# Center for Computational Sciences, University of Tsukuba


筑波大学
University of Tsukuba

## Overview

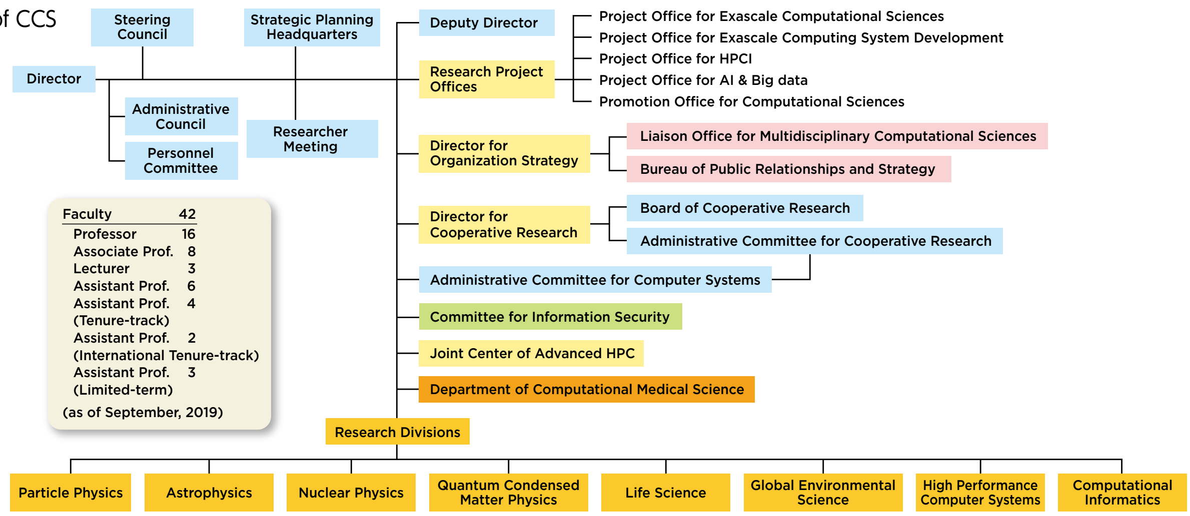
The mission of the Center for Computational Sciences (CCS) is the promotion of "Multidisciplinary Computational Science" through enhanced cooperation between, and the fusion of, computational and computer sciences. To that end, the CCS works toward the development of high-performance computing systems and networks, conducts sophisticated simulations in a variety of scientific research fields, and endeavors to expand the frontiers toward innovative information technology. The scientific research areas of our Center encompass particle physics, astrophysics, nuclear physics, nano-science, life science, environmental science, and information science. On the other hand, the research on computer systems covers high performance computing technology from the architecture to the algorithm and the informatics including big data analysis on large scale storage and database system, and even media science.

CCS had been originally formed as the Center for Computational Physics (CCP) in 1992, then reorganized to current form with the name of CCS on April 2004. In total, we have more than 25 years of history as an ideal research organization to combine computational and computer sciences. The history started with the development of the massively parallel supercomputer CP-PACS, which was ranked as the world fastest supercomputer on November 1996 in TOP500 List. After that, the CCS has been developing ten generations of supercomputer based on the concept of "codesigning" among both application and system scientists together. Currently, the CCS is endorsed as a leading center of advanced research for the Support and Development of Strategic Initiatives in University of Tsukuba. In 2013, our Center and Information Technology Center of the University of Tokyo established a joint organization named the Joint Center for Advanced HPC (JCAHPC) as the first interuniversity supercomputer center in Japan to install and operate Oakforest-PACS system which was ranked as the fastest supercomputer in Japan in TOP500 List of November 2016.

The CCS possesses 8 research divisions and 38 faculty members, and organizes 5 research project offices and a bureau of public relations to strategically promote and spread "Multidisciplinary Computational Sciences". Also, a priority issue and exploratory challenges on Post-K computer are propelled under FLAGSHIP 2020 Project in Japan. Furthermore, a wide variety of multidisciplinary cooperation has been accelerated in Joint Institute for Computational Fundamental Science (JICFuS) and Organization for Collaborative Research on Computational Astrobiology (CAB).

The CCS is playing a significant role as a "national core-center" to provide supercomputer resources as a member of a governmental program High Performance Computing Infrastructure (HPCI) under the Ministry of Education, Culture, Sports, Science and Technology (MEXT) of Japan. The Center also operates its original supercomputer resource sharing program for nationwide researchers, Multidisciplinary Cooperative Research Program (MCRP) to promote scientific projects and encourage the collaboration of interdisciplinary research among computational science and computer science.

Organization of CCS




## Message from the Director

### Taisuke Boku

Director of Center for Computational Sciences,
University of Tsukuba

"Computational Science" is the third kind of approach of science discovery beside traditional "Theory" and "Observation", driven by computational simulation on physical phenomena. The Center for Computational Sciences (CCS) is established to proceed this research methodology by the collaboration between application scientists and computer scientists. In 1992, the Center was organized as the former name of the Center for Computational Physics, then after 12 years of activity, it was reorganized as current form.

The CCS has been developing our original high performance supercomputers based on the concept of "codesigning" where the application scientists and computer scientists collaborate to realize an ideal system to combine their needs and seeds. As a result of our activity, our originally designed supercomputer, CP-PACS was ranked as top of the world in TOP500 List released on November 1996. Moreover, the researchers of CCS coauthored the ACM Gordon Bell Prize on 2011 and 2012, which is the most honorable award for high performance computing and application run in the world.

For the nationwide promotion of computational science, we are providing a half of our supercomputer resources to nationwide computational scientists with free of charge, under the name of "Multidisciplinary Cooperative Research Program (MCRP)".

We also proceed the international collaboration with a number of top-level institutes over the world for high quality of computational science research. Additionally, we are joining to the development of system and application of "Fugaku" Post-K Supercomputer Project (FLAGSHIP2020) under the governmental program.

We will proceed all our research and promotion activities based on our successful history toward the top-level computational and computer science researches in the world.

## CCS Vision of "Multidisciplinary Computational Science"

Computational science is explored by large-scale simulations with high performance computing resources as well as the high-bandwidth networks. The pivot for computational science is the collaboration between wide fields of computational scientists and computer scientists having expertise of computer hardware, software, algorism, and application coding. This collaboration allows us to develop computers best 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 (PACSCS, 2006), and a special-purpose parallel system for astrophysics, the Cosmo-simulator FIRST (2007), have been developed. In 2011, another codesign project for the Highly Accelerated Parallel Advanced system for Computational Sciences (HA-PACS) was launched.

The CCS has been striving to carry out collaborative research with computer scientists in a field of fundamental science for more than 25 years. Currently, in addition to fundamental science (particle physics, astrophysics, and nuclear physics), applied fields are spread to materials science, life science, and global environment. As a result, a wide variety of collaborations among different fields have been initiated. This is a significant potentiality of "Multidisciplinary Computational Science".

## Collaborations and Alliances

As for nationwide alliances, the CCS has entered the T2K alliance, which 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 medial science have been initiated. Also, under the alliance with RIKEN Center for Computational Science (R-CCS, former AICS), the technology for high-performance computing has been explored. Besides, since our university is located in Tsukuba Science City, which is home to many government research organizations, we already have firm connections to a number of major research institutions located there. These include the High Energy Accelerator Research Organization (KEK), the Advanced Institute for Science and Technology (AIST), the National Institute for Materials Science (NIMS), the Meteorological Research Institute (MRI), and the National Institute for Environmental Studies (NIES).

