

## Director's Message



#### RIKEN Center for Computational Science (R-CCS)

has three core objectives, all 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 Al 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 is a next-generation supercomputer that combines simulation and Al to achieve a position of global technological leadership.

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

Furthermore, R-CCS is dedicated to advancing diversity, recognizing it as a vital foundation for driving progress in science, technology, and innovation. We are committed to fostering an inclusive work environment where individuals can thrive regardless of gender, age, nationality, or cultural background. In addition to actively recruiting women and international researchers, we are striving to increase the representation of women in senior research positions.

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 the Science of Computing, by Computing, 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.

# 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 as well as unpredictable and uncertain situations, that ensures the safety and security of the people, and that realizes diverse forms of well-being for each and every individual, "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.

# Advancing Computational Science and Pioneering Future Computing Paradigms to Drive Scientific and Industrial Innovation





#### The Science of Computing

To pursue new technology fundamental to high-performance computing

New technology for the post-Moore era, methodology for AI and big data analysis, etc.

Algorithm and programing models for new devices

New types of computers, new architecture and computational models

#### Synergy and Integration

Collaboration with domestic and overseas industrial enterprises, universities, and research institutes

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

# Apply

#### The Science by Computing

To solve scientific problems and create values using high-performance computing

Research in life science, engineering, meteorology and climate, disaster prevention and mitigation, materials science, space and particle physics, social science, and more by utilizing high-precision analysis and simulation





#### The Science for Computing

To broaden the possibility of high-performance computing by promoting cross-disciplinary exploration

Further evolution of computing (research on optical, quantum, and reconfigurable computing, neuromorphic computing, etc.; development of new materials and devices)

Broaden

Analysis and simulation for new computing technologies



Advancement of computing by new technologies

# 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
- Enhancing operational efficiency to support the realization of carbon neutrality
- Technological development for the "Virtual Fugaku" initiative, which aims to disseminate the software environment developed for Fugaku to other supercomputers
- Research and development of FugakuNEXT, a next-generation HPC infrastructure

# Expanding the Frontiers of Computational Capability

- Development and implementation of computing systems that go beyond conventional architectures to support world-leading "AI for Science"
- Constructing a quantum-supercomputer hybrid platform (JHPC-Quantum Platform)

# Developing Human Resources for the Future 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

# Research Teams and Units

#### **Organizational Chart**

As of May 2025

Director/
Deputy Director

Office of the Fugaku Society 5.0 Initiative Computational Science Promotion 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 Team

High Performance Artificial Intelligence Systems Research Team

Supercomputing Performance Research Team

Large-scale Digital Twin Research Team

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 Research Team

Computational Climate Science Research Team

Complex Phenomena Unified Simulation Research Team

Data Assimilation Research Team

Computational Structural Biology

Computational Disaster Mitigation and Reduction Research Team

Research Team

Digital Materials Science Research Team



### 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 Unit

Quantum Computing Simulation Unit

Quantum-HPC Hybrid Platform Operations Unit

### Al for Science Platform Division

Al for Science Foundation Model Research Team

Learning Optimization Platform Development Unit

Data Management Platform Development 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 Unit



### Operations and Computer Technologies Division

Facility Operations and Development Unit

System Operations and Development Unit

Software Development Technology Unit

Technology Unit

Advanced Operation
Technologies Unit

Data Integration

### Next-Generation HPC Infrastructure Development Division

Next-Generation HPC Infrastructure System Development Unit

Next-Generation HPC Application Development Unit

Next-Generation HPC
Operation Technologies

Advanced HPC Technologies Development Unit

Next-Generation HPC Management Office





#### **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 from institutes in Japan.

#### **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.



#### 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/



