Logo for “AICS”

The three red rectangles in the AICS logo represent racks of the supercomputer, and use the AICS official red. The two circles represent computer and computational science, expressing the desire to achieve new breakthroughs by increasing our specialization and simultaneously promoting exchanges. The C is written in red to mean that it represents both computational and computer science. The design is meant to emphasize the desire of AICS to develop research activities including the development and operation of supercomputers.

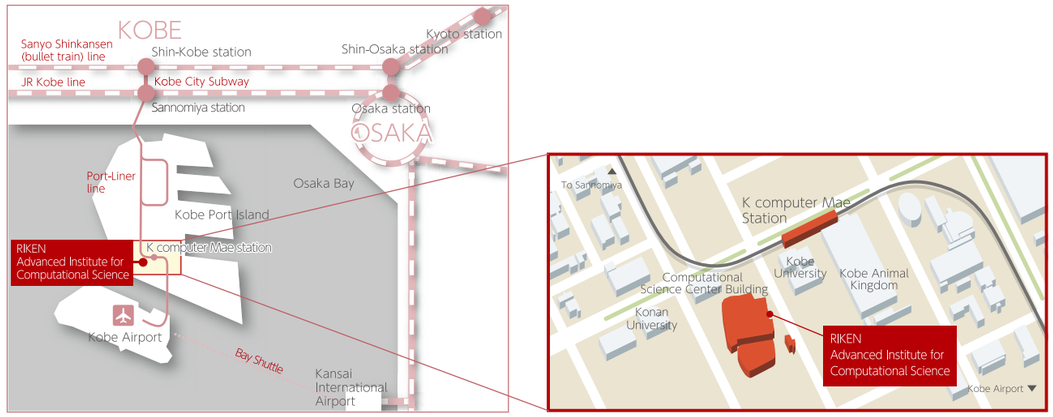
Logo for “K computer”—“京”

In Japanese, the kanji character “京” stands for the number of 10 peta, or 10 to the 16th power, which is the planned processing speed of the computer. The novelty of using a unit for a name made “京” appealing, as did the fact that it was an original name in the domain of science and technology, a field which often gives names and nicknames to new devices. There are some who believe that “京” originally represented a large gate, and that is appropriate too, since the computer represents a new gate to computational science, and the name thus links history with the future. Added to that, the character “京” forms part of “Kei-soku”, which was the unofficial nickname given to the computer at the start of the project, so it is already familiar to those in the computational science community; “京” also seemed the good choice given that kanji characters are full of meaning for Japanese people, who place great value on their sounds and harmony. Since it is only one character, it is simple and easy to understand, and it is also easy for non-Japanese to pronounce. When writing the character for the logo, the popular calligrapher Souun Takeda infused it with the symbolic power of “K computer”— the foundation of Japan’s future in science and technology.

How to Apply to Use the K Computer

In order to use the K computer you must make a project application. Applications can in principle be made by anyone, the qualifications depend on the type of project. For details, please consult the website operated by RIST, the organization responsible for the selection and support for projects on the K computer.

http://www.hpci-office.jp/pages/e_guide/



RIKEN
Advanced Institute for
Computational Science

7-1-26 Minatojima-minami-machi, Chuo-ku,
Kobe, Hyogo 650-0047, Japan
http://www.aics.riken.jp/en/

April 2017

RIKEN 2016-042

RIKEN
Advanced Institute for
Computational Science

RIKEN Advanced Institute for Computational Science

Computer simulations create the future

Computer simulations create the future

While society continues to advance forward thanks to the development of science and technology, we confront ever more serious social problems brought about by rapid change. To confront these many unresolved problems, we must bring together wisdom from around the world and look for the optimal solutions.

To come up with the best solutions to these problems, we must analyze the myriads of elements contained in large volumes of data and recreate the phenomena using computers. It is advanced simulations run on supercomputers that will allow us to look at the future in a scientific way using this science of forecasting.

The RIKEN Advanced Institute for Computational Science (AICS), which is at the forefront of simulations, is charged with the development and operation of the world leading K computer, and is contributing both to the solution of social problems and the raising of industrial competitiveness. AICS is currently working on the co-development of the architecture and applications of the post-K computer, the successor to K, with the goal of being able to perform unprecedented simulations.

Simulations will bring us strength and hope for the future, by helping us to take on the challenges confronting us and achieving breakthroughs that are difficult to even imagine.

