

Director's Message





The objectives of the RIKEN Center for Computational Science (R-CCS) are threefold, centered around supercomputing: one is to target high performance computation itself as a scientific objective, or namely, the "Science of Computing"; another is to apply the enormous computational power thus obtained to solve difficult scientific problems, or namely the "Science by Computing"; finally, to collaborate with other scientific disciplines that contribute to advances in both sciences, or namely, the "Science for Computing." Our goal is to be recognized as one of the global leadership research centers to advance high-end computational science in this regard.

Computational science employs numerous methodologies to essentially recreate various phenomena as computational activities within machines, allowing us to tackle challenging problems faced by humanity. For instance, we can model a phenomenon through a set of physical or mathematical formulas, and by solving these formulas computationally, we achieve a direct "simulation" of the phenomenon. Alternatively, we can analyze vast amounts of data collected by scientific instruments and extrapolate future trends, utilizing the "data science" methodology. Additionally, we can train our "artificial intelligence (AI)" to derive higher-level insights from both simulated and analyzed data. Supercomputers significantly accelerate all these methodologies, empowering the synthesis of innovations to address society's most pressing issues. R-CCS strives to be at the forefront of these activities.

R-CCS is engaged in the research and development of cutting-edge, pioneering technologies that drive the evolution of the entire IT field.

- "Al for Science" to accelerate research processes by applying rapidly advancing AI directly to scientific research, with a focus on developing foundational models for science with Advanced General Intelligence for Science Program (AGIS)* by RIKEN.
- ·Constructing a quantum-supercomputer hybrid platform (JHPC-Quantum Platform) that enables computing in areas previously challenging for traditional supercomputers.
- FugakuNEXT, a next-generation supercomputer that combines simulation and AI and achieve global technological leadership.

We are confident that the outcomes of our efforts will contribute broadly to IT advancements in business and industry, ultimately benefiting national life and economic growth.

Additionally, R-CCS is committed to actively promoting diversity, which is essential for driving science, technology, and innovation. We are fostering a workplace environment where talented individuals can thrive, regardless of gender, age, nationality, or cultural background. We are also prioritizing the recruitment of women and foreign nationals, with initiatives such as women-only recruitment, to address the current underrepresentation of female team leaders (Pls).

As a leading global research center in IT advancements, we will continue to collaborate with domestic and international institutions, taking on cutting-edge challenges and advancing research toward the next generation of Science of, by, and for Computing.

*The concept of "Transformative Research Innovation Platform of RIKEN platforms" (TRIP) aims to organically link outstanding researchers in a broad range of fields of fundamental science and a rich array of research platforms in RIKEN. This is a challenging project to create an innovative research platform that effectively generates new fields of knowledge across research fields. Under the TRIP initiative, "Advanced General Intelligence for Science Program" (AGIS) has been launched to accelerate scientific research using generative AI.

Our Mission

R-CCS Aims to Realize Society 5.0 through High-performance Computing. "The Science of Computing, by Computing, and for Computing"

The realization of Society 5.0, "a society that is sustainable and resilient against threats and unpredictable and uncertain situations, that ensures the safety and security of the people, and that individual to realize diverse well-being," as advocated by Japan, requires the power of high-performance computing (HPC). As a world-leading HPC research center in Japan, based on the slogan, "The Science of Computing, by Computing, and for Computing," we will collaborate with various organizations in Japan and overseas to construct and operate a computing infrastructure that is ahead of its time, while also conducting cutting-edge computational science research that contributes to solving scientific and social issues.

"The Science of Computing, by Computing, and for Computing"

Striving for excellence in science and becoming the cornerstone of Society 5.0



Development of human capital with expertise in advanced computer science and technology

Research in life science, engineering, meteorology and dimate, disaster prevention and mitigation, materials science, space and article physics, social science, and more by



New types of computers, Further evolution of computing (research new architecture and on optical, quantum, and reconfigurable computational models computing, neuromorphic computing, etc. development of new materials and

Analysis and simulation for new computing technologies

Advancement of computing by new technologies

Broaden

Creation of Groundbreaking Science That Paves the Way for the Rest of the World

era, methodology for AI and big data

analysis, etc.

