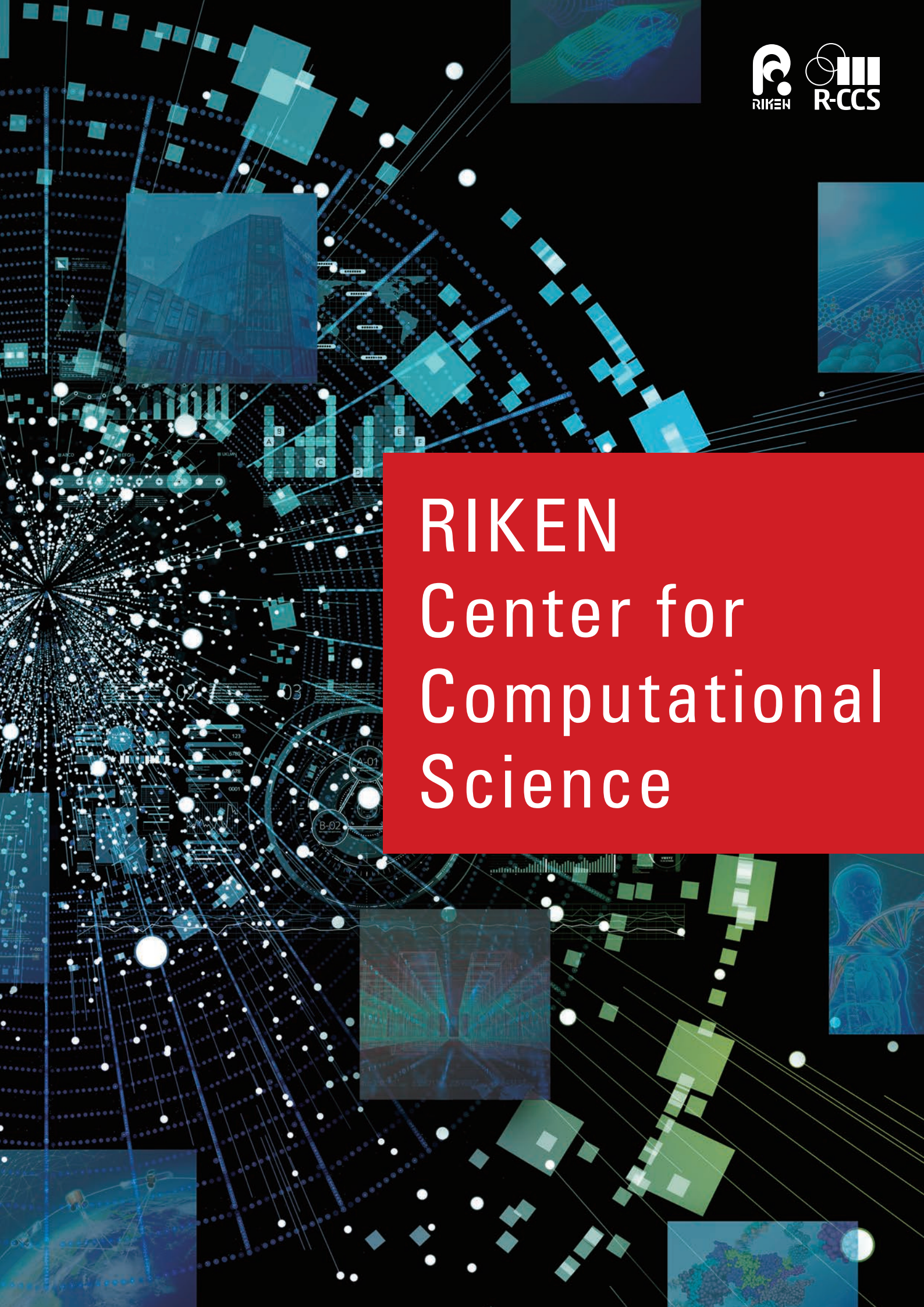


RIKEN Center for Computational Science

Science of Computing, by Computing, for Computing

Director
Satoshi Matsuoka

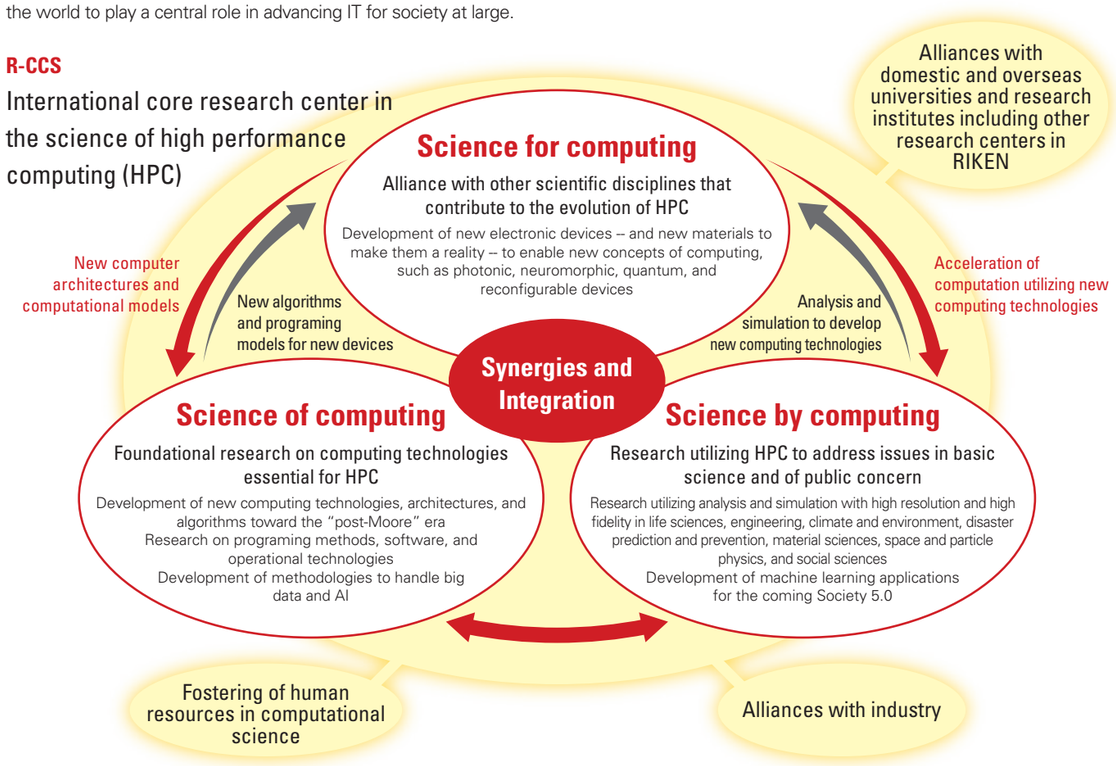
The objectives of the RIKEN Center for Computational Science (R-CCS) are threefold, centered around supercomputing: one is to target high performance computation itself as a scientific objective, or "Science of Computing" ; another is to apply the enormous computational power thus obtained to solve difficult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

Computational science employs multitudes of methodologies to essentially recreate various phenomena as computational activities inside machines, thereby allowing us to challenge difficult problems encountered by mankind. For example, we can model a phenomenon by a set of physical/mathematical formulas, and the machine-driven solution to the formulas will result in direct "simulation" of the phenomenon. Alternatively, we can analyze massive amounts of data gathered on a phenomenon with scientific instruments, and extrapolate future trends, or so-called "data science" methodology. Furthermore, we can train our "artificial intelligence (AI)" to attain higher-level insights on the data, both simulated and/or analyzed. Supercomputers will accelerate all such methodologies by many orders of magnitude, allowing the synthesis of innovations to tackle the most difficult problems confronting society, and R-CCS intends to be at the forefront of such activities.

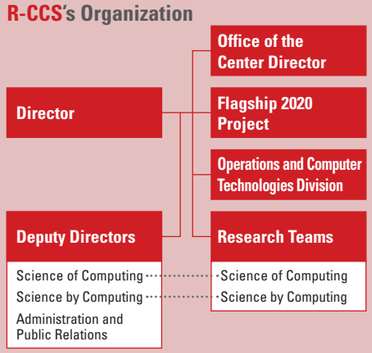
Moreover, research and development of innovative Information Technologies (IT) to advance supercomputing is not only applicable to itself – it is the cutting-edge technology to advance IT as a whole, from Clouds to the Edge. Thus, it will contribute to massive improvements in aspects of the economy and our daily lives that are now heavily reliant on IT. We intend to collaborate with other leadership centers around the world to play a central role in advancing IT for society at large.