Director, AICS
Kimihiko Hirao

Director's Message

The supercomputer is an essential tool for contemporary science and technology. The potential it offers for expanding basic research in areas such as cosmology, elementary particle physics, and the life sciences has been clearly demonstrated. But the supercomputer is equally essential for the development of a wide range of advanced science and technology that is directly related to our daily lives, including scientific global warming forecasts, simulations that will help to minimize damage from earthquakes, tsunamis, torrential rains, typhoons and other natural disasters, genome analysis for gene therapy and protein analysis for drug design, the development of new devices and materials, car crash simulations, jet engine design, and much more.

AICS was founded in July 2010 with the objective of helping the science of forecasting to flourish based on computer simulation. To this end, we are managing the operation of the K computer by maintaining a user-friendly environment and promoting collaborative projects with a focus on the disciplines of computational science and computer science.

After overcoming obstacles such as the disastrous earthquake of March 11, 2011, the K computer was able to take first place in the TOP500 ranking in June and then November 2011. Recently it took top place in Graph500 and HPCG, two new rankings of performance. In addition to its blistering speed and performance, it was designed with ease-of-use in mind, and has gained attention as one of the world's top supercomputers for a wide range of scientific applications.

The K computer today is being used in a wide range of research areas from basic to research to industrial use, and has been responsible for many significant results in the areas prescribed by the government's HPCI Strategic Program as well as by public users. It is also heavily used by private firms and collaborative researchers, leading in some cases to the commercialization of new technologies.

Various joint projects are currently underway to make use of the K computer efficiently. In the strategic field program, priority issues, experts from supercomputer facilities, research institutes, universities and industry have come together to exchange views and carry out research. They are trying to resolve challenging issues, thereby achieving scientific and technological breakthroughs which will help to strengthen Japan's industrial base and solve global issues.

Our goal is to take full advantage of the K computer's capabilities to push Japan to the forefront of computational science and enhance our nation's competitiveness by creating a converging point of global knowledge that will attract scientists from around the world. We hope to live up to the expectations of the Japanese people and the international community by producing exciting results that will amaze the world.

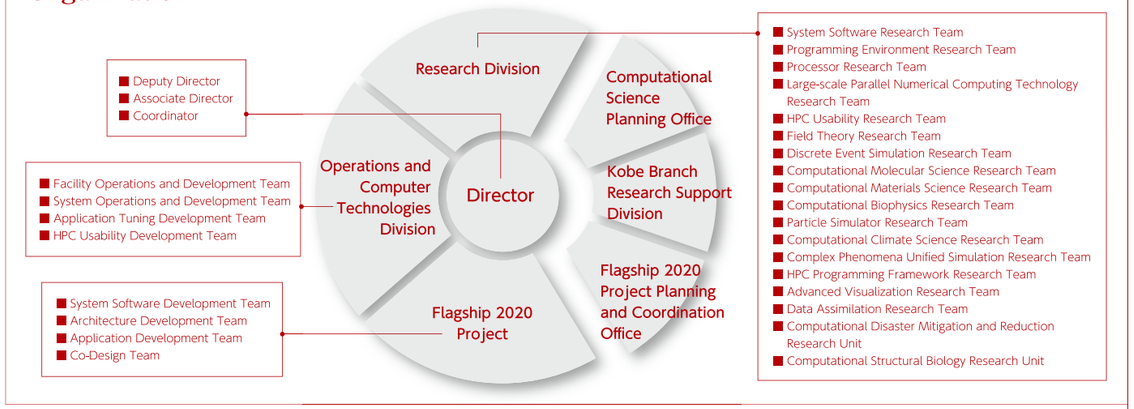
RIKEN has been selected to be the development body of the FLAGSHIP 2020 Project. AICS now has two important missions: one is continuing to operate and manage the K computer and to generate cutting-edge scientific results and technological breakthroughs. The other is to successfully develop the next generation post-K computer. We ask for your support as we work to further expand our programs.

Basic concepts of AICS

AICS aims to establish the science of forecasting based on computer simulation. To this end, AICS does the following:

- Manage the operations of the K computer and maintain a user-friendly environment.
- Generate cutting-edge scientific results and technological breakthroughs by promoting collaborations and the integration of computational and computer science as an international center of excellence.
- Develop the post-K supercomputer and application software for it based on a roadmap for the future of computational science.

