance and durability of energy-related devices such as fuel cells and storage batteries. We run simulations of chemical reactions that occur in these devices at the microscale to understand the reaction mechanisms from a quantum mechanics perspective. The simulation results are used in the design of devices and development of materials to improve device performance. We are also developing computational methods and programs for the simulations, and the code for these has been released in the form of open-source software used widely by researchers both in Japan and abroad.

Emergent gauge field matter (superconductors, strongly correlated matter, topological matter, etc.)

In superconductors, magnetic materials, strongly correlated matter, and topological matter, an emergent gauge field—which differs from an electromagnetic field—is introduced in the mathematical form known as the Berry connection. When considering the function of such matter and their responses to external fields, it is necessary to incorporate the emergent gauge field into the calculations. We are developing such a method and using it to perform material science quantum calculations. Emergent gauge fields give rise to “topological quantum states,” and it is possible to build a quantum computer using the quantum information in these states. The realization of such a computer is also a part of our work. Additionally, we are studying ultrafast dynamics in strongly correlated matter and topological matter irradiated by intense laser beams and electronic state control via laser beams through simulations using theoretical models.



Chief: OTANI Minoru

He graduated from Osaka University in 2000, with a doctor degree. 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 a research associate at the University of Tsukuba (2001), a research associate at the University of Tokyo (2003), a researcher (2008), a senior researcher (2009) and a group leader (2010) in the National Institute of Advanced Industrial Science and Technology (AIST). Since 2021, he has joined the Center for Computational Sciences (CCS) in the University of Tsukuba as a full professor. His major is computational material science.

Biological Function and Information Group

Group Leader: SHIGETA Yasuteru, Professor, Ph.D.
Members: HARADA Ryuhei, Associate Professor, Ph.D. / SHOJI Mitsuo, Assistant Professor, Ph.D. / HORI Yuta, Assistant Professor, Ph.D. / HENGPHASATPORN Kowit, Assistant Professor, Ph.D.

Overview

Biological phenomena are governed by a series of chemical reactions driven by biological molecules such as proteins, nucleic acids, lipids, and sugars. As such, the fundamental molecular mechanisms of biological phenomena can be understood by examining the changes in electronic states and the spatial arrangement of atoms during chemical reactions. In the Biological Function and Information Group, we use computational methods such as first-principles calculations based on quantum theory and molecular dynamics (MD) calculations based on classical (statistical) mechanics to understand the inherent dynamic structure–function relationships in biological molecules and to understand the essence of biological phenomena.

Research Topics

(1) Development of an efficient structure sampling method using MD and machine learning
(2) Reaction analysis of proteins using hybrid Quantum Mechanical/ Molecular Mechanics (QM/MM) methods (photosystem II, hydrogenase, etc.)
(3) Clarifying the mechanism of amino-acid formation in interstellar space and the origin of L-body excess formation (e.g., glycine and alanine formation in interstellar space)

Latest Accomplishments

(1) Protein conformational change is a phenomenon that operates over extremely long timescales, making it difficult to track using conventional MD simulations. We have developed Parallel Cascade Selection MD (PaCS-MD) to efficiently explore protein folding pathways (Fig. 1). Furthermore, we have found that the sampling efficiency can be significantly increased by using machine learning—a method rooted in information science. This method has proven to be suitable for massively parallel environments. We are using the supercomputer at the Research Center for Computational Science to perform such calculations.

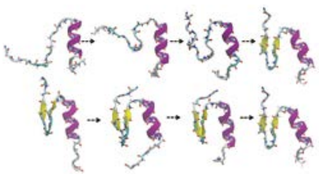


Fig.1 Tryptophan cage folding simulation

(2) Photosystem II has a highly characteristic reaction active center composed of manganese, calcium, and oxygen atoms (Fig. 2) and produces oxygen molecules from water molecules in a multi-step chemical reaction using light energy. We identified the structure–electron–proton transfer changes in this reaction (water-splitting reaction) using a hybrid QM/MM method.

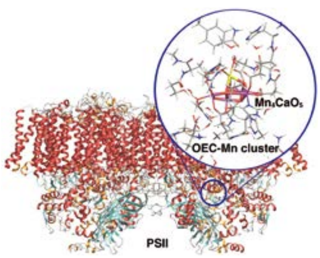


Fig.2 Overall structure and active center structure of photosystem II

(3) Because some of the biomolecules that constitute life have been found in meteorites, there is a possibility that life originated in interstellar space. We are using high-precision *ab initio* methods to comprehensively analyze various reaction pathways for prebiotic amino-acid synthesis and degradation. In collaboration with the Division of Astrophysics, we are studying the molecular evolutionary processes related to the origins of life.

Fig.3 Image of molecular evolution and amino-acid synthesis in interstellar space

(4) Accurate structures of various target proteins derived from SARS-CoV-2 are now available, and there is a need to elucidate the binding mode of various potent drugs to them and to identify novel drug candidates. By using various computational approaches, we aim to accelerate the screening of drug candidates with the highest accuracy and conduct research that contributes to the identification of antiviral drugs.

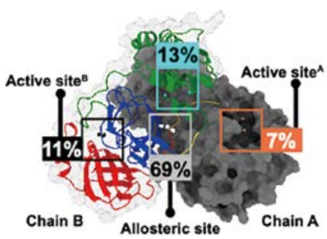


Fig. 4 Image of evaluation of the binding between main protease and inhibitors

Group Leader: SHIGETA Yasuteru, Professor, Ph.D.

He 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. His major is the theoretical biophysics.

Molecular Evolution Group

Chief: INAGAKI Yuji, Professor, Ph.D.
Member: NAKAYAMA Takuro, Assistant Professor, Ph.D.

Overview

Phylogenetic analysis of major phylogenetic groups in eukaryotes: It has been proposed that eukaryotes can be divided into roughly six major phylogenetic groups. We use molecular phylogenetic analysis with multiple gene sequences to infer whether each major phylogenetic group is truly monophyletic and how closely related the groups are. We are also studying the methods for phylogenetic analyses to make unbiased inferences. We are also interested in symbiosis between two distinct unicellular organisms, as multiple symbiotic events played a major role in the early evolution of eukaryotes. We are challenging to elucidate the mechanism underlying symbiotic events by assessing genomic data sampled from diverse organisms.
Earth is inhabited by a wide variety of organisms. For example, we humans have a spine, move our own bodies, and consume foods (other organisms) to survive. The human body is made up of many cells. Although plants are also made up of many cells, their way of life differs significantly from ours. Plants do not move by themselves and do not need to eat food. Instead, they live by photosynthesis, which is based on light energy. Although we do not always realize it, there are a vast number of other species on the planet that we cannot see with the naked eye. These organisms have a wide variety of appearances and lifestyles. All of these organisms on Earth have evolved over a long period of time from a single primitive organism to their present forms. Our research group focuses on eukaryotes—organisms with nuclei in their cells—and aims to understand the evolutionary relationships among the major phylogenetic groups of eukaryotes and their evolutionary paths.
We know that in the evolutionary process of eukaryotes, there have been multiple instances where organisms from completely different phylogenetic lineages have evolved symbiotically in cells and become part of the cells. Such symbiotic events are thought to have contributed substantially to the diversification of eukaryotic organisms, but the mechanism whereby two separate organism lineages fuse into a single organism remains largely unknown. We are working to understand the principles of symbiosis that led to the current diversity among eukaryotes using genomic information and other data.