R-CCS

International core research center in the science of high performance computing (HPC)



R-CCS's Organization



Flagship 2020 Project
- System Software Development Team
- Architecture Development Team
- Application Development Team
- Co-Design Team

Operations and Computer Technologies Division
- Facility Operations and Development Unit
- System Operations and Development Unit
- Application Tuning Development Unit
- HPC Usability Development Unit

Research Teams

Science of Computing
- System Software Research Team
- Programming Environment Research Team
- Processor Research Team
- Large-scale Parallel Numerical Computing Technology Research Team
- HPC Usability Research Team
- Next Generation High Performance Architecture Research Team
- High Performance Big Data Research Team
- High Performance Artificial Intelligence Systems Research Team

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
- Particle Simulator Research Team
- Computational Climate Science Research Team
- Complex Phenomena Unified Simulation Research Team
- Data Assimilation Research Team
- Computational Disaster Mitigation and Reduction Research Team
- Computational Structural Biology Research Team

R-CCS's Activities

Development of a World-leading Supercomputer

R-CCS is the leading member of the development team for the supercomputer Fugaku, which will supersede the K computer, also developed by R-CCS in collaboration with Fujitsu (see the pages inside for details).

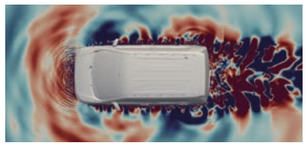
Software Development

R-CCS research teams develop applications, libraries and programming tools for HPC platforms, including Fugaku.

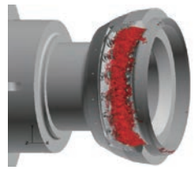
XcalableMP	A programming language designed to improve the performance and the productivity of parallel programming
EigenExa	Software for computation of eigenvalue problems. EigenExa has successfully performed the world's most extensive computation of an eigenvalue problem using all computing processors of the K computer.
GENESIS Generalized-ensemble simulation system	Molecular dynamics and modeling software for bimolecular systems
OACIS	Job management software for large scale simulations
SCALE	Basic library for the analysis and simulation of the climate systems of the Earth and other planets
NTChem	Comprehensive software for *ab initio* quantum chemistry calculations of large and complex molecular systems

Collaboration with Industry

In collaboration with the industrial sector, we established the Consortium for Next Generation Automotive CAE using HPC (CNACH) and the Consortium for Next Generation Combustion System CAE (CNGC). The industry-government-academia collaboration aims to promptly put the R-CCS's achievements into practical application, exchange research information, and share and resolve issues in industry, thereby creating a framework for next-generation manufacturing.



Direct analysis of automobile aerodynamics and acoustics (Courtesy of Suzuki Motor Corporation)



Numerical analysis of combustion flow in aircraft gas turbine combustor

Training Programs

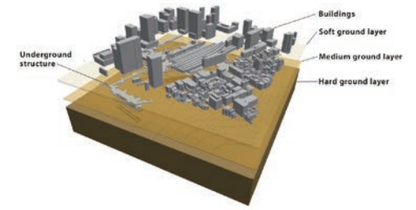
We provide programs for graduate students, early career researchers, and corporate engineers so they can acquire advanced skills in computational science and technology. This helps promote the application of these skills to interdisciplinary R&D and to projects led by the industrial sector. We hold the RIKEN International HPC Summer School, accept interns from Japan and overseas, and conduct other programs.

Notable Achievements since 2018

Director Matsuoka won the Asia HPC Leadership Award at Supercomputing Asia 2019.

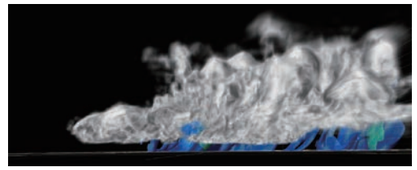
The research group headed by Director Matsuoka received the Best Paper Award at High Performance Computing Conference (HiPC) 2018, an international conference on high-performance computing and data analysis.