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

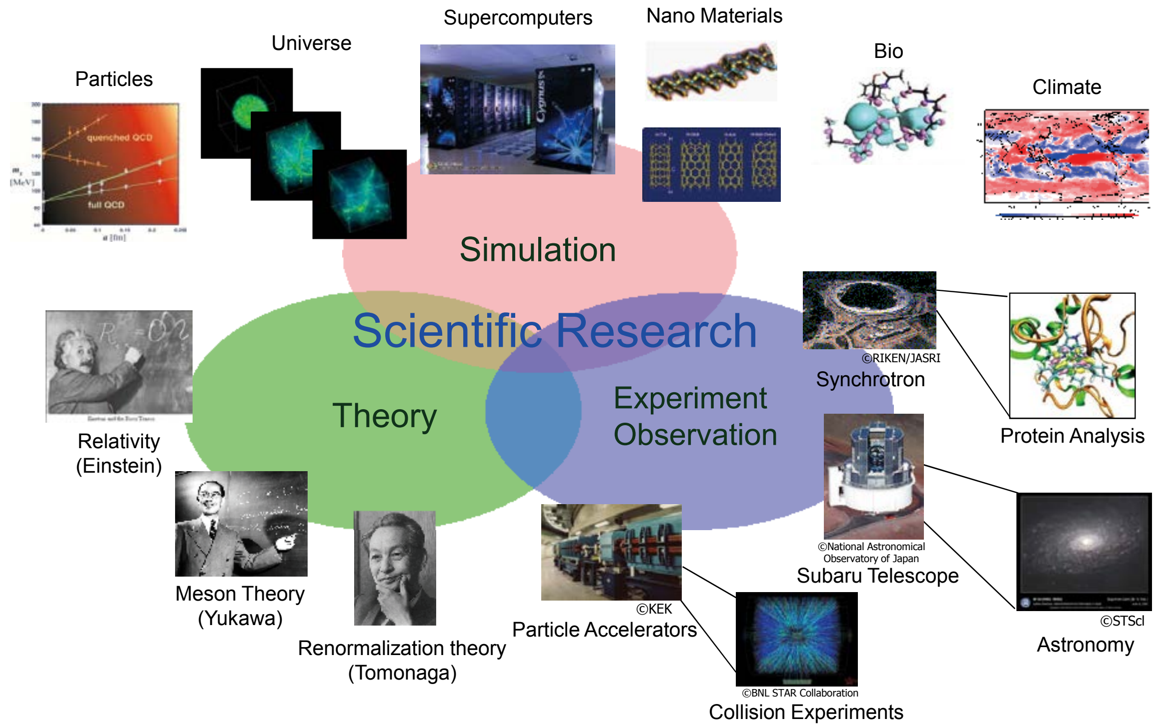
### Chronology of CCS

| | | |
|---|---|---|
| 1992 | April | CP-PACS Project begins (5-year project). Center for Computational Physics (CCP) founded (10-year term). |
| 1993 | August | Computer building 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 Top 500 World Supercomputer List |
| 1997 | April | Research for the Future Program "Development of Next-Generation Massively Parallel Computers" begins (5-year term) |
| 2002 | April | Second 10-year term of the Center for Computational Physics begins |
| 2004 | April | CCP is reorganized, expanded and relaunched as the Center for Computational Sciences (CCS) |
| 2005 | April | Development of Massively Parallel Cluster PACS-CS in the project begins (3-year term) |
| 2007 | March | Second research building 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 |

## Cutting-Edge Research Areas

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

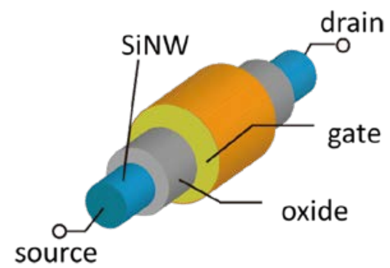
Computational science has shifted the scientific research paradigm to include simulation – along with experiment and theory – as fundamental methods of science. Computer simulation allows us to acquire scientific insights into problems that are too complex or difficult to study analytically using just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




## Awarded Gordon Bell Prize Two Year

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

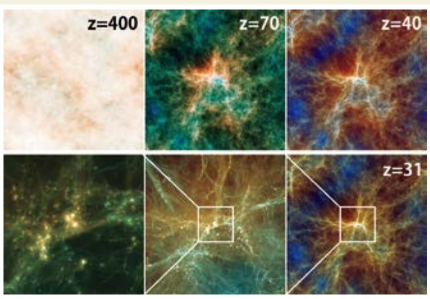
Appraised for the joint research conducted using the K Computer, Center for Computational Sciences (CCS), University of Tsukuba was awarded the Gordon Bell Prize two years in a row.




### 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.

## Cygnus supercomputer system

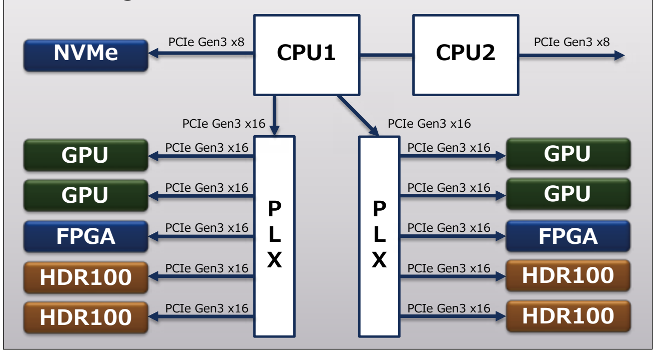
Cygnus supercomputer system demonstrates the 10th generation of PACS series supercomputer developed at the Center for Computational Sciences, University of Tsukuba. It has been operated from April, 2019. It is a large-scale parallel GPU/FPGA cluster system, which consists of 80 compute nodes, each node has GPU and FPGA. The peak performance is 2.4 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 80 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.

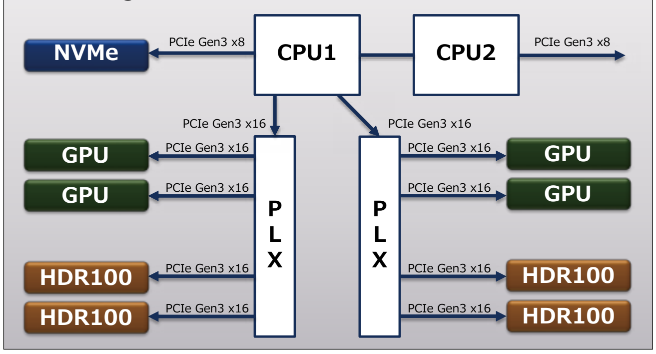

Cygnus

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

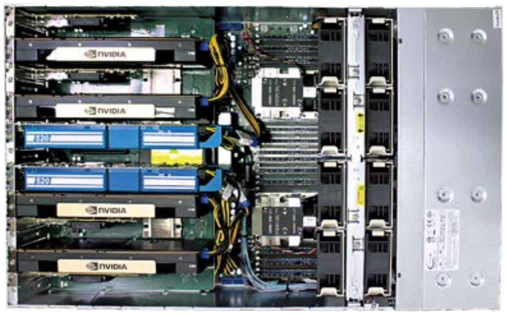



Block diagram of Deneb node




### Specification of Cygnus

| Item | Specification |
|---|---|
| Peak performance | **2.4 PFLOPS Double Precision**<br>(GPU: 2.24 PFLOPS, CPU: 0.16 PFLOPS)<br>FPGA: 0.64 PFLOPS Single Precision |
| Number of nodes | 80 (Albireo nodes 32, Deneb nodes 48) |
| Memory / node | CPU: 192 GB DDR4-2666 (255.9 GB/s)<br>GPU: 32GB × 4 (3.6TB/s) |
| CPU / node | Intel Xeon Gold (Skylake 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<br>(each with 100Gbps interconnect × 4 links/FPGA) |
| SSD / node | 3.2TB Intel SSD DC P4610 |
| Parallel File System | DDN Lustre, RAID6, 2.5 PB |
| Interconnection Network | Mellanox InfiniBand HDR100 × 4 (two cables of HDR200 / node),<br>48 GB/s |
| Programming Language | CPU: C, C++, Fortran, OpenMP<br>GPU: OpenACC, CUDA<br>FPGA: OpenCL, Verilog HDL |
| System Vendor | NEC |



Cygnus node

# Joint Center for Advanced High Performance Computing (JCAHPC)

## Overview

The Center for Computational Sciences (CCS) at 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 is the fastest supercomputer in Japan as on November 2016. It is believed that operating the Center through cooperation and collaboration will promote advanced computational sciences, and contribute to the promotion of academia, science, and technology in Japan.

## Background and History

The advancement of computational sciences through cutting-edge high performance computing (HPC) platforms is vital to maintaining a world-leading position in science and technology in the 21st century. Although the K computer, operated at the RIKEN Center for Computational Science (former AICS), set a new world record in terms of speed since entering shared use in 2012, it was believed that closer cooperation between the ITC group furnishing the HPC platform and the attached advanced institute that operates the supercomputer would be necessary to establish a genuine world-class facility.

As a result, the institutions at 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 large-scale HPC system worthy of becoming the hub of Japan's computational sciences, and to architect an advanced system that exploits many-core technology, which is believed to be the key to future HPC systems. Furthermore, such research and development will proceed in establishing alliances with other organizations for the operating system, programming languages, numerical computation libraries, etc., that comprise the technologies at the heart of the system software. Based on this design and development, the institutions will jointly procure, operate, and administer the supercomputer. As the result of its first primary mission, we successfully procured and installed Oakforest-PACS as the fastest supercomputer in Japan 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.

## Oakforest-PACS

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

In TOP500 list on November 2016, Oakforest-PACS was ranked at No.6 in the world (No.1 in Japan) with 13.55 PFLOPS of Linpack performance out of 25 PFLOPS of the peak performance. The many-core architecture is the most promised general purpose processor technology currently and near future, and wide variety of applications and system software will be developed toward next generation national flagship supercomputer. Actually, it has been contributing to the development of McKernel which is the many-core aware operating system targeting Fugaku (Post-K), the next generation national flagship supercomputer as well as XcalableMP programming language and a number of application programs toward operation on Fugaku. Oakforest-PACS also plays a central role in the supercomputer resource sharing program under HPCI of MEXT.