- •Promotion of computational science that contributes to the development of individual scientific and industrial fields
- •Exploring new computing paradigms that will be the grand challenge of information science in the future

Career Development to Support the Development of Computational Science

- *Training highly skilled computational science and technology professionals with a broad perspective
- •Promoting the exchange of the best talent from Japan and overseas

Construction and Operation of an Advanced and Stable Computing Infrastructure

- •Operation, maintenance, and management of the computing infrastructure, construction of the usage environment, and supply of computing resources
- •Research and development of the next-generation HPC infrastructure (FugakuNEXT)
- ·Construction of an information infrastructure that organically integrates simulation, data, Al and quantum computing (construction of a quantum HPC collaboration platform, promotion of AI for Science)

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Research Teams and Units at R-CCS

Organizational Chart

As of September 2024

Director **Deputy Directors** Computational Science Planning Office

Administrative Division

Research Teams

The Science of Computing

Processor Research Team

Large-scale Parallel Numerical Computing Technology Research Team

Next Generation High Performance Architecture Research Team

High Performance Big Data Research

High Performance Artificial Intelligence Systems Research Team

Supercomputing Performance Research Team

Large-scale Digital Twin Research

High Performance Cloud Systems and Secure Software Research Team



The Science by Computing

Field Theory Research Team

Discrete Event Simulation Research Team

Computational Molecular Science Research Team

Computational Materials Science Research Team

Computational Biophysics ResearchTeam

Computational Climate Science Research Team

Complex Phenomena Unified Simulation Research Team

Data Assimilation Research Team

Computational Structural Biology Research Team

Computational Disaster Mitigation and Reduction Research Team



Operations and Computer **Technologies** Division

Facility Operations and Development Unit

System Operations and Development Unit

Software Development Technology Unit

Data Integration Technology Unit

Advanced Operation Technologies Unit



HPC- and Al-driven Drug Development Platform Division

Biomedical Computational Intelligence Unit

Medicinal Chemistry Applied Al Unit

Molecular Design Computational Intelligence Unit

Al-driven Drug Discovery Collaborative Unit

Quantum-HPC Hybrid Platform Division

Quantum-HPC Hybrid Software Environment

Quantum Computing Simulation Unit

Quantum-HPC Hybrid Platform Operations Unit

Al for Science Platform Division

Learning Optimization Platform Development Unit

Data Management Platform Developmen Unit

Advanced Al Device **Development Unit**

Al Development Computing **Environment Operation** Technologies Unit

Life and Medical Science Application Interface Platform Development Unit

Material Science Application Interface Platform Development



Office of the Fugaku Society 5.0 Initiative



Job Openings

R-CCS recognizes diversity as a major pillar of science, technology, and innovation, and actively recruits the best researchers and engineers from all over the world and all regions, regardless of age, nationality, or cultural background. We also actively support the further advancement of female researchers and promote the recruitment of talented female researchers.





https://www.r-ccs.riken.jp/en/ about/recruit/



Career Development

RIKEN Center for Computational Science (R-CCS) plays a central role in the development of computational science and technology in Japan. R-CCS also actively utilizes the advanced technologies and knowledge accumulated through these activities and cooperates with related institutions to develop the personnel who will support computational science and technology. R-CCS conducts training for graduate students, young researchers and corporate engineers, aiming to develop:

- ·Human capital who can coordinate and integrate computational and computer sciences
- ·Human capital with advanced computational science technology skills
- ·Human capital who will contribute to the promotion of the use of advanced computational science technologies in industry

R-CCS Internship Programs

International internship programs for students from overseas institutes and domestic internship program for students



R-CCS Schools

Schools with lectures, tutorials, exercises, and group work for students and early career researchers.

Joint Graduate School Program

Collaborative programs between RIKEN and Kobe University and Tohoku University.

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from institutes in Japan.

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Supercomputer Fugaku

The supercomputer Fugaku was developed with the aim of contributing to Japan's growth by solving social and scientific issues, and producing world-leading results. As a supercomputer with the world's highest level of comprehensive performance in terms of power efficiency, computational performance, user convenience, ease of use, groundbreaking results, and acceleration functions for big data and AI (artificial intelligence), it is being used in HPC infrastructure to realize Japan's vision of Society 5.0.