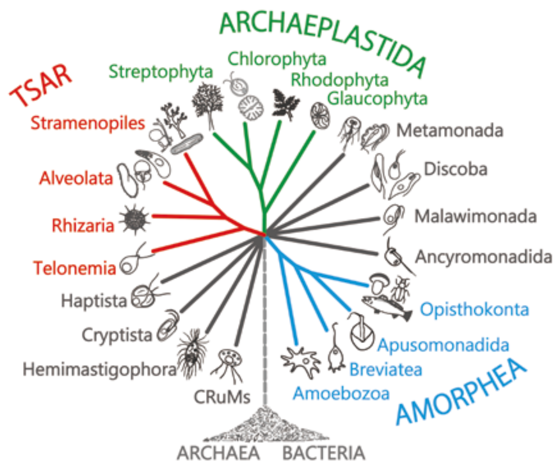


Fig.1 Main lineages of eukaryotes

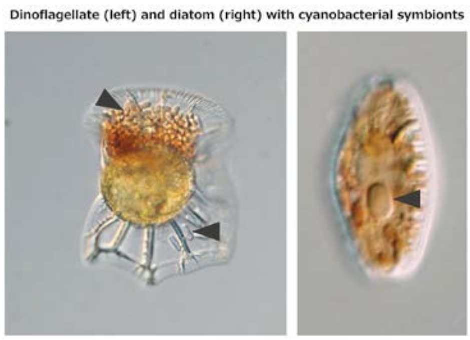


Fig.2 Example of a unicellular eukaryote that coexists with bacteria (arrows)

Research Topics

We endeavor to understand the evolutionary path of eukaryotes by inferring their phylogenetic relationships and performing comparative genomic analyses based on data regarding gene (DNA) sequences and protein amino-acid sequences of existing species. Furthermore, there are many "new" organisms in the natural environment that have yet to be studied, and these undiscovered organisms may hold the key to solving various problems in eukaryotic evolution. We are investigating such organisms that are evolutionarily important but have not yet been investigated. To this end, we are analyzing each organism's evolutionary characteristics by acquiring large-scale genetic and genomic information from eukaryotes from various phyla.
Molecular phylogenetic analysis requires statistical processing using the maximum likelihood method, and computers are used for this purpose. In a nucleotide or amino-acid sequence, "signals" corresponding to past evolutionary events and random changes (called "noise") have accumulated during the evolutionary process. The problem lies in the fact that the amount of noise in the sequence increases over time, while the amount of signal decreases. Therefore, to accurately infer the relationship between major eukaryotic phylogenetic groups that may have diverged in the distant past, it is necessary to analyze large amounts of sequence data. We are using supercomputers to analyze transcriptome data and genome data to handle large amounts of data containing complex genetic information.

Chief: INAGAKI Yuji, Professor, Ph.D.

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

Global Environmental Science Group

Chief: KUSAKA Hiroyuki, Professor, Ph.D.
Members: MATSUEDA Mio, Assistant Professor, Ph.D. / DOAN Quang-Van, Assistant Professor, Ph.D.

Overview

The Division of Global Environmental Science comprehensively plans and promotes research related to weather and climate from the global scale to the urban scale using the global cloud-resolving model "NICAM" with the regional weather model "WRF" and the urban district weather model "LES."
In addition to three dedicated faculty members, the research division has joint researchers within the university. The resident faculty members are Professor Hiroyuki Kusaka, who specializes in studying climates familiar to us, such as urban and mountain climates; Assistant Professor Mio Matsueda, who aims to improve the accuracy of weather prediction using ensemble forecasting; and Assistant Professor Doan Quang Van specializes in regional climate change.

Research Topics

The **Weather Research and Forecasting model (WRF)** is a highly versatile numerical weather prediction/simulation model that was developed mainly by the National Center for Atmospheric Research (NCAR) in the United States and released to the public. In this division, we use the WRF to tackle unsolved problems in familiar meteorological phenomena, such as the urban heat island phenomenon, heavy rainfalls, Foehn wind, and cap and mountain-wave clouds in mountains. We are also conducting research on global warming and urban climate and projecting the future of heat stroke to address issues in society.

Additionally, we have been developing a micro-scale meteorological model (LES model) with extremely high spatial resolution that can reproduce radiations, temperature, humidity, and wind distributions in urban districts, in collaboration with the CCS's Division of High-Performance Computing Systems.

Fig.1 Cap clouds and mountain-wave clouds appearing over Mt. Fuji.

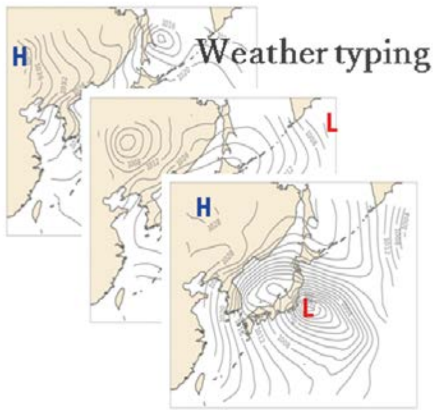


Fig.2 Classification of weather map patterns using machine learning methods

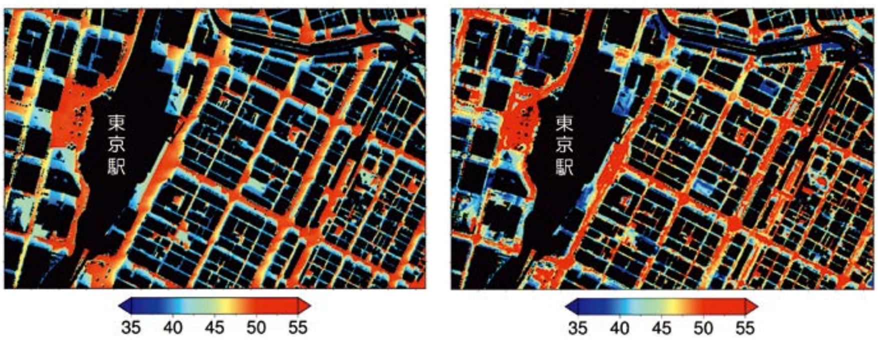


Fig.3 Surface temperature distribution around Tokyo Station. Buildings are shown in black. The left figure shows the results of a simulation with the LES model developed by JCAHPC, and the right figure shows the results of helicopter observation by the Tokyo Metropolitan Institute of Environmental Science.

Chief: KUSAKA Hiroyuki

He graduated from the University of Tsukuba. He assumed his present position after a Researcher at the Central Research Institute of Electric Power Industry, long-term visiting scientist at NCAR, and as a Lecturer and Associate Professor at the Center for Computational Sciences, University of Tsukuba.
He is an expert of the micro-scale and meso-scale meteorology and climatology. Urban heat island effect, foehn phenomenon, downslope windstorms, LES modeling, and climate downscaling in Japan and Vietnam are the main themes. Cap and mountain-wave clouds around the Mt. Fuji is also one of the research themes.

High Performance Computing Systems Group

Chief: BOKU Taisuke, Professor, Ph.D., Director of CCS
Members: TAKAHASHI Daisuke, Professor, Ph.D. / TATEBE Osamu, Professor, Ph.D. / NUKADA Akira, Professor, Ph.D. / TADANO Hiroto, Assistant Professor, Ph.D. / KOBAYASHI Ryohei, Assistant Professor, Ph.D. / FUJITA Norihisa, Assistant Professor, Ph.D. / HANAWA Toshihiro, Visiting Associate Professor, Ph.D.

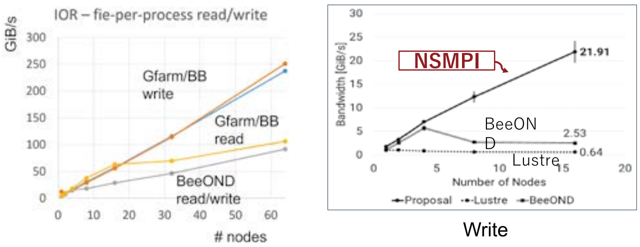
Overview

The High-Performance Computing Systems Division conducts research and development of various hardware and software for High Performance Computing (HPC) to satisfy the demand for ultrafast and high-capacity computing to promote cutting-edge computational science. In collaboration with the Center's teams in domain science fields, we aim to provide the ideal HPC systems for real-world problems.
Research targets a variety of fields, such as high-performance computer architecture, parallel programming languages, large-scale parallel numerical calculation algorithms and libraries, computational acceleration systems such as Graphics Processing Units (GPUs), large-scale distributed storage systems, and grid/cloud environments. Research on high-performance computer architecture is described in "Project Office for Exascale Computing System Research and Development" on p.21.

Research Topics

●Fundamental technologies for parallel I/O and storage systems

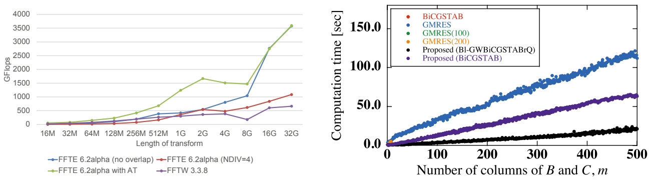
Storage performance has become a bottleneck in large-scale data analysis and artificial intelligence (AI) using Big Data on supercomputers. To reduce this performance bottleneck, we are researching and developing fundamental technologies for parallel input/output (I/O) and storage systems. We developed Gfarm/BB, which can temporarily configure a parallel file system when parallel applications are executed, by utilizing the storage system of a compute node. We also designed and implemented a standard library for parallel I/O (NSMPI), which efficiently utilizes the storage system of a compute node. Both of them exhibit scalable performance depending on the number of nodes and contribute significantly to reducing performance bottlenecks.