Organization



System

What makes the K computer system special?

- It is based on Japanese technology and know-how, developed jointly by RIKEN and Fujitsu
- Over 10 petaflops (LINPACK) performance
- Highly reliable system
- Useful for calculations in a wide range of fields, with ability to make petaflops performance available for real applications.

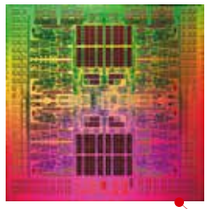
・The system uses CPUs (SPARC64TM VIIIfx, 8 cores, 128 gigaflops) manufactured with 45nm CMOS process technology. To achieve high performance and high scalability to ultra-large-scale systems, the CPU additionally supports SIMD (Single Instruction and Multiple Data) processing, and is furnished with functions for instruction retry as exhaustive error detection/correction, contributing to high performance and reliability in application execution in an environment with huge numbers of CPUs.
・The network between the compute nodes consists of a direct-connection network※1, ensuring high flexibility and scalability and enabling ultra-large-scale connectivity. Users can create application programs adapted to either a one-, two- or three-dimensional torus network, contributing to improvements in usability, fault-tolerance and interoperability.
・With its water cooling system, the K computer maintains a low temperature in the CPU and other LSIs, minimizing the failure rate and reducing power consumption.
・It executes over 300,000 jobs per year. It is operated at the high system usage.※2 (ex. 93.3% in FY2014)
・It offers one of the world' s largest disk storages.

※1 There are two styles of networks, direct-connection networks and indirect-connection networks. In a direct-connection network, the entire network consists of numerous connections between pairs of nodes. In an indirect-connection network, a switch sits between multiple nodes. A three-dimensional torus network is a kind of direct-connection network where the nodes are organized into a three-dimensional structure, and each is linked to six others, forming a ring structure on each dimension.
※2 Excepting scheduled maintenance

Specification

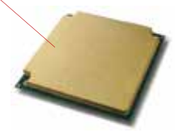
Performance (peak)	10.62PFLOPS	Peak bandwidth	5GB/s×2	CPU	82,944
Total Memory Capacity	1.26PB (16GB/node)	Bisection bandwidth※3	30TB/s	Core	663,552
Network	Tofu interconnect (Logical 3-dimensional torus network)				

※3 Bisection bandwidth is an available bandwidth between the two partitions



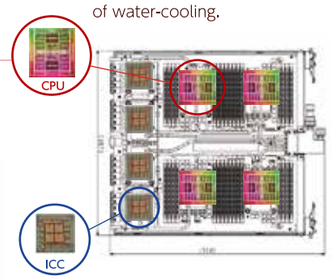
SPARC64™ VIIIfx

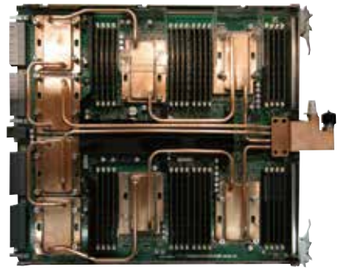
CPU



System board

Four CPUs and four ICCs are mounted on a system board. The metal parts are a module of water-cooling.

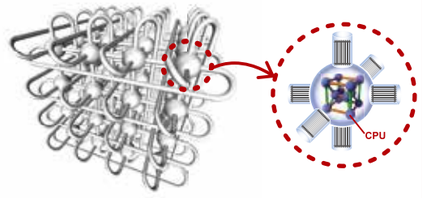




Courtesy of Fujitsu

Rack

Each rack houses 24 system boards, 12 at the top and 12 at the bottom.



Innovative network: Tofu
(6D mesh/torus interconnect)

System

There are 1080 racks on the third floor of the supercomputer room (864 system racks and 216 disk racks).

Awards

(Nov. 2016)

First place in TOP500!

The TOP500 list ranks computers based on their performance on LINPACK, a benchmark program that requires computers to solve a dense system of linear equations, which is a very regular calculation. The K computer took first place in June and November 2011.

First place in HPCG!

HPCG is a new supercomputing ranking that evaluates how they solve symmetric sparse linear system equations, a type of calculation that is frequently used in applications for industry. The K computer took the top spot in November 2016.

First place in Graph500!