Visiting Scientist Tsuyoshi Ichimura and his team created an ultra-high-resolution urban earthquake simulation that combines AI and the latest computational technologies. This earned them a finalist nomination for the 2018 Gordon Bell Prize, awarded to recognize world-leading achievement in applied HPC.



Researcher Atsushi Hori and colleagues proposed a new implementation approach to a third parallel execution model for many-core CPUs. The proposal received the ACM HPDC 2018 Best Paper Award.

A team led by Takemasa Miyoshi conducted research into forecasting sudden torrential rains, using big data assimilation, which won them the Gold Medal at the Yomiuri Techno Forum.



Development of Supercomputer Fugaku

The main goals of Fugaku are to solve various social and scientific issues and to help build "Society 5.0." To this end, Fugaku was developed through co-design of the hardware system and applications in a broad range of fields. Nine target applications were selected from among many candidates, and their characteristics have guided the design of the hardware system. The applications were, in turn, optimized for the hardware system. As a result, application performance is expected to improve up to 100-fold compared with the K computer.

Highlights of Fugaku Computer System

We have been developing the world's best and most versatile system.

We aim to develop the world's most advanced technology that will serve as the international standard through an international collaboration.

We aim to continue K computer's legacy and maintain the competitive advantage in simulation science, and to advance the areas of big data and AI through technological innovation using Fugaku.

Technological Innovations

▷ **Outstanding Computing Performance of the CPU**
The scalable vector extension (SVE) and novel architecture with high-bandwidth memory enable several-fold greater performance of CPUs than that of conventional CPUs in many HPC applications.

▷ **Excellent Energy Efficiency**
The "power knob" and other energy-saving features allow the highest level of energy efficiency in the world as a general-purpose CPU.

▷ **Enriching the "Arm HPC Ecosystem"**
The Arm instruction set is adopted in the Fugaku CPU, making it the most advanced for HPC among all Arm-based processors, of which more than 20 billion units a year are produced. The CPU may be used for cloud computing and IoT in the future. The SVE, designed during Fugaku development, will be a global standard.

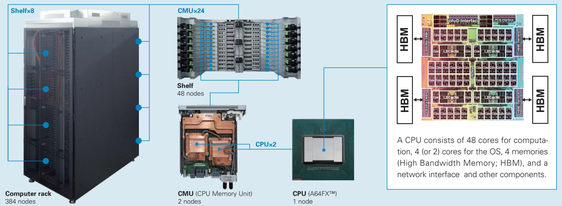
▷ **High Performance for Society 5.0 Applications**
The Fugaku CPU (Fujitsu A64FX™) is expected to provide comparable performance to GPUs for big data and AI/DL applications.

Advances from K to Fugaku

	K computer	Fugaku
CPU architecture	SPARC64™ VIIIfx	A64FX™ (Armv8.2-A, SVE + Fujitsu Extension)
Number of cores	8	48
Peak DP performance per node	0.13 TF	2.7 TF+
Number of nodes per rack	102	384
Main memory capacity	16 GiB	32 GiB
Memory peak bandwidth	64 GB/s	1,024 GB/s
Network performance	20 GB/s	40.8 GB/s
Process technology	45 nm	7 nm FinFET
Power consumption	11 MW	30 - 40 MW (target performance)

Processor Chips and High-density Computer Rack

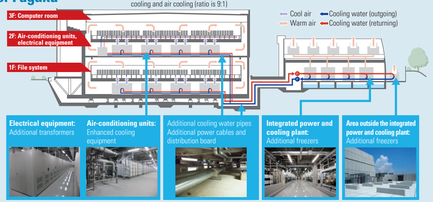
Courtesy of Fujitsu Limited



A CPU consists of 48 cores for computation, 4 (or 2) cores for the OS, 4 memories (High Bandwidth Memory; HBM), and a network interface and other components.

Enhanced Facilities for Fugaku

Fugaku will be installed in the building where the K computer once stood. Most of the facilities for the K computer will be used for Fugaku as well. Since Fugaku will require more electricity and produce more heat waste than the K computer, additional electrical equipment and chillers will be installed. Existing co-generation power plant and high-voltage substation will be used without modification.