Gfarm/BB read and write performance (left) and NSMPI write performance (right)

●High-performance, massively parallel numerical algorithms

FFTE—an open-source high-performance parallel FFT library developed by our division—has an auto-tuning mechanism and is suitable for a wide range of systems (from PC clusters to massively parallel systems). We are also developing large-scale linear computation algorithms. We constructed a method using the matrix structure of saddle point problems that enables faster solutions than existing methods.



Performance of parallel one-dimensional FFT on Oakforest-PACS (1024 nodes) (left) and solution time of saddle point problems (right)

●GPU computing

GPUs were originally designed as accelerators with a large number of arithmetic units for image processing, but they are also able to perform general-purpose calculations. GPUs have been used to accelerate applications but are now used to perform larger-scale calculations, often with longer execution times. In shared systems such as supercomputers, there are execution time limits, but time limits can be exceeded using a technique called checkpointing, which is used to save the application state to a file in the middle of an execution so that the application can be resumed later.
Because the checkpointing technique for applications using only the central processing unit (CPU) is well established, we extended it to the GPU. The GPU has its own memory separate from the CPU, and GPU applications control the GPU with dedicated application programming interface (API) functions from the CPU. We monitor all the calls to these API functions, collect the necessary information to resume execution, and store it in the CPU memory. Additionally, in the pre-processing of saving the checkpoint, the data in the GPU's memory is collected on the CPU side so that they can be saved together in a file. Because we cannot increase the execution time to enable to checkpoints, we must minimize the overhead of monitoring the API. It is important to minimize the number of API functions to be monitored and to save only the data that are needed.

Chief: BOKU Taisuke

He 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 25 years from its establishment and is serving as Director of CCS since 2019. He has participated in the development of most of the supercomputer systems in CCS such as CP-PACS, FIRST, PACS-CS, HA-PACS and Cygnus as an HPC system researcher. All of these systems were designed and developed through discussion and collaboration with researchers in other Center application divisions. His research interests include high performance interconnection networks, large scale cluster system design, parallel programming and tuning for real applications, and most recently, GPU and FPGA accelerated computing.

Database Group

Group Leader: AMAGASA Toshiyuki, Professor, Ph.D.
Members: SHIOKAWA Hiroaki, Associate Professor, Ph.D. / HORIE Kazumasa, Assistant Professor, Ph.D. / BOU Savong, Assistant Professor, Ph.D.

Overview

The management and utilization of Big Data are major issues in computational science. The Department of Data Infrastructure in the Computational Informatics Laboratory is in charge of research and development in the field of data engineering for the utilization of Big Data (Fig. 1). Specifically, we work on data integration infrastructure technology to handle diverse information sources and real-time data in an integrated manner, high-performance large-scale data analysis technology, data mining and knowledge discovery technology for knowledge and patterns found in large-scale scientific data and social media, open data-related technologies for handling various data and knowledge on the Internet in a unified manner, and other such fundamental technologies. We also promote applied research in various fields of computational science in collaboration with the Division of Global Environmental Science, Division of Particle Physics, and Division of Life Sciences at the Research Center for Computational Science, International Institute for Integrated Sleep Medicine (IIIS), Center for Artificial Intelligence Science (C-AIR), etc.

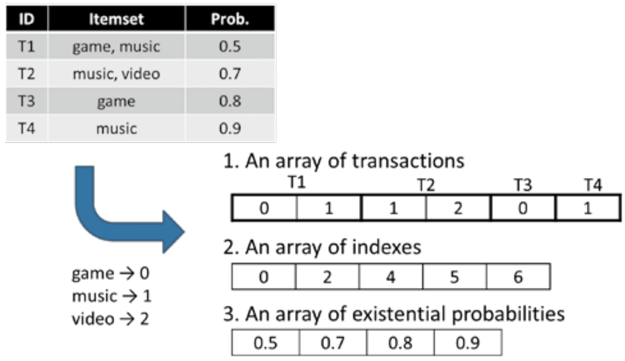


Fig.1 GPU probabilistic frequent item set mining

Research Topics

Big Data infrastructure technology

Research on fundamental technologies for processing and analyzing Big Data characterized by the 3Vs (Volume, Variety, Velocity): 1) development of fundamental systems for linking streams such as sensor data in addition to databases and the Web, etc.; 2) high-performance Big Data analysis technology using massively parallel processing with GPUs, FPGAs, etc.; 3) privacy and security in Big Data processing; and 4) open data-processing infrastructure such as RDF and LOD.

Data mining and knowledge discovery

Research on data mining and knowledge discovery methods for various types of data: 1) various analysis algorithms for text, images, graphs, etc.; 2) social media analysis and mining; and 3) biological data analysis using machine learning.

Utilization of scientific data

Research aimed at the management and utilization of explosively growing scientific data: 1) operation and development of the GPV/JMA large-scale meteorological database and the JRA-55 archive; 2) operation and development of the JLDG/ILDG lattice QCD data grid; and 3) advancement of genomic and biological data utilization using machine learning.

Latest Accomplishments

Big Data infrastructure technology

We are working on research and development of heterogeneous stream integration infrastructure systems, stream/batch integrated Big Data-processing infrastructure, and ultrahigh-performance data analysis methods using GPUs.

Data mining and knowledge discovery

We are working on research and development of high-speed analysis algorithms for large-scale graphs and images, advanced metadata extraction algorithms that significantly improve the scope of social-media use, etc.

Utilization of scientific data

We are developing and operating the GPU/JMA archive and the JRA-55 archive, which are databases for archiving numerical weather data (GPV) published by the Japan Meteorological Agency (JMA), and making them available to researchers (Fig. 2).

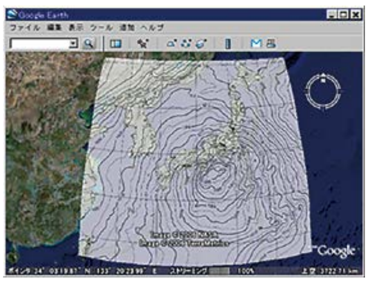


Fig.2 Viewing weather maps using Google Earth

Group Leader: AMAGASA Toshiyuki

He received B.E., M.E., and Ph.D. from the Department of Computer Science, Gunma University in 1994, 1996, and 1999, respectively. He is currently a full professor at the Center for Computational Sciences, University of Tsukuba. His research interests cover database systems, data mining, and database application in scientific domains. He is a senior member of IPSJ, IEICE, and IEEE, and a member of DBSJ and ACM.

Computational Media Group

Chief: KAMEDA Yoshinari, Professor Ph.D.
Members: KITAHARA Itaru, Professor, Ph.D.

Overview

In contrast to ordinary supercomputers, which require pure data-processing efficiency and speed, computational science that processes information related to humans requires that the time axis of information processing be aligned with that of humans. We are therefore conducting research on the global expansion of human society and its surrounding environments (living spaces, urban environments, etc.). We propose a new framework of computation using computational media as a mediator to present the information obtained by integrating observed data and simulation results in a form that is easy for humans to understand and to feed back to human society.
Specifically, we are implementing large-scale intelligent information media by integrating sensing functionality for real-world information, ample computing functionality for processing diverse information, and large-scale database functionality for selecting and storing information on a computer network. Our research efforts are focused on the computational medical business.

Research Topics

- Methodology for acquiring vision based skills through sports-related video analysis and virtual reality (VR) use
- Proposal of a video viewing method to observe a work space
- Multi-viewpoint video presentation system that work online
- Multi-viewpoint video presentation system that automatically reconfigures points of gaze and switches points of view
- Precise measurement of human behavior and real-time visual feedback
- Integration of deep learning and 3D point cloud processing
- Matching of past and current images based on correspondence search
- 3DCG virtual surgery

Latest Accomplishments

Measurement and analysis of visual search activities in sports

We proposed a VR system that allows both soccer players and coaches to measure active visual exploratory activity patterns. The main objective of this research is to analyze the ability of soccer players to “read the game” in pressure situations. By using head-mounted display technology and biometrics, including head- and eye-tracking functions, we can accurately measure and analyze the user’s visual search movements during a game.

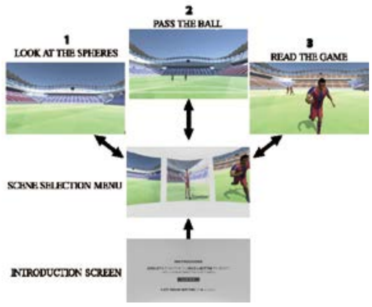


Fig.1 Measurement of visual search movement in VR space

Omnidirectional multi-view image viewing method using 3D image processing and generative adversarial networks (GANs)

We propose an omnidirectional multi-view image viewing method using 3D image processing and GANs. With structure from motion, we can estimate the camera parameters and 3D information of the targeted workspace from the omnidirectional multi-view images and generate the free viewpoint image with an arbitrary viewpoint image rendering process based on the depth information to achieve smooth viewpoint movement. The quality of free viewpoint image is improved by deep learning using a GAN to achieve high-quality omnidirectional multi-viewpoint image viewing.