The K computer has taken first place as well on the Graph500 ranking, which evaluates the capability of computers to handle big data by performing a breadth-first search in a large undirected graph. It has taken first place on five lists during the period from June 2014 to November 2016.

Winner of the Gordon Bell Prize!

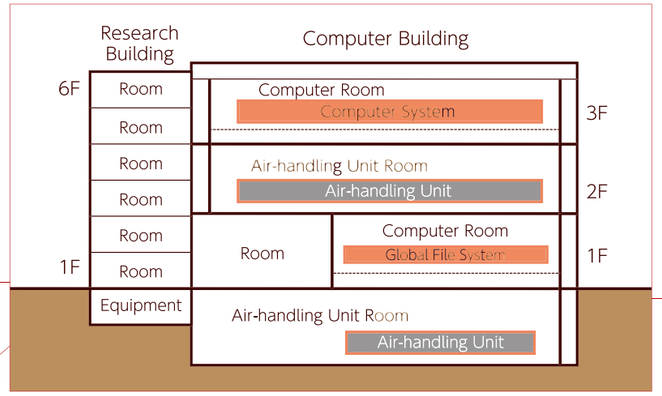
This award is given for publications based on excellent achievements in developing either hardware or applications. The award was set up in 1987 by Gordon Bell, a renowned American computing scientist, to promote the development of parallel processing technology. Work done on the K computer received the award in 2011, for calculations of the electronic state of silicon nanowires, and in 2012 for work on the gravitational evolution of dark matter in the early Universe.

First place in the HPC Challenge Awards!

This benchmarking program uses 28 items to evaluate the overall performance of supercomputers from a variety of angles. There are two classes, one where computers compete for performance under the benchmark and a second where the elegance of programming languages for using the benchmark is evaluated (for class 1, awards are given in four different areas). Work on the K computer has gained both prizes.

Facilities

Leading-edge technology provides the infrastructure for K computer's stability



< Site Area > Approx. 2 ha (semi-industrial zone)
<Power Utilities> 77 kV high-voltage power substation, with co-generation station (approx. 5MW)
<Cooling Facilities> Steam type absorption refrigerator (Waste heat recovered from co-generation system)
High-efficiency inverter turbo cooling unit.

Earthquake and Salt Resistant and Durable Facility

- K computer consists of 864 cabinet racks, at approximately 1,350 kg per cabinet. (In addition, 216 cabinet racks of magnetic disks are installed.)

Bringing out the best performance of the K computer and keeping it running

◆Foundation

- Ground improvements of the reclaimed area (20 m) were conducted to build up soil bearing capacity and as a countermeasure against liquefaction (Kobe City) .
- 2m spread foundation + settlement-control pile foundation, using the improved area as a base supporting layer.

◆Earthquake Resistance

- The Research Building and Computer Building are base-isolated structures.
  Laminated rubber base isolators are installed at 49 locations.
  In addition, lead dampers and U-shaped stiffness dampers are installed to quickly suppress earthquake vibrations.
- Earthquake resistance grade S (Main functions can be maintained even if a large earthquake with JMA scale intensity of 6-upper occurs.)

◆Durability (Salt Damage Countermeasures for Coastal Zone)

- Anti-corrosion measures are implemented in important structures.
- Components with superior salt damage resistance are used: aluminum panel outer walls for the Computer Building, glass outer walls for the Research Building.

◆Structure of the Computer Room

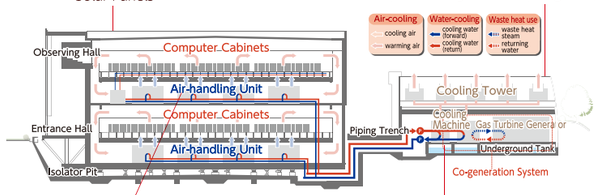
- The computer room does not have any pillars, in order to accommodate shorter lines and uniformity during interconnections in the supercomputer and to secure flexibility in installation layout.
- Floor load capacity is 1 ton/m^2 for the floor with computers.

Environmental Considerations

Reduction of Running Costs and Environmental Load

Solar Panels

Cooling Source Building
(Shape enhancing sound dissipating effect)



Combined Air-water Cooling System
(Building Scheme)

Air-handling Unit

Cooling Source Building

◆ Energy Savings

- Highly efficient devices are employed (top runner system) to achieve performance target to be the most energy-efficient device (top runner) or higher.
- Waste heat from power co-generation is effectively utilized.
  - ✔ Waste heat is recovered and reused for cooling and heating the facility.
  - ✔ Energy use is highly efficient (overall efficiency ≥ 75%) and better than commercial thermal power generation.
- Solar panels are installed on the computer building roof, generating 50 kW maximum power.