**Oakforest-PACS**

## Provision of Computing Resources

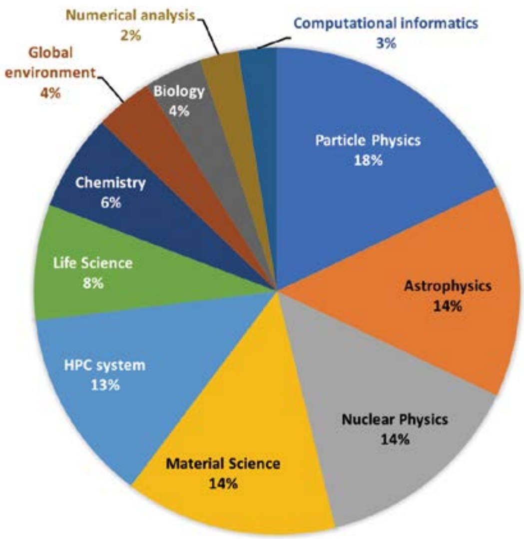
The mission of the Center for Computational Sciences (CCS) focuses on promoting research efforts in computational sciences where scientists of various fields do not simply employ computers, but also work in close collaboration with computer scientists to develop computers that are most suitable for scientific investigations. Since 2002, the CCS has been providing computer resources to researchers in Japan in order to facilitate nationwide progress in computational sciences. Since 2007, these activities have been reinforced by enhanced links with computer sciences through the promotion of the Multidisciplinary Cooperative Research Program (MCRP). Since 2010, the Center has been recognized as a national core-center, Advanced Interdisciplinary Computational Science Collaboration Initiative (AISCI). Under the MCRP, the CCS not only provides the computing resources, but also supports research meetings, short-term employments, and travels of researchers.
Until 2018, the MCRP consisted of the following three programs: (1) Multidisciplinary Pioneering Program (MPP) (2) Priority Subjects Promoting Program (PSPP) (3) Cooperative Research Promoting Program (CRPP). Since 2019, we have divided the MCRP applications into different categories according to magnitude of requested resources.

In order to allow overseas researchers to submit MCRP proposals, the English application forms and the English online submission system have been made available. Because of this, the number of overseas users has significantly increased.
The CCS is calling for proposals of the MCRP in the computational sciences (including particle and nuclear physics, astrophysics, material sciences, chemistry, life sciences, global environmental sciences, and biology), and in the computer sciences (including high performance computing systems, computational informatics, and numerical analysis). Computational facilities that can be used under the MCRP include the PACS-CS (2007-2011), FIRST (2009-2011), T2K-Tsukuba (2008-2013), HA-PACS (2013-2017), COMA(PACS-IX) (2014-2018), Oakforest-PACS operated by JCAHPC (2017-), and Cygnus (2019-).
The numbers of MCRP-approved projects conducted since 2010 are shown in the table. In recent years, more than 60 projects have been approved each year. The percentage of each research field of proposed projects in MCRP-2019 is shown in the graph, and demonstrates that the projects include a variety of fields in natural sciences and engineering.

### Numbers 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 |

### Ratio of each field in the proposed projects for 2019




### Past symposiums organized by the CCS
**(including MCRP report meetings)**

10th symposium on “Discovery, Fusion, Creation of New Knowledge by Multidisciplinary Computational Sciences”
Oct. 15-16, 2018, University of Tsukuba

The 25th Anniversary Memorial Symposium of CCS, Univ. Tsukuba and 9th symposium on “Discovery, Fusion, Creation of New Knowledge by Multidisciplinary Computational Sciences”
Oct. 10-11, 2017, Tsukuba International Congress Center

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

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

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

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

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

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

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

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

# Particle Physics Group

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

## Overview

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

## Research Topics

- Precision measurement of hadron spectra
- Precise determination of fundamental parameters in QCD (strong coupling constant and quark masses)
- Investigation of hadron structures and hadron-hadron interactions based on QCD
- Direct construction of nuclei from quarks
- Investigation of QCD phase structure including high-temperature states (the beginning of universe) and high-density states (inside a neutron star)
- Application of tensor renormalization group to lattice quantum field theories

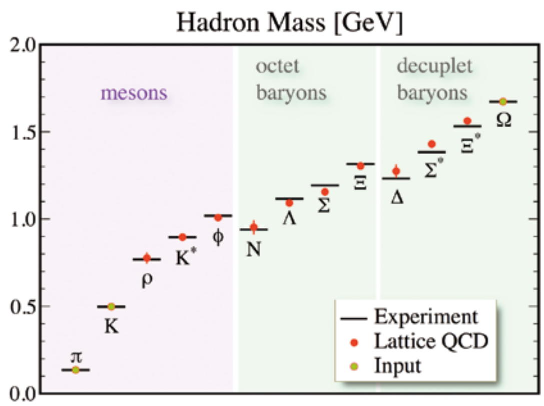



**Fig.1 Hadron masses with lattice QCD in comparison with experimental values**

## Latest Accomplishments

Since the physical point simulations with the physical quark masses have been made possible thanks to algorithmic improvements and increasing computational resources in recent years, lattice QCD simulations are now in the stage of precision measurements at 1% error levels. This is a significant improvement from the previous 10% error stage. In the latest studies, the results for the hadron masses obtained by our lattice QCD simulation had almost reproduced the experimental values (Fig. 1). In addition, extremely large scale simulations allow us a detailed investigation of the internal structure of hadrons. For example, Fig. 2 shows our lattice QCD results for the proton electric form factor (□, ◯) in comparison with the experimental one (red curve). Both results show a good agreement.

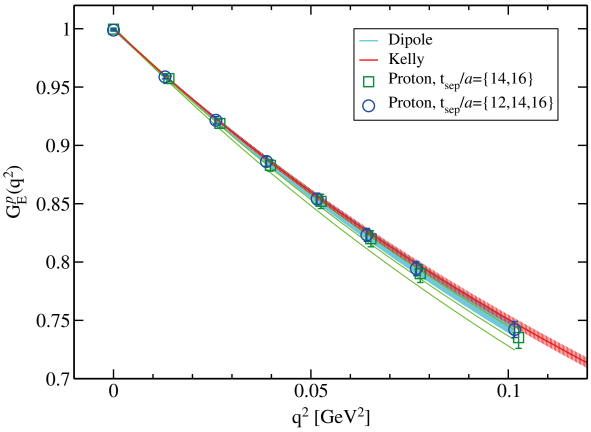



**Fig.2 Proton electric form factor with lattice QCD in comparison with experimental values**

### Chief: Yoshinobu Kuramashi

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

# Astrophysics Group

**Chief**: Masayuki Umemura, Professor, Ph.D. **Members**: Ken Ohsuga, Professor, Ph.D. / Masao Mori, Associate Professor, Ph.D. / Hidenobu Yajima, Associate Professor, Ph.D. / Kohji Yoshikawa, Lecturer, Ph.D. / Alexander Wagner, Assistant Professor, Ph.D. / Kenji Furuya, Assistant Professor, Ph.D. / Naohito Nakasato, Visiting Associate Professor, Ph.D.

## Overview

The universe is believed to have been born 13.8 billion years ago with the Big Bang. The universe continued to expand, gradually decreasing in temperature and density. The first hydrogen atoms appeared 3.8 million years after the big bang, in the epoch of recombination. The temperature of the universe then was 3000 K, no stars or galaxies existed, only small density fluctuations with amplitudes at the 0.01% level.

Recently, many young galaxies existing in the universe already 600 million years since the Big Bang have been discovered. This tells us that the universe has undergone a major transformation between 3.8 and 600 million years after its birth, a transformation generally linked to galaxy formation. The processes, however, by which galaxies are born is still shrouded in mystery.

Since the formation of the first galaxies, the universe continued to expand and evolve, and the galaxies clustered to form the large-scale structure of the cosmos. The formation of galaxies and the evolution of the universe is believed to be underpinned by the ubiquitous existence of dark matter.

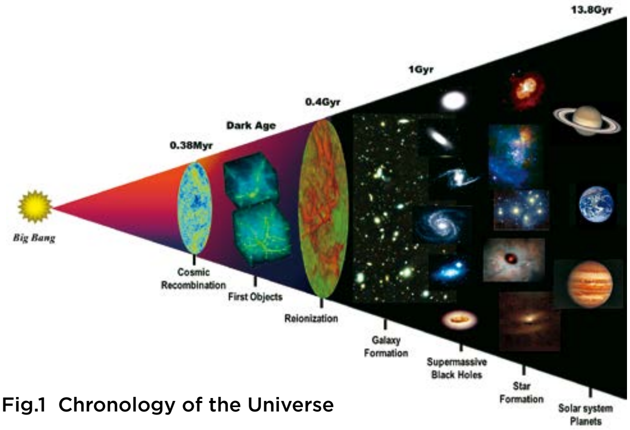



Fig.1 Chronology of the Universe

## Research Topics

In Astrophysics, we seek to understand, using fundamental laws of physics, the birth of the first stars and galaxies, the light they emit, the formation and evolution of galaxies and galaxy clusters, the formation and evolution of black holes and active galactic nuclei, and the formation of stars and planets. We pursue these aims by accurately solving radiative transfer equations and relativistic radiation-hydrodynamic equations and thereby realistically simulating the interaction between radiation and matter, and the multi-constituent, multi-bodied nature of the formation and evolution of astrophysical objects. We frequently begin a project by making analytical advances and numerical estimates of the important physics involved in the problem, before launching large scale numerical simulations on supercomputers hosted at the Center for Computational Sciences.