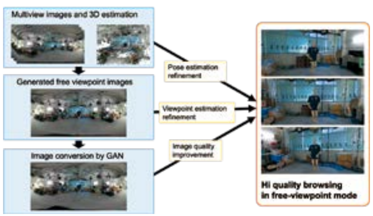


Fig.2 Omnidirectional multi-view image viewing method overview

Visualization of time-series changes in 3D reconstruction of cultural heritage buildings

Investigating the degree of deterioration, damage, renovation, or alteration of cultural heritage buildings over time is an important issue. Continual image capturing from one viewpoint over a long period of time is impractical. In this research, by using a self-encoder (auto-encoder) and guided matching, we succeeded in precisely visualizing time-series changes by accurately aligning past and present images of the target building.

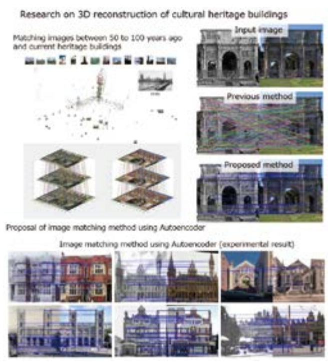


Fig.3 Superposition of past and present images using the proposed method

Chief: KAMEDA Yoshinari, Professor, Ph.D.

He received his Bachelor of Engineering degree, his Master of Engineering, and his Doctor of Philosophy from Kyoto University in 1991, 1993, and 1999. He was an assistant professor at Kyoto University until 2003. He was a visiting scholar in AI Laboratory at MIT in 2001-2002. In 2003, he joined University of Tsukuba and is now a full professor. His research interests include intelligent enhancement of human vision, virtual reality, mixed reality, computer vision, and intelligent support for handicapped people and smart transportation society.

Department of Computational Medical Science

Head: AMAGASA Toshiyuki, Professor, Ph.D.

Objectives

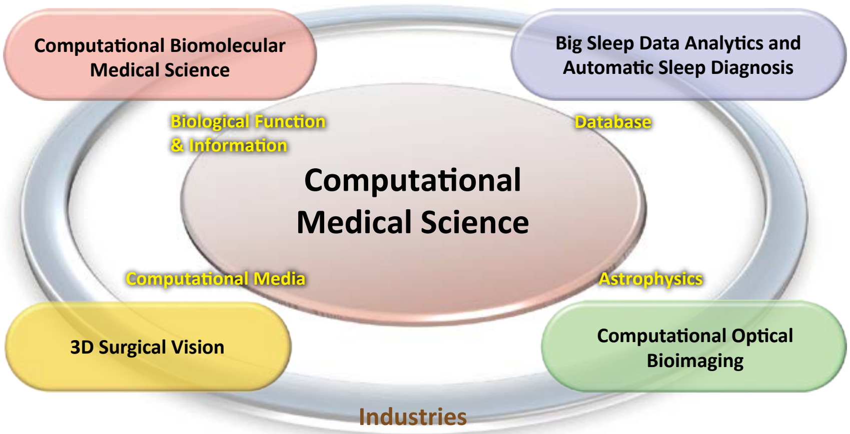
For the development of novel technologies for medical care, there has been hitherto conducted “medicine and engineering cooperation”, which is the cooperation between medical scientists in private enterprises and engineers in academic institutes, or “medicine, science and engineering cooperation” including natural scientists as well. Owing to recent rapid strides in computational science, state-of-the-art computational techniques have been developed, and they have established an indispensable research method comparable to theory and experiments. Besides, the technology of big data and machine learning has made remarkable progress in the fields of database and computational media. In Center for Computational Sciences, University of Tsukuba, we promote “Computational Medical Science”, which initializes a novel approach of “medicine and computation cooperation” by incorporating cutting-edge computational sciences into medical science. In this department, we explore medical technologies based on the latest development of computational methods, imaging technology, and machine/deep learning, in cooperation of computational sciences in physics, life science, database technology, computational media engineering with medical science and industries. For the objectives, we propel four projects of (1) Computational Biomolecular Medical Science, (2) Big Sleep Data Analytics and Automatic Sleep Diagnosis, (3) 3DCG Virtual Surgery, and (4) Computational Optical Bioimaging, in pursuing mutual cooperation and synergy.

Prof. SHIGETA Yasuteru
Assoc. Prof. HARADA Ryuhei
Assist. Prof. Kowit Hengphasatporn
Dr. MORITA Rikuri
Dr. SHIMOYAMA Hiromitsu

Collaborations:
Medicine, Biology, Physics

Prof. AMAGASA Toshiyuki
Pro. KITAGAWA Hiroyuki (IIIS)
Assist. Prof. HORIE Kazumasa

Collaborations:
Sleep Medicine/Science, Medicine, Engineering



Prof. Yoshinari Kameda
Prof. Itaru Kitahara
Dr. Chun Xie

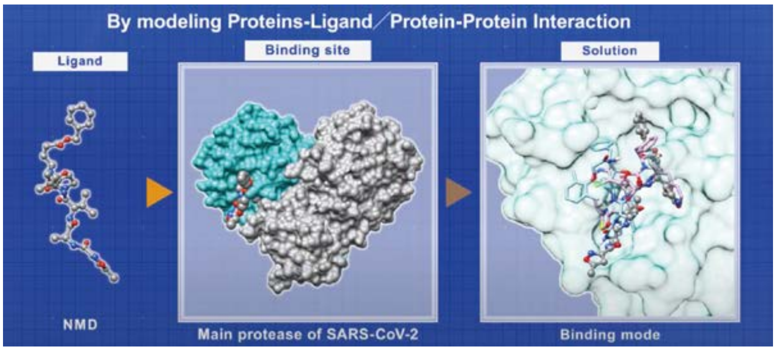
Collaborations:
Medical Science, Engineering, Art

Prof. UMEMURA Masayuki
Assoc. Prof YAJIMA Hidenobu

Collaborations:
Biomedical optics, Mathematics

Computational Biomolecular Medical Science

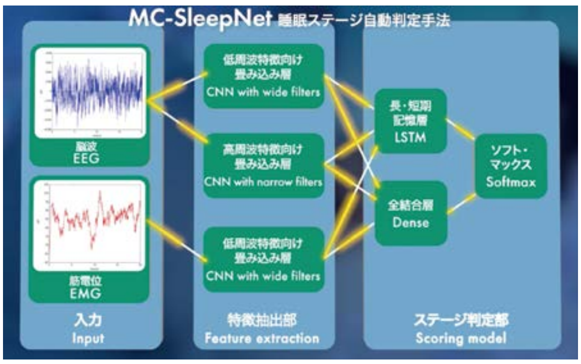
In conventional drug development, one has aimed to develop small molecular drugs with low side effects that have both high selectivity and the binding ability for a specific target. In order to support them, in silico technology has been advanced in recent years, with the expectation that it will be possible to reduce the cost to 100 billion yen per drug for ten years. However, despite many attempts, few cases have been put to practical use because of the limitation of the small-sized drugs. One of the new drug targets is the middle-sized drugs such as cyclic polypeptides and DNA/RNA aptamers. In this group, we conduct researches on reaction pathway analysis using first-principles calculation and analysis of substrate-protein binding process using molecular dynamics calculation for drug discovery targeting on middle-sized molecules. In particular, the computational methodologies for the membrane permeability, p*K*a, and redox potential prediction are developed.



Overview of docking simulations for the main protease of SARS-CoV-2

Big Sleep Data Analytics and Automatic Sleep Diagnosis

Sleep plays an important role in people's daily lives. Sleep disorders could cause various illnesses. There are a lot of scientific questions that need to be answered about sleep. Quantitative and accurate measurements and analysis of sleep are fundamental issues in sleep research. Sleep polysomnography (PSG) is a commonly used sleep measurement method. PSG attaches many sensors to the subject and continuously measures and records various biological data such as brain waves, respiratory movements, and eye movements throughout the night. In PSG, the burden and cost of the subject are large, and measurement over a long period is impossible. Moreover, analysis of the acquired data depends on manual inspection by human experts, and it is impossible to analyze large-scale data. In response to the increasing social interest in sleep in recent years, some methods have been developed to easily measure sleep status using a smartphone or the like. However, at present, there is still no means to conveniently measure sleep as accurately as human experts. This research aims to realize automatic sleep analysis and diagnosis by integrating sleep big data analysis, machine learning and new sensing technology, and to pioneer a new computational medical science field.