◆ Air Conditioning System in Computer Room

- A hybrid cooling system, using combined air-water cooling, is used in the computer cabinets to efficiently remove generated heat.

◆ Reuse of Rainwater and Blow-down Water in Cooling Tower

- Water is reused for plant irrigation and lavatories.
- Water is stored in multi-purpose water tanks in underground pits and used as water supply for various areas.

◆ Noise Reduction

- Consideration for the surrounding environment is given through a building shape that enhances the sound dissipating effect.

Research

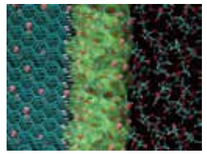
Some examples of scientific results using the K computer

Multi-scale Multi-physics Heart Simulator UT-Heart

A human heart model, which can function like a real heart both physically and biologically, was created on the K computer. Starting from the movements of molecules within cells, it seamlessly linked the contraction/relaxation of the muscle, the pulsation of the heart and the resultant blood flow to perform the simulation.

HPCI SPIRE Field 1
UT-Heart, Inc., Fujitsu Limited, RIKEN

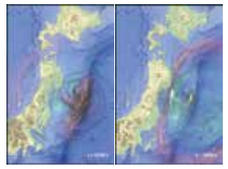
Using the K Computer to Elucidate the Circulation Between the Electrolyte and Electrodes and Film Formation in a Lithium Ion Battery



Extensive DFT-MD simulations on the K computer have revealed the atomistic mechanisms of electrolyte decomposition and subsequent interphase (SEI) film formation, which are crucial for the performance and safety of lithium ion batteries.

HPCI SPIRE Field 2
National Institute for Materials Science, Yoshitaka Tateyama, Keitaro Sodeyama and FUJIFILM Corporation, Yukihiro Okuno, Keisuke Ushirogata / J. Am. Chem. Soc. 2013, 135, 11967–11974.

Seismic- and Tsunami-Wave Propagation of the 2011 Off the Pacific Coast of Tohoku Earthquake derived from the Tsunami-Coupled FDM Simulation



A simulation was performed to simultaneously synthetize the strong shaking, ground motion, and resultant tsunami from a powerful earthquake. The K computer allowed for an algorithm to be developed for earthquake tsunami, so that the shaking and tsunami could be calculated simultaneously.

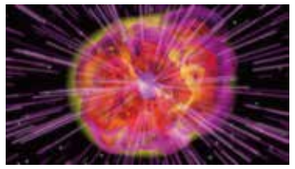
HPCI SPIRE Field 3
Earthquake Research Institute, The University of Tokyo, Maeda Takuto, Furumura Takashi / Maeda et al., Bull. Seism. Soc. Am., 2013, 103, 1456–1472.

Automobile Drag Simulation: Recreating the Flow of Air around a Moving Car

The development of vortices in the air around a moving vehicle has an impact on the fuel consumption and driving stability. By modeling the movement of a vehicle and flow of air around it, the K computer makes it possible to look simulate tiny vortices that could not be modeled previously.

HPCI SPIRE Field 4
Kobe University, Hiroshima University, RIKEN AICS, MAZDA Motor Corporation

K Computer Simulation Provides Support for Theory that Neutrino-Heating Is Involved in Supernovae



Using the K computer, researchers performed large-scale simulations demonstrating the possibility that supernovae are triggered by a neutrino-heating mechanism. In this study, the researchers performed the calculation under a natural assumption close to the real situation, and found strong evidence to support the neutrino-heating hypothesis.

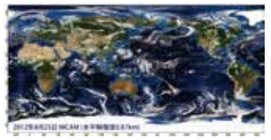
HPCI SPIRE Field 5
Tomoya Takiwaki, Kei Kotake, Yudai Suwa ©NAOJ

Tire Technology Developed Using K Computer Revealed at Motor Show

Using a simulation on the K computer, scientists examined data on the high-resolution internal structure of rubber and its molecular movements from the SPring-8 synchrotron facility and J-PARC proton accelerator facility, to reveal the mechanism of breaking and heating inside rubber.

