Special Contribution
Japan's K computer Project

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1. Introduction

The TOP500 List of the world's most powerful supercomputers is announced twice a year, in June and November. Japan's K computer,[note)] which is being jointly developed by RIKEN and Fujitsu Limited, surprised the world on June 20, 2011, when it was ranked the world's top supercomputer, achieving a LINPACK benchmark performance of 8.16 PFLOPS despite being only partially completed. ("FLOPS" is the number of floating-point calculations that can be performed per second. PFLOPS, where "P" corresponds to "peta," is equal to 10^{15} FLOPS.) This score far surpassed that of the other computers on the list. The entire K computer, from the processors at its heart to its main components such as boards, racks, interconnects, and cooling equipment, is the culmination of a unified effort within Japan, from development to manufacturing. Indeed, it is a pure, homegrown supercomputer. The power of a supercomputer is broad in nature, and for a nation, it can be an index of its scientific, technical, and manufacturing abilities. By taking the top position on the TOP500 List, the K computer reflects the high level of Japanese science and technology and the robust state of *monozukuri* (innovative manufacturing and engineering) in Japan.

A high execution efficiency of 93% and 28 consecutive hours of operation without a failure during LINPACK measurements have demonstrated the high stability and reliability of the K computer. Development of the K computer, which is a general-purpose supercomputer slated for use in a wide variety of fields, began with the aim of achieving the world's most advanced, top-performing supercomputer at 10 PFLOPS by its completion date of June 2012. Yet, in November 2011, the K computer achieved a performance level of 10.51 PFLOPS, surpassing its score in June of that year. At that level, the K computer was again ranked No. 1 in worldwide supercomputer performance, thereby taking the top position on two consecutive TOP500 Lists.

In 2002, when Japan's supercomputer known as the Earth Simulator became the fastest in the world, topping supercomputers in the United States, it was viewed by some as a threat to the dominant position that the United States had held throughout the world in science and technology. For this reason, the Earth Simulator came to be called "computnik" in reference to the Sputnik satellite of the former Soviet Union that came as a surprise and a shock to the United States at the time of its launch. However, the ten-year period following the appearance of

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note) "K computer" is the English name that RIKEN has been using for the supercomputer of this project since July 2010. "K" comes from the Japanese word "Kei," which means ten peta or 10 to the 16th power.

the Earth Simulator saw a drop in Japan's international competitiveness in a number of areas. Japan's supercomputer was no exception, and its ranking in the TOP500 dropped. It was during this time that Europe and the United States came to realize the important role of the supercomputer in science and technology and accordingly took on supercomputer development with an all-out effort. In recent years, China as well has undertaken the development of supercomputers for the welfare of the nation.

International competition in supercomputer development is now intense. The reason is clear: the supercomputer is an indispensable tool for advancing science and technology in the modern age and increasing the international industrial competitiveness of a nation. A cutting-edge supercomputer is essential to acquiring knowledge and making discoveries in the natural sciences and performing advanced simulations. It is a necessary tool for taking science to a new level, driving technical innovation, and developing new products. The supercomputer is vital to the research and development of groundbreaking science and technology directly connected to everyone's life. This includes, of course, fundamental science, such as studies on the formation of the universe after the Big Bang, the research of elementary particles, the search for new quantum phases in material science, and the explanation of complex biological phenomena. But a supercomputer can also be used to make predictions about global warming, reduce harm to people and damage to property by predicting earthquakes, tsunamis, torrential rainfall, and typhoons or hurricanes, analyze the human genome to provide a basis for gene therapy, discover new drug candidates by protein analysis, design new substances, develop new devices and materials by simulations at the atomic level, perform automobile collision simulations, and design jet engines.

The K computer is scheduled to be completed in June 2012 with shared use of its facilities to begin in the fall of 2012. A great number of people eagerly await access.