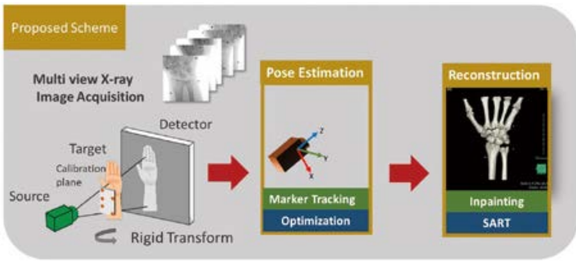


Scheme for an automatic sleep stage determination method using deep learning

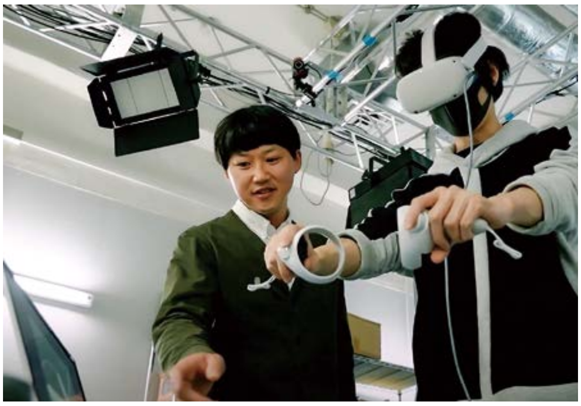
Demonstration of sleep data acquisition using a home sleep measurement device

3D Surgical Vision

Although the safety of surgery has improved urgently due to advances in medical technology, the upper limit of patient survival is always surgical cancer, the number one cause of death in Japan, and the 1st treatment option is surgery. On the other hand, doctors vary in skills because of increased knowledge and skills that need to be acquired and lost due to medical progress (regional disparities in 5-year survival rates for cancer resection are more than 10%). Since education takes about 15 years, there is a shortage of surgeons and there are concerns that the problem will become even more serious. Until now, research and development on virtual surgery using IT technology has been carried out, however there are not many implementation examples of surgical navigation systems based on 3D visual information. Our research aims to realize “3D surgical navigation system” that integrates “3DCG simulation” used by doctors for preoperative examination and “on-site navigation” based on 3D Computer Vision technology. Supporting surgeons with an intuitive understanding of proper instructional procedures and advanced medical techniques can improve the level of surgery. In addition, by utilizing technologies such as 3DCG modeling and Augmented Reality (AR), we realize a remote diagnosis and VR treatment system, which aim to correct regional disparities in medical technology. Furthermore, by applying our technologies to laparoscopic surgery, a surgical procedure with less physical burden on the patient can be possible.



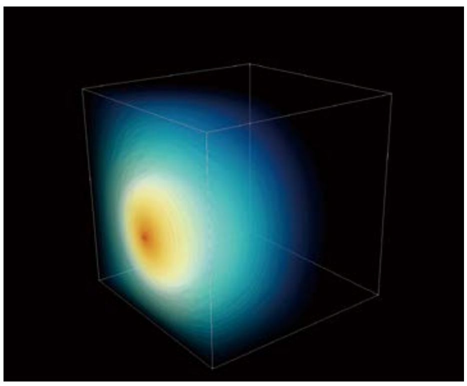
Scheme for 3D reconstruction from multi-view X-ray images



Demonstration of surgical navigation using computer media technology

Computational Optical Bioimaging

Recent years, the technology of optical imaging is extraordinarily developing, and thereby molecular processes in live cells and tissues can be pursued. At present, the imaging methods such as X-ray CT or MRI are widely applied, and mainly detect the alteration of morphology at a level of organs and tissues. However, these methods are subject to the risk of significant exposure and require a large-scale apparatus or a specialized measurement room. On the other hand, the optical imaging can dynamically visualize multi-level function and morphological alteration in molecules and organs, and possesses a lot of advantages such as no exposure, non-invasion, bed side inspection, low cost, low restraint, and high time –resolution. Thus, it allows us to make automatic and remote diagnosis, monitoring, and screening and is applicable to new-born babies and infants without side effects like CT or MRI. Since biological tissues are strong scattering media, a sophisticated technology of computational science is required to extract the local information from scattered light. The study for the practical realization at clinical settings has not been thitherto sufficient. In this project, we aim at developing a safe technology of CT with near-infrared imaging under the cooperation among the construction of light propagation models based on radiative transfer equation (RTE), the inverse-problem analysis based on mathematical methodology, and the experiments of medical optics for biological tissues.



Radiative transfer simulation assuming pulsed light irradiation of a living body

Project Office for Exascale Computational Sciences

Develop Computational Sciences with the Full Performance of the Machine

Head: YABANA Kazuhiro, Professor, Ph.D., Deputy Director of CCS

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, and large-scale computers with Field Programmable Gate Arrays (FPGAs) in addition to GPUs, 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 was a massively-parallel supercomputer equipped with GPU accelerators, and in Oakforest-PACS in Joint Center for Advanced High Performance Computing (JCAHPC), the fastest supercomputer in Japan equipped with processors of Many Integrated Core architecture, under close cooperation with the Project Office for Exascale Computing System Development, which is the organization promoting the development of new computers. Currently, developments and adjustments of computer codes that run efficiently at Cygnus, equipped with both GPU and FPGA, and at Fugaku, the flagship machine in Japan have been a central issue at the Office. Since it is believed that the massively parallel supercomputers of the future will be mainly equipped with GPU and other computation accelerators, we are also focusing on efforts to the development of applications that efficiently use GPUs through the use of a newly introduced Pegasus.

Activities of each field in the Project Office for Exascale Computational Sciences

	Scientific Target	Theory/Model, Numerical methods
Particle Physics	- High precision calculations of the standard model of particle physics - Physics beyond the standard model - Physics at finite temperature and density - Phase transition of quantum many body system	- Iterative solver for linear equations with large sparse matrices - Dense matrix-matrix multiplication - Extraction of eigenvalues and singular values
Astrophysics	- Dynamics of accretion disks around black holes - Elucidation of dark matter and neutrinos by the large-scale structure of the universe	- General relativistic radiation magnetohydrodynamic simulation - Vlasov and Boltzmann simulations in a six-dimensional phase space
Nuclear Physics	- Exploring nuclear structures with describing various many-body correlations	- Projection and configuration mixing calculations - Eigenvalue problem of large sparse matrices
Material Science	- Light-matter interaction, ultrafast electronic dynamics - Electrochemistry reaction at surface/interfaces	- (Time-dependent) density functional theory - Real-time, real-space finite difference method - Effective screening medium method
Life Science	- Analyses of enzymatic reaction in living body - Large-scale phylogenetic analyses on eucaryote	- Fragmented molecular orbital method - Real space Car-Parrinello molecular dynamics method
Global Environmental Science	- Exploring arctic oscillation - Exploring urban climate and local wind	- Efficient solution of Poisson equation - Similarity retrieval of high-dimensional data
Computational Informatics	- Information management and knowledge discovery in massive scientific data	- Efficient processing of large graphs - Cluster analysis over large-scale scientific data
Mathematical modeling and algorithms	- Large-scale parallel computational methods in computational sciences	- Parallel algorithms for a generalized eigenvalue problem of dense matrices - Development of eigenvalue calculation software for sparse matrices – z-Pares, CISS

Introduction of Research Projects Offices

Project Office for Exascale Computing System Research and Development

Developing advanced fundamental technologies for ExaFLOPS and beyond

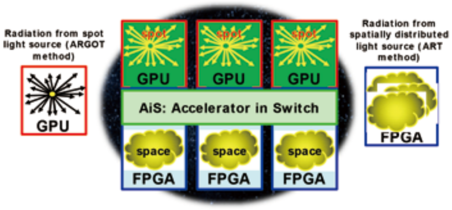
Head: BOKU Taisuke, Professor, Ph.D., Director of CCS

A parallel supercomputer system's peak computing performance is expressed as follows: node (processor) performance × number of nodes. Thus far, performance improvement has been pursued by increasing the number of nodes, but owing to problems such as power consumption and a high failure rate, simply increasing the number of nodes as a means of performance improvement is approaching its limit. The world's highest performing supercomputers are reaching the exascale, but to reach this level and beyond, it is necessary to establish fault-tolerant technology for hundreds of thousands to millions of nodes and to enhance the computing performance of individual nodes to the 100TFLOPS level. To achieve the latter, a computation acceleration mechanism is promising, which would enable strong scaling of the simulation time per step.