HPCG

500 CERTIFICATE

Mary Jackson Marty Bullion

HPL-AI

Development History

April 2014 Launched the FLAGSHIP 2020 project to develop the successor to the K computer

March 2019 Started manufacturing

May Determined the name of the successor to the K computer to be the supercomputer "Fugaku"

December Started the installation of Fugaku

April 2020 Started use of the Program for Promoting Research on the Supercomputer Fugaku, Ministry of Education, Culture, Sports, Science and Technology

Used Fugaku partially for countermeasures against COVID-19

May Completed the installation of Fugaku

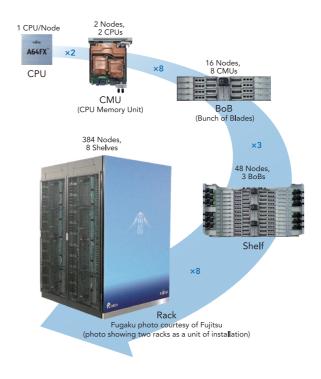
June Achieved the world's top ranking in four benchmark test categories (First time ever to be the best in four categories simultaneously)

March 2021 Started shared use

Total Number of Nodes

The total number of nodes* in Fugaku is 158,976 (432 racks).

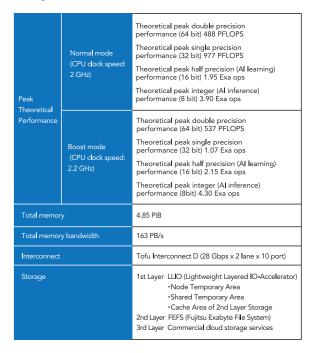
*In high performance computing, a management unit is often called a node. For example, a node can be a cluster of CPUs and memory that runs a single operating system.



Performance

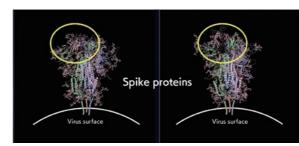
Fugaku can be run in a normal mode (CPU clock speed of 2 GHz) and a boost mode (CPU clock speed of 2.2 GHz), and the peak theoretical performance in each mode is summarized in the table below.

The high memory bandwidth is also one of the features of Fugaku.

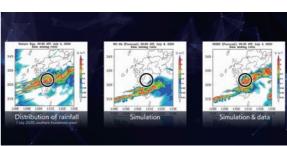


Research Using Fugaku

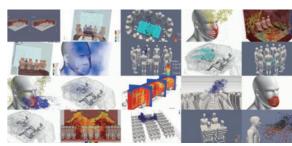
Examples of research using Fugaku are showcased in articles and videos. Be sure to take a look.



Understanding How Molecules Move Inside the Cell (video)



Making "Storm Cloud Train" Forecasting More Accurate (video)



Studying How Droplets & Aerosols can Transmit Viruses (video)



Creating a New Platform for Drug Discovery (video)





Press Releases





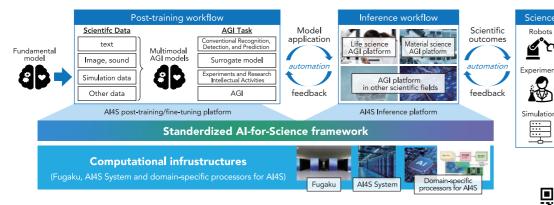
R-CSS Challenges

Aiming to Realize "Al for Science"



RIKEN is spearheading the Transformative Research Innovation Platform (TRIP)*, an interdisciplinary initiative designed to foster groundbreaking scientific advancements. Within this initiative, the AI for Science Platform Division is tasked with a critical role: the establishment, management, and continuous enhancement of the computational infrastructure essential for the creation of generative AI models, also known as Foundation models, tailored for scientific discoveries. This division's responsibilities extend to the integration of the 'Fugaku' supercomputer, with a novel AI-dedicated supercomputing system. This integration is aimed at developing foundational software that significantly advances

the capabilities of training and inference processes in AI for science. In addition to the mainstream pursuit of upscaling a large supercomputing infrastructure for AI for Science, we will also investigate computational paradigms that surpass the traditional reliance on GPUs, enhanced speed, efficiency, and energy conservation in AI tasks. The overarching goal of these endeavors is to catalyze innovation across various scientific domains by the application of advanced AI for Science. By expediting the scientific research cycle and broadening the scope for exploration within scientific fields, RIKEN's TRIP initiative stands to make substantial contributions to the advancement of scientific knowledge and its applications.