Sumitomo Rubber Industries, Ltd.

Deep Convections Are Realistically Simulated in the First Ever Sub-kilometer Global Simulation by Using K Computer



We successfully conducted the first ever global atmospheric simulation with 0.87 km grid spacing and described the convection features. This will advance the understanding the mechanisms of cloud disturbances (e.g. Tropical cyclone) which are sometimes accompanied by heavy rainfall and cause the severe disaster.

JAMSTEC and AORI/The University of Tokyo (HPCI SPIRE Field3) collaboration with RIKEN AICS. Visualized by RIKEN AICS, Computational Climate Science Research Team, Ryuji Yoshida.

Outline of development of the post-K computer

RIKEN was selected to carry out development of the post-K computer designed to be the successor of the K computer under the Ministry of Education, Culture, Sports, Science, and Technology's FLAGSHIP 2020 Project. We are currently engaged in the development work with the aim to launch the new computer around 2020.

Top priority on problem-solving research

During development, highest priority will be given to creating a system capable of contributing to the solution of various scientific and societal issues. For this, the hardware and software will be developed in a coordinated way (Co-design), with the aim to make it usable in a variety of fields.

World-leading performance

Create the most advanced general-use system in the world.

Improve performance through international cooperation

While leveraging Japan's strengths, cooperate internationally to achieve world-leading technologies of the highest quality and become the international standard.

Continue the legacy of the K computer

Make the fullest use of the technologies, human resources, and applications of the K computer project for developing the post-K system.

Research Subjects of the post-K computer

The Ministry of Education, Culture, Sports, Science and Technology has chosen AICS to develop the post-K computer which is expected to lead the world in research outcomes.

Health and longevity

Priority Issue 1

Innovative computing infrastructure for drug discovery

RIKEN Quantitative Biology Center, and 6 other institutions

Priority Issue 2

Personalized and preventive medicine using big data

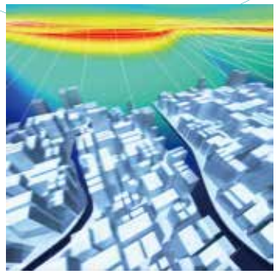
The Institute of Medical Science, the University of Tokyo, and 4 other institutions

Disaster prevention / Environment

Priority Issue 3

System for integrated simulation of earthquake and tsunami hazard and disaster

Earthquake Research Institute, the University of Tokyo, and 4 other institutions



Priority Issue 4

Meteorological and global environmental predictions using big data

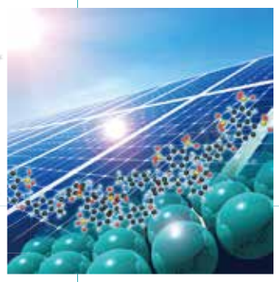
Japan Agency for Marine-Earth Science and Technology (JAMSTEC), and other 5 institutions

Energy issues

Priority Issue 5

New technologies for 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

Industrial competitiveness enhancement

Priority Issue 7

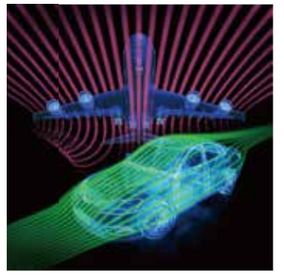
Creation of new functional devices and high-performance materials

The Institute for Solid State Physics, the University of Tokyo, and 9 other institutions

Priority Issue 8

Development of innovative design and production processes

Institute of Industrial Science, the University of Tokyo, and 7 other institutions

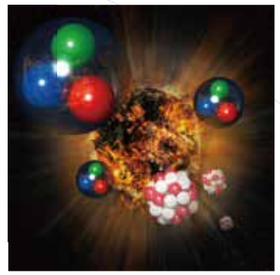


Basic science

Priority Issue 9

Elucidation of the fundamental laws and evolution of the universe

Center for Computational Sciences, University of Tsukuba, and 10 other institutions

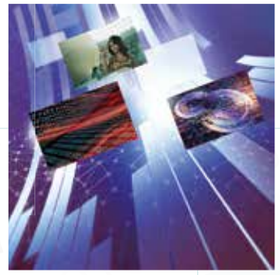


Exploratory Challenges

Four project areas are now under consideration based on survey research for challenges to be undertaken on the post-K computer.

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 Earths) 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