In the Next Generation Computing Systems Laboratory, we are conducting research on fundamental technologies for the next generation of HPC systems based on the concept of Cooperative Heterogeneous Acceleration with Reconfigurable Multidevices (CHARM). FPGAs play a central role in this research and are applied to the integration of computation and communication against the backdrop of dramatic improvements in the computation and communication performance in these devices. Since 2017, we have been developing and expanding PPX (Pre-PACS-X), a mini-cluster for demonstration experiments based on the idea of using FPGAs as complementary tools to achieve the ideal acceleration of computation for applications where the conventional combination of CPU and GPU is insufficient. Cygnus—the 10th generation supercomputer of the PACS series—was developed as a practical application system and began operating in the 2019 academic year. The following is an introduction to the main technologies being developed here.

Developing applications that jointly use FPGAs and the GPU

In collaboration with the Division of High-Performance Computing Systems and Division of Astrophysics, we developed the ARGOT code, which includes the radiation transport problem in the simulation of early-universe object formation, so that it would run fast on a tightly coupled GPU and FGPA platform. The entire ARGOT code can now be run on a 1-node GPU+FPGA co-computation, which is up to 17 times faster than a GPU-only computation. Additionally, we developed a DMA engine that enables high-speed communication between the GPU and FPGAs without using the CPU. Furthermore, through joint research with the Division of Global Environmental Science and the Division of Quantum Condensed Matter Physics, we are working on GPU/FPGA acceleration of application codes being independently developed at JCAHPC.



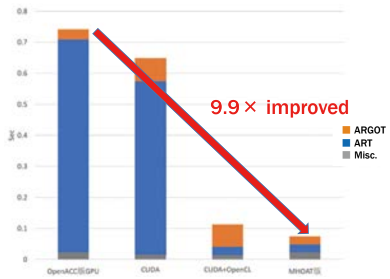
GPU-FPGA cooperative execution by CHARM for ARGOT code

OpenCL interface for FPGA-to-FPGA high-speed optical networks

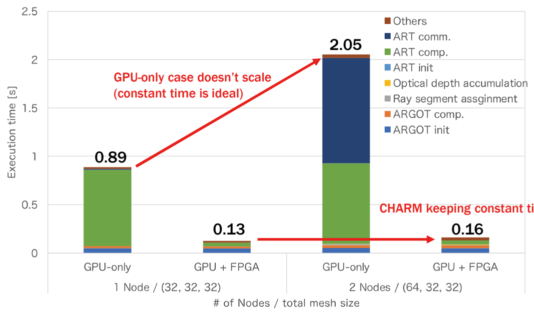
We developed CIRCUS (Communication Integrated Reconfigurable CompUting System) as a communication framework that facilitates the use of FPGA-to-FPGA networks with physical performance levels of 100 Gbps. It is easy to use at the user level and achieved high-performance communication (90 Gbps—90% of the theoretical peak performance of 100 Gbps) on the Cygnus supercomputer. Additionally, we applied this framework to the FPGA offload portion of the ARGOT code and confirmed that parallel FPGA processing can be performed smoothly.

Unified GPU–FPGA programming environment

In collaboration with the RIKEN Center for Computational Science and Oak Ridge National Laboratory in the United States, we are developing an OpenACC translator called MHOAT, which enables FPGA and GPU joint programming using only OpenACC. We aim to apply the concept of CHARM to a wide range of applications by making it available in a simple programming environment.



GPU (OpenACC or CUDA) vs CHARM (CUDA+OpenCL or MHOAT)
⇨ MHOAT is the best with 10× speed of OpenACC GPU



Weak scaling execution time with 2 nodes on CHARM (CUDA+OpenCL) programming

Project Office for HPCI

Establishing a system for promoting computational science at the Joint Institute for Computational Fundamental Science (JICFuS)

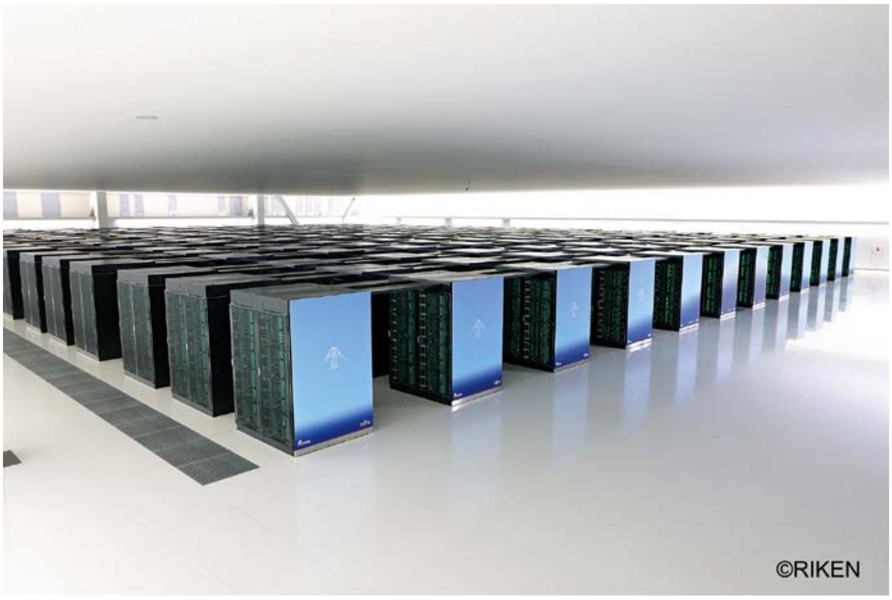
Head: KURAMASHI Yoshinobu, Professor, Ph.D.

History of the High Performance Computing Infrastructure (HPCI) project and the Joint Institute for Computational Fundamental Science (JICFuS)

The innovative HPCI project was planned in the early 2010s with the supercomputer K computer at its core, aiming to build and promote the use of HPCI to establish an innovative computing environment that satisfies diverse user needs. Among the initial goals of the project were to create breakthrough results using HPCI and to establish a system for promoting computational science in major fields. In the HPCI Strategic Program, which was promoted for five years (2011–2015), five fields were selected as strategic areas requiring the computing resources of the K computer and are expected to make major breakthroughs in society and academia. The fifth area—"Field 5: The origin of matter and the Universe"—is a field of fundamental physics focusing on elementary particles, atomic nuclei, and astrophysics. The Joint Institute for Computational Fundamental Science (JICFuS)—a joint research organization led by the University of Tsukuba's Center for Computational Science, the High Energy Accelerator Research Organization (KEK), and the National Astronomical Observatory of Japan (NAOJ)—was the strategic organization driving the research and development of Field 5. Although the K computer was shut down in August 2019, the JICFuS continues to play a role in advancing computational science in the field of fundamental physics.

New supercomputer "Fugaku" and future utilization of HPCI

Since the 2014 academic year, the research and development project of a new supercomputer that will succeed the K computer (officially named "Fugaku" in May 2019) has been ongoing, and nine priority issues were highlighted for application development and research development related to issues in science and society that should be prioritized following the K computer. Among them, "Priority Issue 9: Elucidation of the fundamental laws and evolution of the universe" is an extension of the research and development in HPCI Strategic Program Field 5, and the University of Tsukuba's Center for Computational Science and seven sub-institutes were designated as leading institutions. The Center for Computational Science at the University of Tsukuba also participated in "Priority Issue 7: Creation of new functional devices and high-performance materials to support next-generation industries (CDMSI)" as a designated institution. In addition to the priority issues , four exploratory research projects were selected as challenging new research projects to be undertaken in the post-K computer era. Among them, the CCS has participated in "Exploratory Challenge 1: Frontiers of basic science: Challenging the limits" and "Exploratory Challenge 3: Elucidation of the birth of exoplanets (second earth) and the environmental variations of planets in the solar system" as a designated institution. After the aforementioned preparation period, the Fugaku supercomputer became available for public use in March 2021, and a result creation acceleration program aimed at its early strategic use is being promoted along with general-use research topics. The Project Office will continue to promote application development and research and development for the utilization of Fugaku and HPCI and aim to make achievements in science, as well as advance the development of computational science in the field of fundamental physics by holding study groups and research meetings that break the boundaries in the fields of elementary particles, atomic nuclei, and astrophysics.



Fugaku

Introduction of Research Projects Offices

Promotion Office for Computational Sciences

Promote Social Contributions and Human Resource Development in Computational Sciences

Head: TAKAHASHI Daisuke, Professor, Ph.D.

The Promotion Office for Computational Sciences promotes human resource development programs related to computational science in collaboration with graduate schools, educational activities such as summer-school programs, and making social contributions to the community, e.g., through the dissemination of information related to advanced research at the CCS.