## Achievements to date

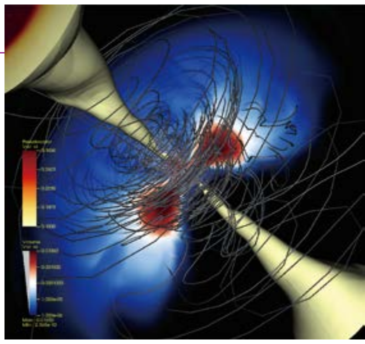


Fig.2 Accretion disc and jet around a black hole

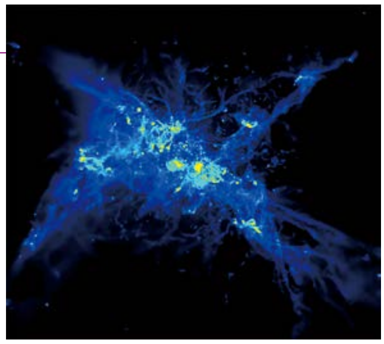


Fig.3 Simulation of cosmological galaxy formation simulation in the early universe

Fig. 2 depicts an accretion disc around a black hole and a jet emanating from the black Hole's ergosphere as calculated by general-relativistic radiation-magnetohydrodynamic simulations. Matter attracted by the formidable gravitational force of the black hole forms an accretion disc and, little by little, gets sucked into the black hole. In the accretion disc, gravitational energy is released, and an enormous swathe of photons is emitted. The force of the photons is so strong that it can lift off material from the accretion disc in the form of jets that can escape the gravity of the black hole.

Fig. 3 shows the formation of the first galaxies in the early universe, as calculated with state-of-the-art cosmological hydrodynamic simulations. In the era of galaxy formation, gas efficiently accretes along cosmic filaments onto galaxies, triggering massive bursts of star-formation in the galaxies. Those stars eventually explode in supernovae, which drives out much of the gas in the galaxies, rapidly quenching star-formation. The star-formation history in the early universe is, thus, very intermittent; it is a self-regulating cycle of bursts of star-formation and quiescence.

### Chief: Masayuki Umemura

University of Tsukuba, Center for Computational Science (Professor)

Doctor of Science. 1987, Ph.D. University of Hokkaido. 1989, Assistant Professor at the National Astronomical Observatory of Japan. 1993, Associate Professor at the University of Tsukuba, Center for Computational Sciences. Full Professor since 2004. Research expertise in theoretical astrophysics, in particular radiation hydrodynamics and galaxy formation, and the formation of supermassive black holes.

# Nuclear Physics Group

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

## Overview

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

## Research Topics

Density functional theory (DFT) has been developed for universal and quantitative description of nuclei. Fig. 1 shows a chart of nuclear deformation in the ground state, obtained with the DFT calculation. Furthermore, the time-dependent density functional theory (TDDFT) enables us to study response and reaction of nuclear systems. We have developed numerical codes to study photonuclear reaction, giant resonances, low-lying elementary modes of excitation, and heavy-ion collision. From these numerical calculations, we have succeeded to achieve a number of new insights into microscopic mechanisms of nuclear reactions, spontaneous breaking of symmetry, and quantum fluctuations. In addition, these results contribute to understanding element-synthesis process behind explosive stellar phenomena, such as supernovae.
Many attempts for synthesis of new elements have been performed using collisions of two heavy nuclei in accelerator facilities in the world. Recently, the naming right is awarded to a team in RIKEN, leading to the first element name by Japanese, “Nihonium”, of element 113. Fig.2 shows a study on possible reaction producing element 120. In most of heavy nuclei, protons and neutrons are paired and condensed in the ground state (pair condensation). This was confirmed in the calculation of Fig. 1. This leads to nuclear superfluidity and significantly affects many properties of structure and reaction. However, its effects on nuclear reaction, such as pair transfer and dynamical shape evolution, have not been well understood. We are currently developing real-time simulation in the 3D space for collisions of superfluid nuclei, and microscopic determination of nuclear reaction path based on theories of large amplitude collective motion. Recently, we have studied nuclear fission problems, and have found out production mechanism of fission fragments around xenon inside nuclear reactors. In Fig. 2, we show how the nuclear shape of $^{240}$Pu changes during the fission process. The larger fragment (lower fragment in Fig. 2) is deformed in the pear shape, which leads to an energy gain in the isotopes around xenon. The present results of simulation also agree with experimental data.

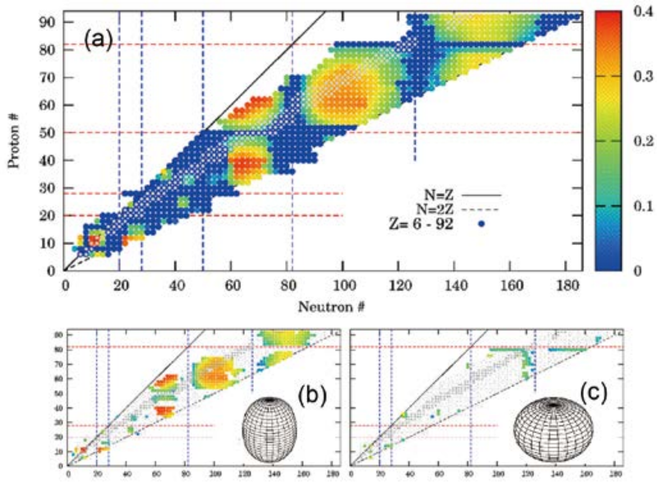



Fig.1 (a) Chart of nuclear deformation. Among those with relatively large deformation, (b) prolate shapes, and, (c) oblate shapes.

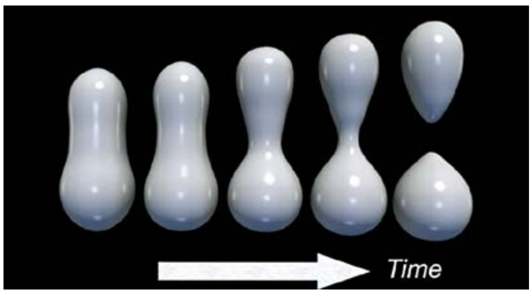



Fig.2 Simulating nuclear fission of the Pu nucleus in real time. The time span from the left to the right ends is about 2×10$^{-20}$ s.

### Chief: Takashi Nakatsukasa

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

# Quantum Condensed Matter Physics Group

**Chief**: Kazuhiro Yabana, Professor, Ph.D., Deputy Director of CCS **Members**: Hiroyasu Koizumi, Associate Professor, Ph.D. / Xiao-Min Tong, Associate Professor, Ph.D. /Nobuya Maeshima, Lecturer, Ph.D. / Shunsuke Sato, Assistant Professor, Ph.D. / Tomoya Ono, Visiting Professor, Ph.D.

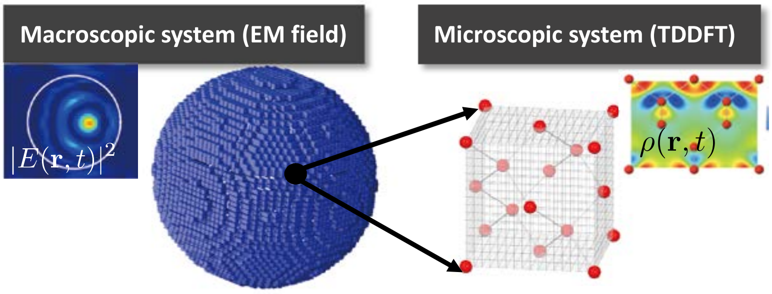
## Overview

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

## Research Topics

### Light-matter interactions

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

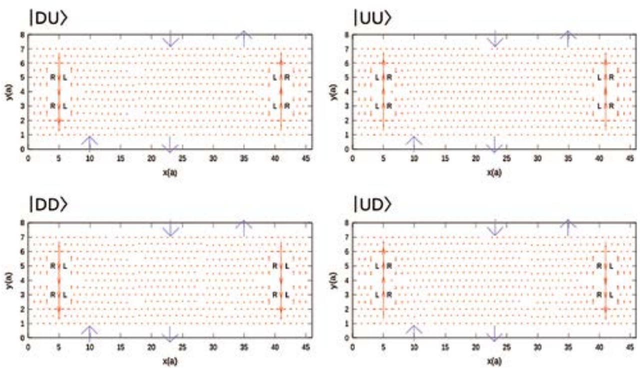



### Development of first-principles, real-time and real-space simulation code for optical science

In current frontiers of optical science, innovative simulation methods describing light-matter interaction from microscopic electronic dynamics are required. As such computer code, we develop a first-principles computational code SALMON (Scalable Ab-initio Light-Matter simulator for Optics and Nanoscience) that is based on density functional theory and utilizes real-space and real-time method, under close collaborations with computer scientists in the Center and researchers in physics and optics world-wide. SALMON is developed as an open-source software, and can be downloaded from the website, https://salmon-tddft.jp.