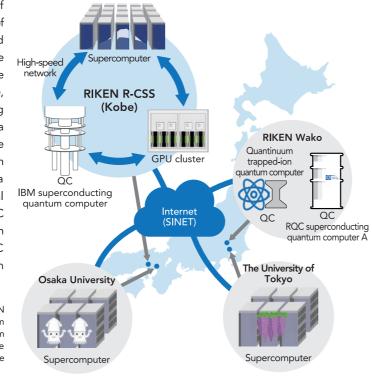
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Construction and Technical Development of a Quantum-HPC Hybrid Platform

As part of the Transformative Research Innovation Platform of RIKEN platforms (TRIP)*, RIKEN is working to enable exploration of uncharted computable capabilities through highly integrated quantum computers (QC) and supercomputers (high performance computing (HPC)). Meanwhile, it is essential to organically integrate and utilize HPC in order to put QC into practical use. Therefore, R-CCS aims to promote the full-scale use of QC by developing system software that integrates QC and HPC and constructing a platform for quantum research. Furthermore, in order to accelerate this research and development, we are conducting JHPC-quantum project with SoftBank, The University of Tokyo, and Osaka University, with support from the New Energy and Industrial Technology Development Organization (NEDO), to build QC-HPC hybrid computing platform with technology for deploying quantum and HPC hybrid software and enable the service by QC-HPC hybrid applications as a service (PaaS) developed in this research and provided by networks in the post-5G era.

In addition to the superconducting quantum computer A at the RIKEN Wako Branch, a trapped-ion quantum computer from Ouantinuum will be installed at the Wako Branch, and a superconducting quantum computer from IBM will be installed at the Kobe Branch. These quantum computers will be connected to the R-CCS Fugaku and the supercomputers at The University of Tokyo and Osaka University.



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Virtual Fugaku: Your Personal Fugaku, Empowering the World

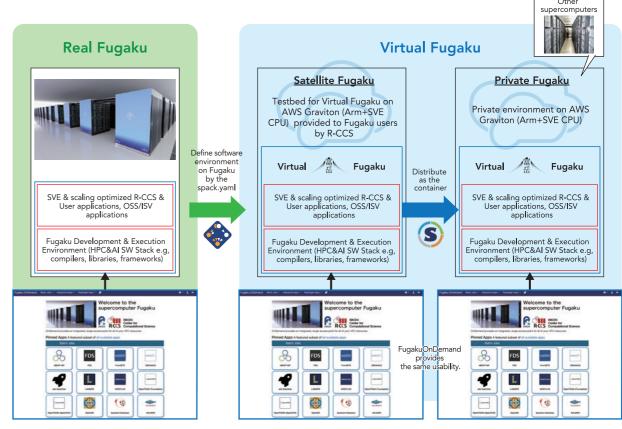


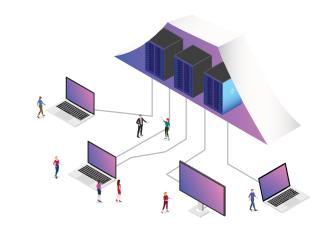
It is no exaggeration to say that the new value created continuously by the supercomputer Fugaku is supported by a highly developed software environment. Since the development of Fugaku began, R-CCS has developed and maintained an exceptionally high-quality software environment using methods such as co-design, and has continued to update it with cutting-edge software technology since its launch. This high-quality and sustainable software environment, which can be considered a cutting-edge research platform, will be made available for use on computers and cloud services beyond Fugaku. This is Virtual Fugaku.

Virtual Fugaku is a development environment that has

the potential to become a global standard. Application programs developed on Virtual Fugaku can be run not only on Fugaku but also on any computers and cloud services that have installed Virtual Fugaku, contributing to the groundbreaking expansion of the software ecosystem for supercomputers.

R-CCS has begun providing Satellite Fugaku as an environment for experiencing Virtual Fugaku and testing individual programs. Additionally, we are also providing Private Fugaku, which allows users to utilize Virtual Fugaku in cloud services and other environments by containerizing it with container virtualization technology.