	Course Name
Specialized Subjects	Principles of Software Engineering
	Topics in Computational Science I
	Data Engineering I
	Programming Environment
	Basic Computational Biology
	Advanced Course in High Performance Computing
	Special Lecture on Numerical Simulation
	Advanced Course in Computational Algorithms
	Adaptive Media Processing
	Frontier Informatics A
	Frontier Informatics B
Basic Subjects	Experiment Design in Computer Sciences
Interdisciplinary Foundation Courses	Computational Science Literacy
	High Performance Parallel Computing Technology for Computational Sciences

Personnel Development

Graduate School Dual Degree Program

he graduate school houses a Master's program and a doctoral program. Doctoral candidates usually study a specialized field through both programs. However, in computational science, it is necessary to conduct research in scientific fields such as physics, environmental sciences, and biology while making advanced use of computers, and complex expertise related to both science and computers is necessary. To satisfy this need, we are promoting the Dual Degree Program at the graduate school, where students can simultaneously pursue research in a scientific field in the doctoral program and computer research in the Master's program, allowing them to obtain both a doctoral degree in science and a Master's degree in computer science.

Computer Science English Program

To satisfy the needs of increasing numbers of international students, we established the Informational Science and Engineering English Program as part of the Master's program in Information Science and Engineering as a program that students can complete in English only. Fourteen courses and research guidance conducted in English will enable students to obtain a Master's degree.

Social Contribution

Cooperation with other institutions

Within Japan, we have close collaborative relationships with RIKEN and other research institutions in Tsukuba. We have also established international research ties such as through the International Lattice Data Grid (ILDG) —an international data sharing project in particle physics—and conducted exchanges with the University of Edinburgh in the UK and the Lawrence Berkeley National Laboratory in the US. We will continue to strengthen and develop the domestic and international research collaborations that we have cultivated and use them as a bridge to facilitate exchange between researchers and students to conduct joint research.

Mt. Tsukuba Project

Meteorological observations are conducted at the summit of Mt. Tsukuba (877 m), and meteorological data such as the air temperature and humidity are continuously recorded and made available to the public for use in research and educational activities and to contribute to society.

Information transmission

In cooperation with the Bureau of Public Relations and Strategy, we welcome domestic high-school students and overseas university students to visit our school, and we open our school to the public to improve exchanges with local people in Tsukuba City and the Kanto region. Additionally, staff are actively involved in onsite classes and support groups as individual members of faculty.

Project Office for AI & Big Data

Promoting big data and AI research exploiting supercomputers

Head: AMAGASA Toshiyuki, Professor, Ph.D.

Big data analysis is used to find information buried in data by analyzing data that are so vast and complex that they are difficult for ordinary computers to handle, and AI technology enables highly accurate discrimination and prediction that were previously unachievable by applying machine-learning methods such as deep learning to large amounts of training data. The Project Office for AI & Big Data is engaged in the application of big data and AI technology in various fields of computational science, the promotion of big data and AI research using supercomputers, and collaboration with C-AIR at the University of Tsukuba and other institutions.

Application of big data and AI technology in various fields of computational science

There are active attempts at uncovering new knowledge by applying big data analysis or machine learning to large amounts of data being accumulated in various fields of science. One of the most well-known examples of this is in bioinformatics. The Center for Computational Science is driving the application of big data and AI technology in various fields of computational science through collaboration with other departments in related fields.

Advancing big data and AI research using supercomputers

Big data analysis and AI require enormous computational resources (computing power and memory). Thus, supercomputers are considered to be among the most suitable environments for performing big data analysis and AI, and major supercomputers are increasingly being used for such applications. The Project Office for AI & Big Data promotes big data analysis and AI research using supercomputers operated by the Center for Computational Science.

Collaborating with C-AIR at the University of Tsukuba and other institutions

In addition to the aforementioned activities related to promoting big data and AI, we collaborate with the Center for Artificial Intelligence Research (C-AIR) at the University of Tsukuba, along with other institutions.

A meeting of project office for AI & big data

Project Office for High Performance Computing System Development and Operation

Developing and operating a supercomputer through co-design

Head: TATEBE Osamu, Professor, Ph.D.

The High-Performance Computing System Development and Operation Office designs and develops supercomputers through a co-designing process with applications from the Divisions of Particle Physics, Astrophysics, Nuclear Physics, Quantum Condensed Matter Physics, Life Sciences, Global Environmental Science, and Computational Informatics before actually operating them at the CCS. In designing a supercomputer, it is important to improve not only the computing performance but also the application performance, which requires improving computing, memory, network, and storage performance in a well-balanced manner. In addition, the use of computing acceleration mechanisms is becoming essential to improve the computing and memory performance, yet the application side must take action to fully utilize the performance. A co-design process that considers the development of the computer side and the application side simultaneously will improve the application performance and lead to developments in computational science, data-driven science, and AI-driven science.

Cygnus

In December 2022, we introduced Pegasus, a big memory supercomputer with GPU and persistent memory. Not only has the computing performance been improved by using state-of-the-art CPUs and GPUs, but DDR5 memory has been installed to greatly increase memory bandwidth, which is essential for improving application performance. It is also equipped with persistent memory to expand memory capacity and improve storage performance, which is especially important for data-driven and AI-driven science. User authentication incorporates two-factor authentication for enhanced security, and access is available via Jupyterhub and Nextcloud for improved convenience. The system will be operated on a trial basis until March 2023, with full-scale operations beginning in April 2023.

In addition, we have been operating a GPU/FPGA system Cygnus since April 2019. Cygnus is a mixed GPU and FPGA architecture developed in the Next Generation Computational Systems Development Laboratory, where FPGAs are used not only to supplement GPU acceleration but also for high-speed networking between FPGAs. This has enabled acceleration of computation for ARGOT applications being developed in the Division of Astrophysics.

Pegasus

Project Office for Society-Academia collaboration in computational sciences

Promote society-academia collaboration of computational technologies and simulation programs

Head: OTANI Minoru, Professor, Ph.D.

The University of Tsukuba's Fourth Mid-term Goals and Mid-term Plans aim to foster joint research between academia and society that addresses real-world needs, and to generate innovative solutions that drive social change. To this end, we have set up the Office for Society-Academia Collaboration in Computational Sciences in FY2022. This new office will enhance industry-academia partnerships within the Center and facilitate the practical use of computational technologies and simulation programs developed within the Center.

Society-Academia collaboration in computational sciences

Our aim is to use computational sciences and technologies to tackle social challenges and drive industrial development. We will apply these tools to various areas, such as resolving environmental problems, devising medical diagnostic methods, improving social systems and disaster prevention measures, and addressing other pressing societal issues. In the manufacturing industry, we will actively employ computational science and technology to optimize production processes and develop new materials, and foster collaborations between academia and industry to advance these goals.

In collaboration with Bureau of Public Relationships and Strategy

Working with the Bureau of Public Relationships and Strategy in the Center for Computational Science, we will promote awareness of the computational technologies and simulation programs we are developing among diverse audiences. We will use our website and social media channels to share a range of information, including news about seminars focused on social implementation, updates on research outcomes, and details about collaborative researches with industry. Our aim is to maximize transparency and foster further collaborations.

Activities

- Work closely with headquarters for international industry-university collaboration to establish large-scale joint research projects.
- Collaborate with the Bureau of Public Relationships and Strategy to publicize the industry-academia collaboration activities of faculty members affiliated with the Center through the Center's website and other channels.
- Organize study groups and other initiatives to facilitate alignment between the Center's research themes and the needs of the industry.
- Develop and deliver tutorials that leverage the supercomputing capabilities available at the Center.
- Explore opportunities for actively utilizing data generated by computational science in collaboration with companies.

Liaison Office for Multidisciplinary Computational Sciences

Toward Formation of the International Hub of Computational Sciences

Head: INAGAKI Yuji, Professor, Ph.D.

At the Center for Computational Sciences, we conduct researches based on the central concept of “multidisciplinary computational sciences” that are based on collaboration and cooperation among various scientific fields including computer sciences. The Liaison Office of Multidisciplinary Computational Sciences is part of the CCS’s efforts to create an international hub for computational sciences.

Multidisciplinary collaboration

Collaboration between different fields is necessary to promote multidisciplinary computational sciences. In 2011, a research group consisting of RIKEN, the University of Tsukuba, the University of Tokyo, and Fujitsu was awarded the Gordon Bell Prize for High Performance Computing—a renowned prize in the field of HPC—for its work on the first-principles calculations of the electronic structure of 100,000-atom silicon nanowires using the K computer. This is just one of the achievements of the longstanding multidisciplinary collaboration that occurs at the CCS—collaboration that we will continue to promote.