### Strongly correlated materials and topological materials

Strongly correlated materials or topological materials whose properties depend on the shape of the material exhibit interesting properties that cannot be explained by the band theory. We develop a numerical method to study properties of these systems including electronic states, phase transitions, optical responses, and perform a research toward developing new quantum information devices.




### Chief: Kazuhiro Yabana

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

# Biological Function and Information Group

**Chief**: Yasuteru Shigeta, Professor, Ph.D. **Members**: Ryuhei Harada, Associate Professor, Ph.D. / Mitsuo Shoji, Assistant Professor, Ph.D. / Hiroaki Nishizawa, Assistant Professor, Ph.D. / Yuta Hori, Assistant Professor, Ph.D.

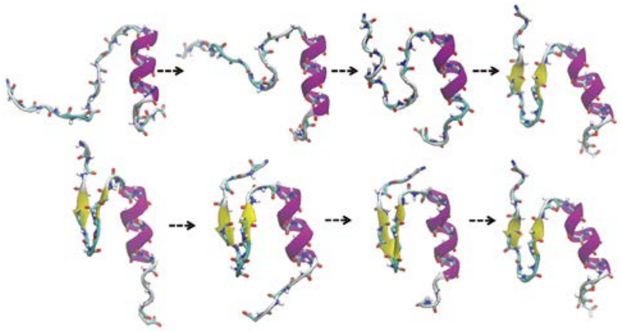
## Overview

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

## Research Topics

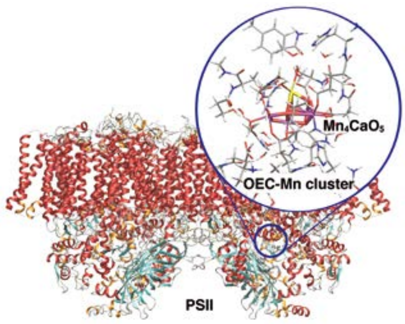
### Structural transitions of proteins for understanding its function.

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



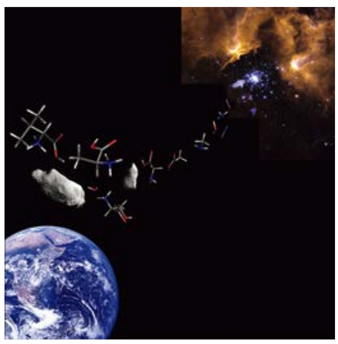
### Enzymatic reaction analyses by using hybrid QM/MM calculations

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




### Origin of amino acids and its enantiomeric excess in space

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



## Chief: Yasuteru Shigeta

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

# Molecular Evolution Group

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

## Overview

**Building the global phylogeny of eukaryotes**

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

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

## Research Topics

**Analyzing 'phylogenomic' data comprising >100 gene sequences**

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

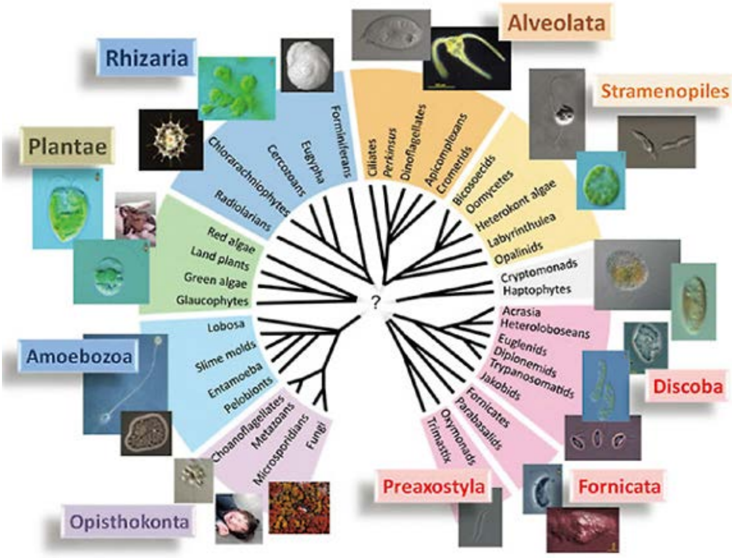



Fig.1 Tree of eukaryotes

## Current ongoing projects

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

### Group Leader: Yuji Inagaki

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

# Global Environmental Science Group

**Chief**: Hiroyuki Kusaka, Professor, Ph.D. **Members**: Hiroshi L. Tanaka, Professor, Ph.D. / Mio Matsueda, Assistant Professor, Ph.D. / Quang-Van Doan, Assistant Professor, Ph.D.

## Overview

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

## Research Topics

### NICAM (Non-hydrostatic ICosahedral Atmospheric Model)

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

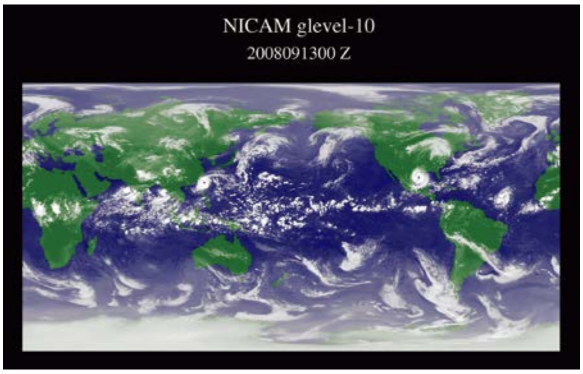



Fig.1 Numerical simulation of the general circulation of the atmosphere produced by 7-km resolution NICAM. NICAM-based modeling accurately predicted the evolution and movements of Typhoon Sinlaku and Hurricane Ike in 2008.

### WRF (Weather Research and Forecasting), CM1 (Cloud Model 1), and CCS-LES (Large Eddy Simulation) models

WRF, which is a compressible, non-hydrostatic numerical weather prediction model, is a collaborative development of the National Center for Atmospheric Research (NCAR), the National Centers for Environmental Protection (NCEP), etc. CM1, which is a compressible, non-hydrostatic numerical atmospheric model for idealized simulations, is developed in NCAR and PSU. Climate downscaling to the urban areas, heavy rainfalls in the urban areas, downslope windstorms, gap winds are studied with the WRF and CM1. Our group has been developing a new LES for urban areas (CCS-LES). Urban heat island is studied with the CCS-LES model.

Fig.2 Cap and Tsurushi clouds around Mt Fuji.

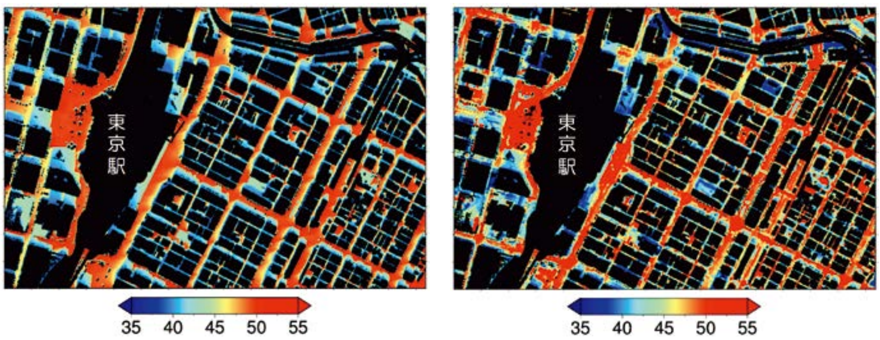



Fig.3 Road skin temperature distribution estimated by the CCS-LES model (left) and helicopter observation (right). Black indicates buildings.

### Chief: Hiroyuki Kusaka

Prof. Kusaka 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 pehomenon, downslope windstorms, LES modeling, and climate downscaling in Japan and Vietnam are the main themes. Cap and Tsurushi clouds around Mt. Fuji is also one of the research themes.

# High Performance Computing Systems Group

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

## Overview

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

Our research targets, which are spread across various HPC technologies, include high performance computing architecture, parallel programming language, massively parallel numerical algorithms and libraries, Graphics Processing Unit (GPU)-accelerated computing systems, large scale distributed storage systems, and grid/cloud technology. The following are among our more recent research topics.

## Research Topics

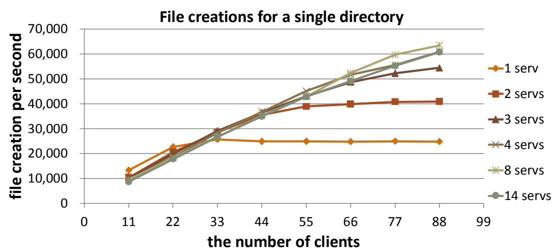
### A multi-hybrid accelerated computing system

Graphics processing units (GPUs) have been widely used in HPC systems as accelerators by their extreme peak performance and high memory bandwidth. To enhance the sustained performance even on strong scaling, we combine GPU and field programmable gate arrays (FPGAs) to compensate the weakness of these devices with each other, utilizing FPGA for reconfigurable computation and external communication over nodes with its high speed optical network. This system concept is called Accelerator in Switch (AiS) and we believe that it offers better strong scaling. Our brand-new supercomputer Cygnus incorporates this concept and it has been in operation since April 2019. We develop a set of supporting modules for application users as well as high performance applications on this concept.