Co-design

Science of Computing

Design systems with parameters that consider various application characteristics

Science by Computing

Select representatives from hundreds of applications signifying various computational characteristics

Fugaku

Enabling the world's highest performance and greatest usability

High accelerating ability in large-scale applications

Wide range of use

Target Applications

Nine applications in a broad range of fields with various characteristics were selected to create a highly versatile computer. The R-CCS researchers are conducting research to evaluate and enhance the performance, and to develop new algorithms and methods for implementation. These efforts will maximize the outcomes of the Fugaku project.

- **GENESIS** — Calculates protein conformational dynamics
- **Genomon** — Genome analysis
- **GAMERA** — Analyzes seismic wave propagation in crust and urban areas
- **NICAM+LETKF** — Global atmospheric simulation assimilating Earth observation data
- **NTChem** — Clarifies molecular structures
- **ADVENTURE** — Large-scale computational mechanics simulation
- **RSDFT** — Elucidates properties of materials
- **FrontFlow/blue** — Analysis of turbulent flow and noise
- **LQCD** — Computes properties of elementary particles

Priority Issues

These social and scientific issues were selected in 2014 as priorities for the successor of the K computer. The institutions listed here are engaging in activities to address these issues.

Category		Issues	Organizations
Achievement of a society that provides health and longevity	Priority Issue 1	Innovative drug discovery infrastructure through functional control of biomolecular systems	RIKEN Center for Biosystems Dynamics Research and 6 other institutions
	Priority Issue 2	Integrated computational life science to support personalized and preventive medicine	The Institute of Medical Science, the University of Tokyo and 4 other institutions
Disaster prevention and global climate problems	Priority Issue 3	Development of integrated simulation systems for hazards and disasters induced by earthquakes and tsunamis	Earthquake Research Institute, the University of Tokyo and 4 other institutions
	Priority Issue 4	Advancement of meteorological and global environmental predictions utilizing observational "Big Data"	Japan Agency for Marine-Earth Science and Technology (JAMSTEC) and other 5 institutions
Energy problems	Priority Issue 5	Development of new fundamental technologies for high-efficiency energy creation, conversion/storage and use	Institute for Molecular Science, National Institute of Natural Sciences and 8 other institutions
	Priority Issue 6	Accelerated development of innovative clean energy systems	School of Engineering, the University of Tokyo and 11 other institutions
Enhancement of industrial competitiveness	Priority Issue 7	Creation of new functional devices and high-performance materials to support next-generation industries (CDMSI)	The Institute for Solid State Physics, the University of Tokyo and 9 other institutions
	Priority Issue 8	Development of innovative design and production processes that lead the way for the manufacturing industry in the near future	Institute of Industrial Science, the University of Tokyo and 7 other institutions
Development of basic science	Priority Issue 9	Elucidation of the fundamental laws and evolution of the universe	Center for Computational Sciences, University of Tsukuba and 10 other institutions

Exploratory Challenges

These challenges were selected in 2016 as new projects for the K computer's successor. Research on how to meet the challenges is now in progress.

Exploratory Challenge 1	Frontiers of Basic Science: Challenging the Limits
Exploratory Challenge 2	Construction of Models for Interaction among Multiple Socioeconomic Phenomena
Exploratory Challenge 3	Elucidation of the Birth of Exoplanets [Second Earth] and the Environmental Variations of Planets in the Solar System
Exploratory Challenge 4	Elucidation of How Neural Networks Realize Thinking and Its Application to Artificial Intelligence

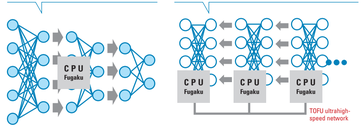
What Fugaku Will Offer

AI & Data Science Research

Next-generation AI created by deep learning will require enormous computational power of large-scale supercomputers. Fugaku is equipped with CPUs with the architecture suitable for convolution computing, which is essential for deep learning, and a high-performance network system. Thus, Fugaku will be the top-rated supercomputer in the world for AI and data science research. At R-CCS, researchers are developing AI applications of the future. Taking advantage of the power of Fugaku, their efforts will advance AI and data science research.