International collaboration

As part of our international collaborative projects, the University of Tsukuba has concluded collaborative agreements with the University of Edinburgh (UK) and the Lawrence Berkeley National Laboratory (US). Every year, the University of Tsukuba holds a symposium with the University of Edinburgh’s Parallel Computing Centre (EPCC)—a workshop with the Lawrence Berkeley National Laboratory in the United States—and holds the HPC winter school and mini-workshops with the Korea Institute for Science and Technology Information (KISTI) to further the exchange of research in computational sciences.

Interdisciplinary Development Program

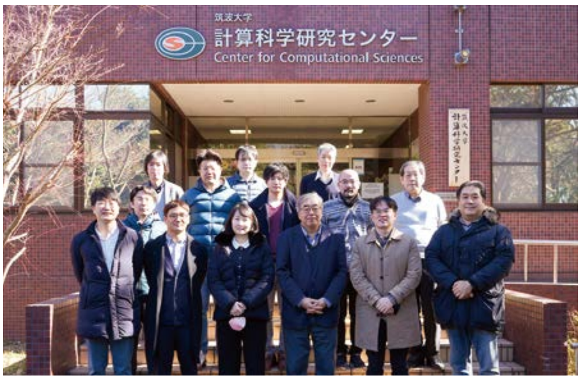
The Interdisciplinary Development Program promotes research that focuses on multidisciplinary collaboration. These include projects involving collaboration between the fields of computational physics (science) and numerical analysis (engineering) to generate a highly efficient computational code and conduct large-scale simulations using this code, as well as projects in which different fields that share methods in the field of computational science collaborate organically to develop new research and make significant progress. This program is conducted in collaboration with the Multidisciplinary Cooperative Research Program (MCRP) of the CCS.

Organization for Collaborative Research on Computational Astrobiology

In the past decade, astrobiology has attracted considerable attention owing to observations of exoplanets and interstellar molecules. In collaboration with the fields of computer science, space science, life sciences, and planetary science, the Organization aims to investigate the key processes involved in the origin of life in the universe using the first-principles calculations and to establish astrobiology as a computational science. The main research topics are interstellar molecular biology, planetary life science, and star/planet formation. At present, the University of Tsukuba is playing a central role in this project, and 51 researchers from 20 research institutes are participating.

Collaboration workshop between CCS and the university of Edinburgh, 2022.

Collaboration workshop between CCS and Lawrence Berkeley National Laboratory, 2019.



Japan-Korea HPC Winter School and CCS-KISTI workshop, 2022.

Bureau of Public Relations and Strategy

Supporting the development of the Center for Computational Sciences and the advancement of computational science

Head: KITAHARA Itaru, Professor, Ph.D.

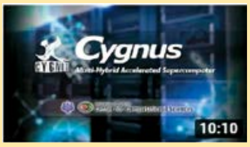
The Bureau of Public Relations and Strategy was established in 2016 to support the promotion of strategic projects at the CCS in addition to public-relations activities for the development of the CCS and the promotion of computational science. The office also collaborates with the Promotion Office for Computational Sciences and the Liaison Office for Multidisciplinary Computational Sciences to support the CCS's research activities and conduct public-relations activities.

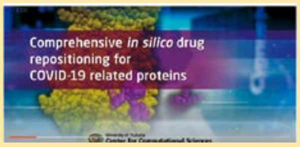
Press release

The CCS's research activities and achievements are shared with the media and public and have been featured in many national newspapers, TV programs, and online news publications.

Contents

A large amount of information is communicated via our website. (https://www.ccs.tsukuba.ac.jp/)
Brochures for the public and researcher interviews are also available for viewing on the website.
Videos introducing our supercomputers and researches are posted on our YouTube channel.



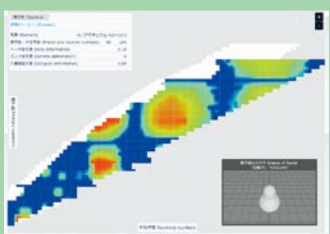


CCS Tour / Open day

The CCS's activities and supercomputers are introduced at organized visits by junior and senior high-school students, university information sessions, public open houses in April, and other such events. We welcome more than 2,000 visitors annually.

Projects, symposiums, and conferencing support

We are supporting a weather-observation project at the summit of Mt. Tsukuba that is being conducted jointly with the Tsukubasan Shrine. We are also engaged in public-relations activities for the JCAHPC and Oakforest-PACS—a supercomputer established in cooperation with the University of Tokyo's Information Technology Center. We also support the creation of tools for public disclosure of research results and manage booths at major supercomputing conferences (SC and ISC) held in the US and Germany every year.



Interactive Nuclear Chart & Periodic Table "InPACS"

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Access

Airport Bus

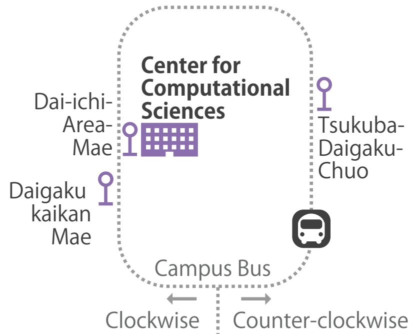
Narita Airport: About 60 minutes from Narita Airport by bus bound for "Tsukuba Center".
Take a bus at the bus stop at the Terminal 1, the Terminal 2, or the Terminal 3.
Haneda Airport: About 120 minutes from Haneda Airport by bus bound for "Tsukuba Center".
Take a bus at the bus stop No.6 in the International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

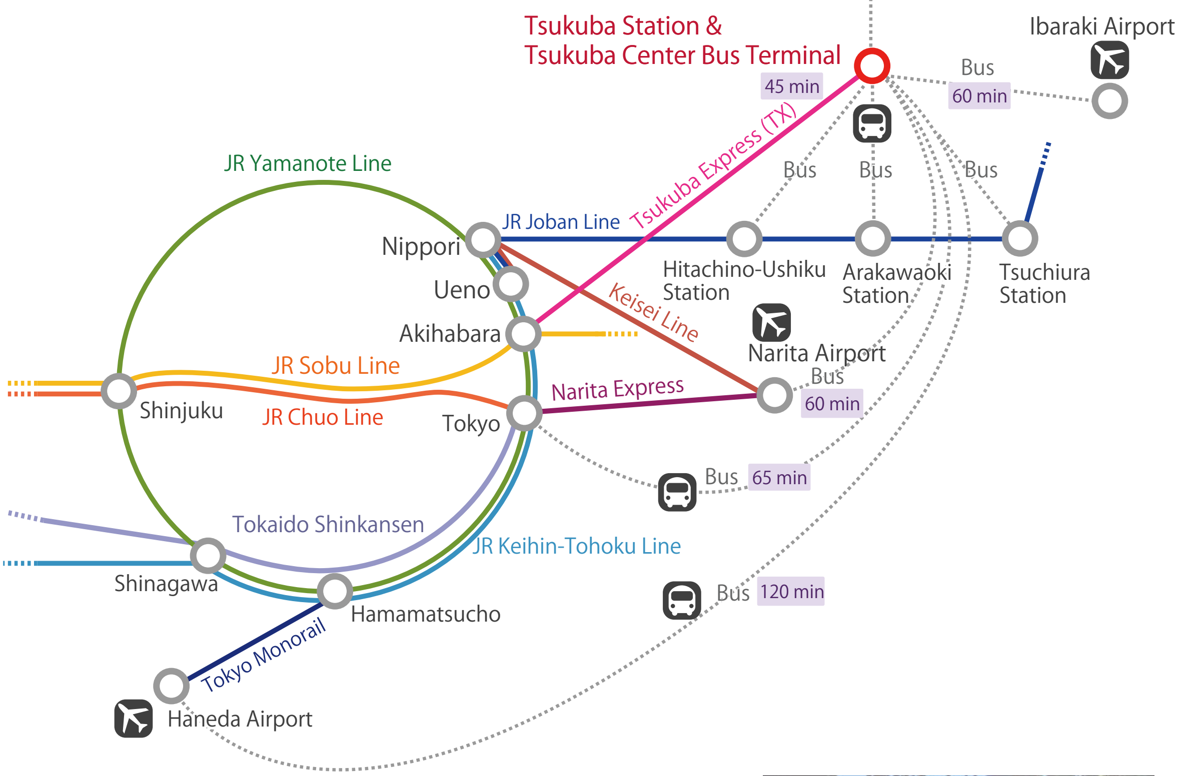
Tsukuba Express (TX)

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

From Tsukuba Center (Tskuba Station)

Please take a bus bound for "University Loop-line On-campus Bus [Tsukuba Daigaku Junkan Bus] (clockwise)" or "Tsukuba Daigaku Chuo".
The nearest bus stop from CCS is "Dai-ichi Area Mae".
It takes about 10 minutes by bus.





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