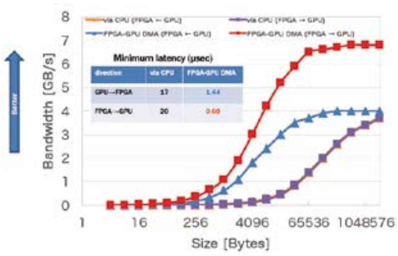
### XcalableMP

XxcalableMP is a PGAS-base large scale parallel programming language. In future supercomputer generations, which are expected to have millions of cores and distributed memory architecture, traditional message passing programming would strongly reduce software productivity.

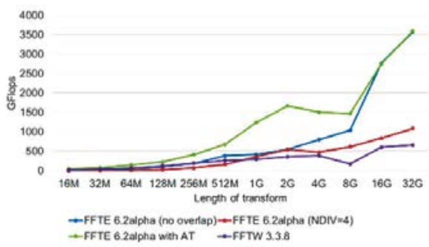
This language provides OpenMP-like directive base extension to C and Fortran to permit a global view model of data array handling in the manner of Partitioned Global Address Space (PGAS) concept as well as local-view modeling when describing highly tuned parallel programs. We are extending the target platform to the computation node with accelerators such as GPU and FPGA.



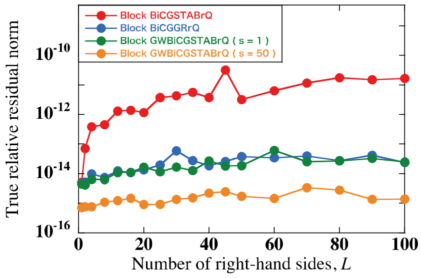

Meta-data server scalability of PPMDS




GPU-FPGA DMA performance for multi-hybrid acceleration




Performance of parallel 1-D FFT on Oakforest-PACS




Accuracy of the approximate solutions among three Block Krylov subspace methods

### Chief: Taisuke Boku

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

# Database Group

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

## Overview

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

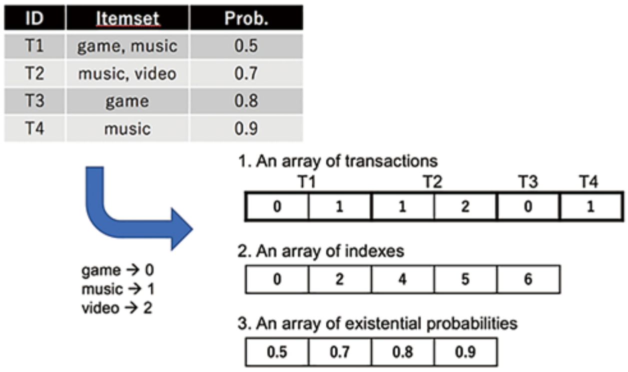



Fig.1 Frequent Pattern Mining using GPU

## Research topics

### Big Data Processing Frameworks

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

### Data Mining Algorithms

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

### Scientific Data Management

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

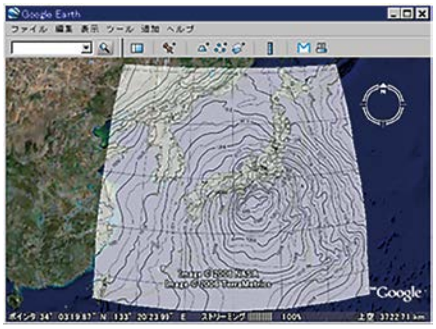



Fig.2 Meteorological Databases

### Chief: Hiroyuki Kitagawa

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

# Computational Media Group

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

## Overview

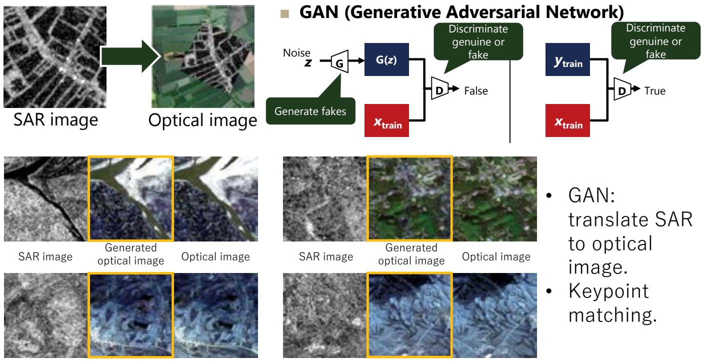
Our group aims to establish a new paradigm of computational media that can be used in our science study and our surrounding environment. On human-computer interaction, process speed and data flow speed should be fit to humans. This means any computational media should count the response time of humans and their ability to understand information provided from computer side. Our research covers the framework of computational science research scenes, human society system, daily life situations, and city-size environments. Our ultimate goal is to build a new, human-friendly, and intelligent media on the basis of computational sciences.

## Research Topics

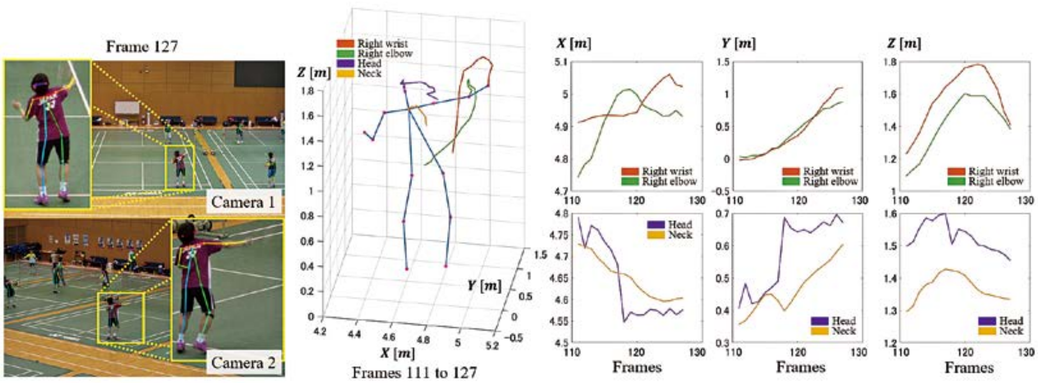
- Expansion of research areas to human society, living space, and city environment
- Intelligent and human-friendly feedback method to show the unified shape of real observation data and simulation result
- Computer vision and image processing technologies on computational medical science
- Advanced application of computational media on sport performance analysis and skill development


We have been working on visual activity analysis on sport scenes. One of the example is to analyze the human visual behavior on deciding the pass course under a pressured scene in soccer game situation. The figure shows one of our prototype systems on which a subject can see the virtual soccer where any motion are being measured.

One of our city-size research works is the image alignment between multi-modal images using advanced computer vision techniques. Since the sensors and their images have different intrinsic properties, a special intelligent approach should be invented to achieve the precise alignment. Out advanced computer vision technologies can make it possible.




As for the sport applications, one of our research works is focusing on the very precise investigation of 3D human pose estimation on badminton games. We have been conducting a joint-research work with Japanese national badminton team.




### Group Leader: Yoshinari Kameda

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

# Department of Computational Medical Science

Head: Masayuki Umemura, 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.

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.

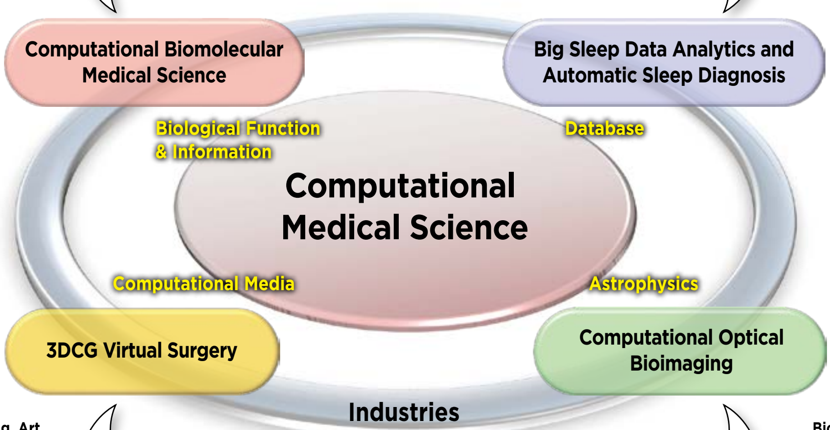
Sleep plays an important role in people's daily lives. Sleep disorders could cause various illnesses. There are a lot of scientific questions that need to be answered about sleep. Quantitative and accurate measurements and analysis of sleep are fundamental issues in sleep research. Sleep polysomnography (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.