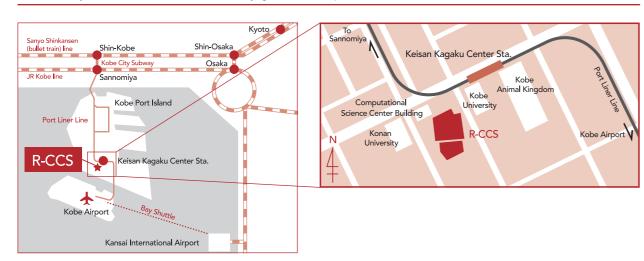


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Directions RCCS Wako Branch R-CCS Tokyo Branch R-CCS Yokohama Branch

R-CCS Kobe (Supercomputer Fugaku)

7-1-26 Minatojima-minami-machi, Chuo-ku, Kobe, Hyogo 650-0047, Japan



From the nearest Port Liner station

(Keisan Kagaku Center Station)

3 min. walk from Keisan Kagaku Center Station on the Port Liner train. Come out of the gate and proceed to the right. Take the escalator to the ground level, and go straight. The R-CCS buildings will be on your left front.

To the nearest Port Liner station

(Keisan Kagaku Center Station)

[From the bullet train (JR Shinkansen) station]

Get off the bullet train (JR Shinkansen) at Shin-Kobe Station, and transfer to the Kobe City Subway. At the first stop, Sannomiya, transfer to Port Liner bound for Kobe Airport. Ride the Port Liner for approximately 15 minutes and get off at Keisan Kagaku Center Station.

[From Kobe Airport (UKB)]

UKB - (Port-Liner) - Keisan Kagaku Center Station (5 minutes)

There is no visitor parking at the location. Please use public transportation. Please contact us for special needs for a large group or handicapped persons.

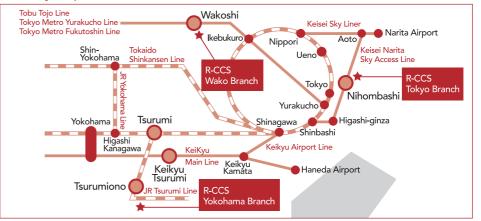


https://www.r-ccs.riken.jp/

en/directions/



< Railway Map of Kanto Locations>



R-CCS Tokyo Branch (Office of the Fugaku Society 5.0 Initiative)

Nihonbashi 1-chome Mitsui Building, 15th floor, 1-4-1 Nihonbashi, Chuo-ku, Tokyo 103-0027, Japan



By Public Transportation

Directions from the Nearest Stations

[From Nihombashi Station]

Directly connected via the B12 and C1 exits from the Tokyo Metro Tozai Line (T10), Ginza Line (G11) and Toei Asakusa Line (A13). [From Tokyo Station]

 $\,$ 6 min. walk from the Yaesu Central gate of the JR Line and Tokyo Metro Marunouchi Line.

1 min. walk from the Subway Nihombashi Station stop of the Metro Link Nihonbashi loop-line bus. (free bus service)

R-CCS Wako Branch

2-1, Hirosawa, Wako, Saitama 351-0198, Japan



By Public Transportation

Directions from the Nearest Station

[From Ikebukuro Station to Wakoshi Station]

- •Tobu Tojo Line: Express and Semi Express (approx. 12 minutes)
- •Tokyo Metro Yurakucho Line: Local (approx. 19 minutes)
- •Tokyo Metro Fukutoshin Line: Express (approx. 14 minutes)

[From Wakoshi Station to RIKEN]

On foot: The institute is about a 15-minute walk from the station. Bus: Approx. 10 minutes (Bus #39 bound for Oizumigakuen) Taxi: Approx. 10 minutes

R-CCS Yokohama Branch

1-7-22 Suehiro-cho, Tsurumi-ku, Yokohama, Kanagawa, 230-0045, Japan



By Public Transportation

Directions from the Nearest Stations

[By Bu

Take the #08 bus from Platform 8 at the East Exit of Tsurumi Station (also accessible from the West Exit of Keikyu Tsurumi Station) and get off at the RIKEN Shidai Daigakuin Mae bus stop. The institute is across the street. All buses from this platform are bound for Fureyu.

[By Train]

A 15-minute walk from JR Tsurumiono Station (JR Tsurumi Line), which is directly accessible by transfer from JR Tsurumi Station.

Use the taxi stand at the East Exit of JR Tsurumi Station or the West Exit of Keikyu Tsurumi Station. The trip takes about 10 minutes.

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