① High performance deep neural network convolution

② High performance and ultra-scalable network for massive scaling model & data parallelism

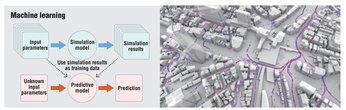


Massive scale deep learning on Fugaku

What Fugaku Will Offer

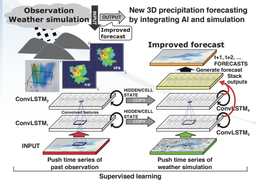
Convergence of High-Performance Computing and AI

R-CCS is pursuing the convergence of high-performance computing and AI in two reciprocal ways: acceleration of simulation with AI, and acceleration of AI with high-performance computing. For instance, AI is used to search parameters needed for a simulation, or to interpolate and extrapolate the trajectories in simulations. Likewise, high-performance computing is used to organize training data for AI and to accelerate the training processes.



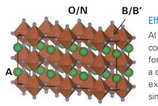
Suggestions for workable evacuation plans

Simulations based on people's behavior and characteristics will enable AI to learn the relationship between people's behavior and evacuation time and efficiency to suggest workable evacuation plans.



New 3D precipitation forecast

State-of-the-art machine learning technology enhances 3D precipitation forecast by integrating precipitation observation and weather simulation.



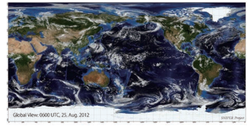
Efficient material design

AI will select the chemical compounds most suitable for a given purpose from a database consisting of experimental data and simulation results.

What Fugaku Will Offer

Simulation

With up to 100-fold improvement in application performance over the K computer, Fugaku allows for higher resolution, longer duration, and more scenarios of simulations. With Fugaku, advances in a wide range of fields are expected, from social issues in our daily lives to fundamentals of sciences.

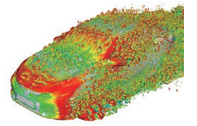


Highly accurate weather forecasts

Global weather simulations allow for accurate prediction of the course and intensity of a typhoon.

Advancing basic science

Movements of all molecules in a cell can be recapitulated to help understand how cells function.

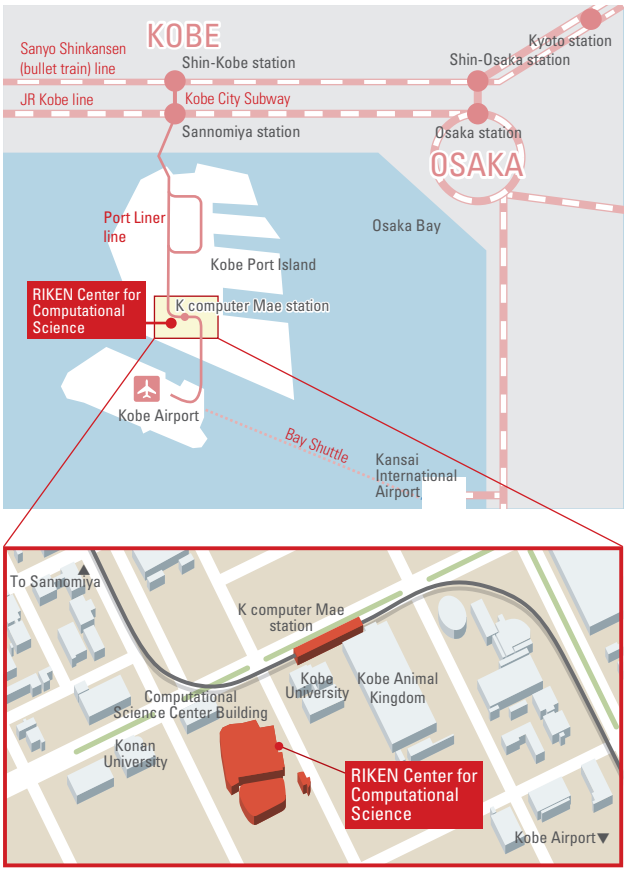


Revolutionizing automobile engineering

Simulations of automotive aerodynamics yield results that far exceed data from wind tunnel tests, greatly improving the efficiency of automobile engineering.

The R-CCS Logo

The three red rectangles in the R-CCS logo represent racks of the supercomputer in the official color of R-CCS. The two circles represent computer science and computational science, expressing the desire to achieve breakthroughs by increasing the specialized knowledge and promoting exchange of ideas. The second "C" is in red to emphasize that it represents both computer science and computational science. The logo symbolizes the commitment of R-CCS to research activities including the development and operation of supercomputers.



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