Prof. Yasuteru Shigeta
Assoc. prof. Ryuhei Harada
Assis. prof. Hiroaki Nishizawa

**Collaborations:**
**Medicine, Biology, Physics**

Prof. Hiroyuki Kitagawa
Prof. Toshiyuki Amagasa
Assis. prof. Kazumasa Horie
Dr. Leo Ota
Dr. Ryusuke Miyamoto

**Collaborations:**
**Sleep Medicine/Science, Medicine, Engineering**




Prof. Yoshinari Kameda
Prof. Itaru Kitahara
Assis. prof. Hidehiko Shishido

**Collaborations:**
**Medical Science, Engineering, Art**

Prof. Masayuki Umemura
Assoc. prof. Hidenobu Yajima
Dr. Makito Abe

**Collaborations:**
**Biomedical optics, Mathematics**

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.

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.

# Project Office for Exascale Computational Sciences

## Develop Computational Sciences with the Full Performance of the Machine

Head: Kazuhiro Yabana, 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, massively-parallel computers equipped with many-core processors, which may play a central role in future large-scale computing, to say nothing of ordinary massively-parallel computers combining a multitude of CPUs. Due to advances of such diverse computers, it becomes a difficult task for researchers to make computations with the full power of each machine.

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

The services of this Office are not restricted to the Center alone, but extend outside to promote nationwide collaborations. To date, it has conducted analyses and examinations of hot spots for major applications to ensure that they show high efficiency in the Highly Accelerated Parallel Advanced system for Computational Sciences (HA-PACS), which is a massively-parallel supercomputer equipped with GPU accelerators, and in 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 feld-programmable gate array (FPGA), have been a central issue at the Office.

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

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

# Project Office for Exascale Computing System Development

## Empirical Research for Exascale Computing

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

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

In the Project Office for Exascale Computing System Development, we have been researching the next generation of accelerated computing systems under the new concept of accelerated computing named Accelerator in Switch (AiS) and Multi-Hybrid Accelerated Supercomputing. Currently, the main player of accelerated supercomputing is Graphics Processing Unit (GPU). However, GPU is not a perfect solution to apply to all fields of application although it provides the highest theoretical peak performance, high memory bandwidth and high performance/power ratio because its performance depends on a large degree of SIMD parallelism and is bottlenecked by frequent communication and conditional branches in the code. AiS is a new concept through our collaborative researches under codesigning among multiple application fields and HPC research. We apply Field Programmable Gate Array (FPGA) additionally to GPU.

Under the concept of AiS, we introduced the first platform as the proof-of-concept system named Cygnus as the prototype of 10th generation of PAX/PACS series supercomputer at the CCS (see p.4 "Supercomputer systems").

To realize the concept of AiS and show the performance of our solution, we have been developing elementary system parts such as high speed interconnection between FPGAs over nodes, GPU-FPGA fast data transfer, and programming environment for such a complicated multi-device system.

### High speed inter-node communication

The latest high-end FPGAs are equipped with their own optical communication link up to 100Gbps of performance. We use this feature for high-level parallel programming on multiple FPGAs over nodes by originally developed communication layer. It is provided as Verilog HDL modules which can be invoked from user level OpenCL code as like as ordinary communication library. We achieved very high speed and low latency communication on the user level OpenCL code.

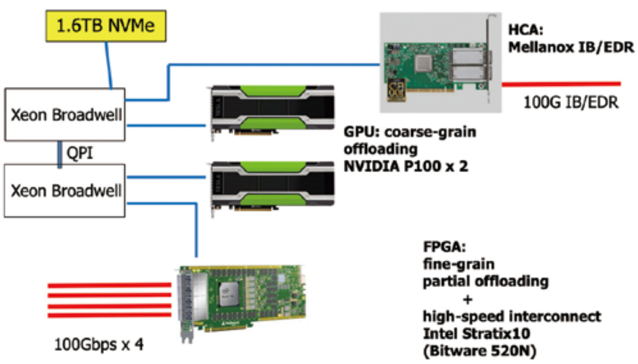
### GPU-FPGA DMA

In the concept of AiS, we combine GPU computing for absolute floating operation power and FPGA for flexible computation and high performance communication. To combine these devices, it is required to establish high-speed data transfer among them within a node. We developed GPU-FPGA Direct Memory Access (DMA) module which can be called from user-level OpenCL. It realizes very low latency communication over PCI-Express without redundant data copy through the host CPU memory and provides easy programming method for users on OpenCL level.

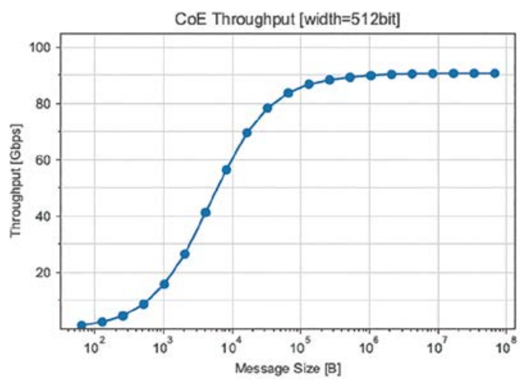
### PPX (Pre-PACS-X)

Before installation of Cygnus, the CCS constructed a testbed system of PACS-X Project named Pre-PACS-X (PPX). It is a minicluster system with 13 computation nodes where each node consists of two Intel Xeon CPU sockets, two NVIDIA GPU (Tesla V100 or P100) and an Intel FPGA board (Arria10) from 2016.

Each node is also equipped with 1.6 TByte of NVMe as local storage and testbed for network accessible storage device through 100Gbps of InfiniBand EDR. We have been developing the basic function and FPGA supporting modules to realize multi-hybrid accelerated supercomputing on Cygnus.




PPX node configuration




FPGA-to-FPGA communication performance on 100Gbps link

# Project Office for HPCI

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

Head: Yoshinobu Kuramashi, Professor, Ph.D.

### HPCI Plan and Strategic Program Field 5

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

In the HPCI Strategic Program, which had been operated from FY2011 to FY2015, five potential fields were identified as strategic fields that not only required K computer resources, but also were expected to yield significant social and scholarly breakthroughs. "Field 5: The origin of matter and the Universe" was one of these. This field dealt with fundamental physics, primarily concerning elementary particles, the atomic nucleus, and astrophysics. The institution (strategic institution) that successfully led Field 5 research and development for five years was the Joint Institute for Computational Fundamental Science (JICFuS), which is a joint research organization combining the University of Tsukuba's Center for Computational Sciences (CCS), the High Energy Accelerator Research Organization (KEK), and the National Astronomical Observatory of Japan (NAOJ). The K computer was shut down at the end of August, 2019.

### Toward the New Supercomputer "Fugaku"

The post-K computer development plan under the FLAGSHIP 2020 Project, initiated by the Ministry of Education, Culture, Sports, Science and Technology in 2014, has set the target of developing (1) the next generation flagship supercomputer of Japan (the successor of the K computer) along with (2) a wide range of applications that will address top 9 priority social and scientific issues. "Priority Issue 9: Elucidation of the fundamental laws and evolution of the universe" led by the CCS, University of Tsukuba and 10 other institutions is essentially the successor of "Field 5: The origin of matter and the Universe" aiming at new developments. The CCS also joins "Priority Issue 7: Creation of new functional devices and high-performance materials to support next-generation industries (CDMSI)". In addition to the priority issues, there are four exploratory challenges selected to be tackled using the post-K computer. The CCS joins two of them: "Exploratory Challenge 1: Frontiers of basic science: Challenging the limits" and "Exploratory Challenge 3: Elucidation of the birth of exoplanets (second earth) and the environmental variations of planets in the solar system". In May 2019 the post-K computer was named "Fugaku", which is another name of Mt. Fuji. The new supercomputer will be installed after disassembling the K computer. As a core institution of priority issues and exploratory challenges, the project office promotes the accomplishment of research and development targets.


K Computer

# Liaison Office for Multidisciplinary Computational Sciences

## Toward Formation of the International Hub of Computational Sciences

Head: Yoshinari Kameda, Professor, Ph.D.

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

### Cooperation among Different Fields

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

### International Cooperation

As for international cooperation, partnership agreements have been concluded between University of Tsukuba and the University of Edinburgh in the UK, as well as with Lawrence Berkeley National Laboratory in the US. Furthermore, as part of the efforts to deepen the computational science research exchanges, the CCS and the University of Edinburgh Parallel Processing Center (EPPC) are currently hosting joint symposiums, and the Center is cosponsoring workshops with Lawrence Berkeley National Laboratory.

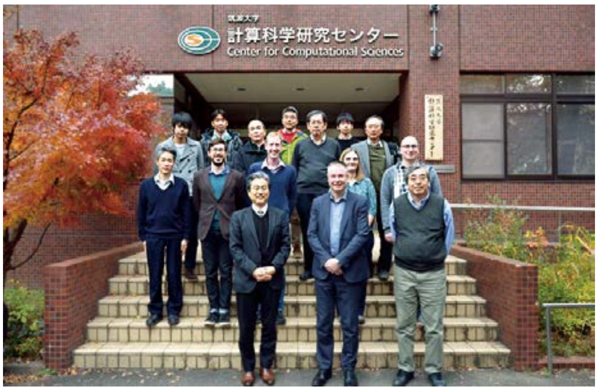
### Multidisciplinary Pioneering Program

The multidisciplinary pioneering program encourages the promotion of research efforts that require collaboration and cooperation among divergent scientific fields. Cooperation between the computational physics (science) and numerical analysis (engineering) fields in order to implement calculation code with high execution efficiency and to perform the necessary large-scale simulations using the code is one of our program activities. There are also projects that aim at new research deployments and developments by facilitating organic cooperation among different fields utilizing the same techniques in computational science. The multidisciplinary pioneering program has support from the collaborative multidisciplinary program of the center.

### Organization for Collaborative Research on Computational Astrobiology

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

These research efforts are focusing on the analysis of the potentials of interstellar molecular biology, planetary biology, and the astrophysics of star and planet formation.




Collaboration workshop between CCS and the university of Edinburgh, 2017.


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


Japan-Korea HPC Winter School, 2019.

# Promotion Office for Computational Sciences

## Promote Social Contributions and Human Resource Development in Computational Sciences

Head: Daisuke Takahashi, Professor, Ph.D.

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

### Personnel Development

#### Graduate School Dual Degree Program

The graduate school consists of master's programs and doctoral programs. Doctoral candidates usually study a specialized field through both programs. However, since sophisticated computer skills and experience are necessary to advanced research in scientific fields such as physics, global environment, and biology, a broad level of expertise in both science and computer technology is required for computational science doctoral candidates.
The Promotion Office for Computational Sciences promotes dual degree programs to meet this need. The dual degree program makes it possible to obtain a doctorate in a scientific field along with a master's degree of computer science simultaneously, by a doctoral program in scientific field and a master's program in computer science.

#### Computational Science English Program

In response to the increasing numbers of international students from overseas, the Computational Science English Program was established as a master's program in computer science that can be completed in English. As shown in the table, this program provides English lectures in 13 subjects, along with English language research guidance aimed at assisting master degree candidates in successfully obtaining their degrees.

#### Campus-wide Courses for Graduate Students

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

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

### Social Contribution

#### Cooperation with other institutions

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

#### Mt. Tsukuba Project

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

#### Dissemination of Information

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

# Project Office for AI & Big Data

## Promoting big data and AI research exploiting supercomputers

Head: Toshiyuki Amagasa, Ph.D.

Recently, big data an AI have attracted a great deal of public attention. In big data analysis, we analyze a massive amount of complex data that cannot be processed by ordinary computers, whereas, in AI, we can achieve ultimately highly precise classification or prediction, that cannot be possible by existing technologies, by applying machine learning techniques, such as deep learning, against a massive training data. The mission of the promotion office of big data & AI covers promoting applications of big data/AI technologies to the research activities in the divisions in CCS, promoting big data/AI research exploiting supercomputers and promoting collaborations with the center for artificial intelligence research (C-AIR) and other institutes.

### Promoting the application of big data/AI technologies to research divisions in computational sciences

In various scientific areas, it has become very active to apply big data analysis or machine learning techniques to massive data for discovering new knowledge. One of the most well-known examples is *bioinformatics*. We promote applications of big data/AI techniques to different research domains in computational sciences by the collaboration between the divisions of computational sciences and the divisions related to big data/AI.

### Promoting big data/AI research exploiting supercomputers

It is known that substantial computer resources (both CPU and memory) are mandatory to perform big data analysis/AI. For this reason, supercomputers are considered to be one of the most suitable environments for performing big data analysis/AI. Thus, in major supercomputers, the number of such use cases have been growing. We promote to use the supercomputers at CCS in the research activities in big data analysis/AI.

### Collaboration with the center for artificial intelligence research (C-AIR) and other institutes

We promote the collaborations with the center for artificial intelligence research (C-AIR) at our university and other institutes concerning the above activities related to big data/AI.

A meeting of project office for AI & big data

# Bureau of Public Relations and Strategy

Head: Yasuteru Shigeta, Professor, Ph.D.

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

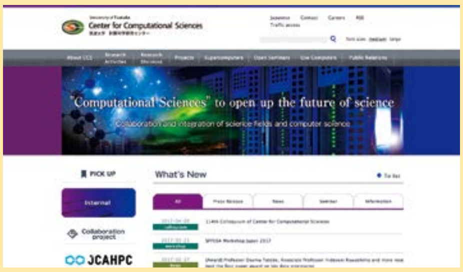
## Press release

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

Articles and the photos of press conference

## Contents

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





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

## CCS Tour / Open day

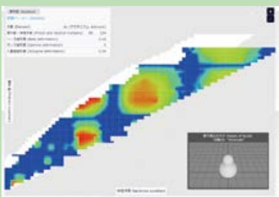
At the CCS tour for high school students, Open day in spring, and Open Campus in summer, we show our research activities and the supercomputer of the center. About 2000 people a year visit the CCS.

## Projects, symposiums, and conferencing support

- Public relations activities on the Mt. Tsukuba project
- Support to Joint Center for Advanced HPC (JCAHPC)
- Support to make communication tools for public about research outputs
- Booth design and management support at SC

etc.

Leaflet of Mt. Tsukuba Project



Interactive Nuclear Chart & Periodic Table "InPACS"

SC18

# Access

## Airport Bus

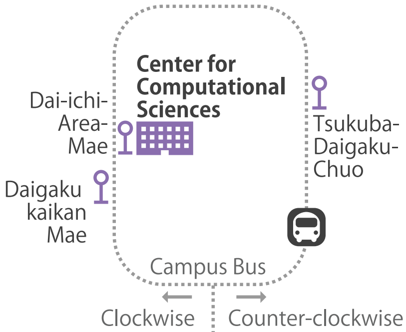
**Narita Airport**: About 60 minutes from Narita Airport by bus bound for “JR Tsuchiura station”.
Take a bus at the bus stop at the Terminal 1, the Terminal 2, or the Terminal 3 and get off at “Tsukuba Center”.
**Haneda Airport**: About 120 minutes from Haneda Airport by bus bound for “Tsukuba Center”.
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.

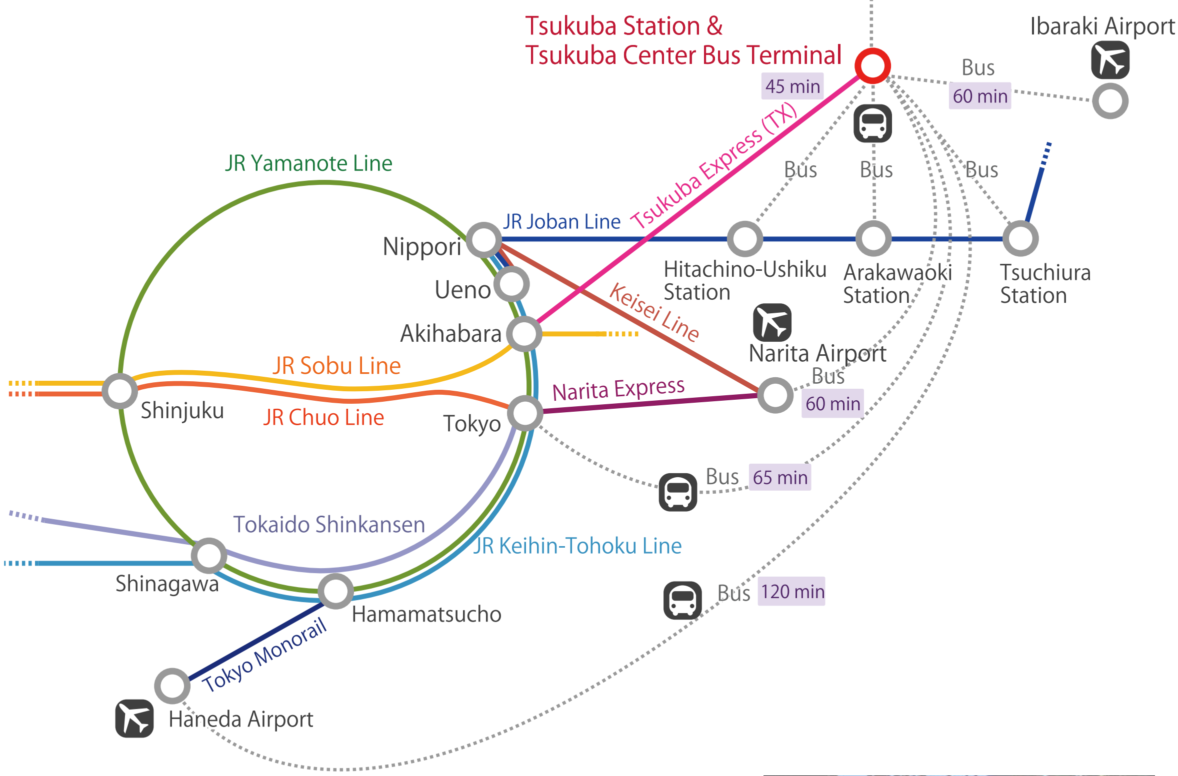
## Tsukuba Express (TX)

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 (Tsukuba Station)

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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