2. Project overview

In 2006, Japan initiated a development project for the next-generation supercomputer "the K computer" as a critical technology for the nation. The goals of this project were as follows:

1) Develop and install the most advanced and powerful supercomputer in the world with a LINPACK performance of 10 PFLOPS
2) Generate breakthroughs in science and technology and boost Japan's international industrial competitiveness by making maximum use of the K computer
3) Establish a world-class research and educational institute for computational science in the city of Kobe

This project envisioned supercomputer use in a wide range of fields in computational science and technology. To this end, the Japanese government began promoting supercomputer-related strategic programs in fiscal year (FY) 2009. It selected five key fields with the aims of achieving breakthroughs in science and technology through strategic use of the K computer and of establishing a nationwide system for supporting science and technology in those fields into the future. These five strategic fields of fundamental research are 1) life sciences including drug manufacture, 2) new materials and energy generation, 3) disaster prediction and prevention in relation to climate change, earthquakes, tsunamis, etc., 4) next-generation *monozukuri,* and 5) research of the universe and elementary particles and astronomy-related studies. For each of these fields, the aim is to reach a world-class level of research and to take that research to even higher levels through the use of the K computer.

The next-generation supercomputer project received its budget in FY2009, and in addition to the three goals described above, it also aimed to create and promote the use of a high-performance computing infrastructure (HPCI) centered about the K computer to meet the diverse needs of users seeking supercomputer processing. The HPCI Consortium was launched in FY2010 to oversee the construction of an HPCI, and specific preparations have since been taken toward the formal inauguration of an HPCI and the start of operations in FY2012. As the core institute of the HPCI Consortium, the Advanced Institute for Computational Science described in the next section is expected to play a central role in the expansion of computational science and technology across Japan.

3. Advanced Institute for Computational Science

RIKEN established the Advanced Institute for Computational Science (AICS) in July 2010. It is an organization charged with operating and managing the K computer and pursuing research and development in computational science and computer science. At AICS, coordination and collaboration between computational science and computer science is expected to drive research and development on a shared infrastructure in a wide variety of fields in computational science and technology, research and development of high-performance computational techniques to make full use of the K computer, and fundamental research and development that looks 10 and 20 years into the future. AICS aims to create a new field of study called "interdisciplinary computational science" and seeks to become a driving force behind computational science and technology in Japan as well as a world-class research and development institute. Maintaining a top position in science and technology in the world is closely related to maintaining national security. Japan seeks to be a country with a sense of presence in the international community through science and technology rooted in Japanese culture and sensitivity. As part of this effort, AICS seeks to make a significant impact.

The massively parallel and high-performance computer systems now being developed require advanced computational techniques to enable the benefits they offer to be exploited. The K computer is an ultra-advanced supercomputer, and if Japan is to promote computational science centered about this computer, creating an institute to nurture advanced research and to develop highly competent personnel is a matter of urgency. This makes it important that research and development in computational science be linked with related fields such as computer science and mathematical science. Taking an interdisciplinary approach to such a variety of fields is the key to making progress in computational science and creating new theories and techniques. This approach is centered about a common axis formed by shared algorithms, infrastructure software, methodologies, modeling, common techniques, numerical analysis, and architecture. An infrastructure for developing and utilizing a massively parallel computer must be constructed without delay to enable the use of future computers on the "exa" scale (100 times 10 peta; i.e., 10^{18}) and beyond, and whether the K computer—the forerunner of those future computers—can be used at an advanced level is a key enabler in that endeavor. At the same time, broadening the range of computer use is essential to advancing simulation techniques, and promoting an ongoing program of systematic research and personnel development is indispensable given the future evolution of computers. Although progress in developing massively parallel systems is anticipated, it is clear that research in conventional fields and areas is limited by the inherent inability of such research to make effective use of massively parallel computers. From a medium- to long-term perspective, ongoing research and development in computational techniques, computer systems, and computational science is essential to driving next-generation computational science beyond the use of the K computer.

The Research Division of AICS consists

of research and development teams grouped under computational science and computer science. **Table 1** lists the fields of research. The computational science department has been organized to provide a comprehensive, cross-sectional view of the main methodologies of computational science with the aim of constructing a shared infrastructure for advanced use of the K computer. This department consists of the following research and development teams covering the fields of quantum systems, particle systems, continuous systems, complex systems, and discrete systems.

- Computational Materials Science Research Team
- Computational Molecular Science Research Team
- Computational Biophysics Research Team
- Particle Simulator Research Team
- Field Theory Research Team
- Discrete Event Simulation Research Team (tentative)
- Computational Climate Science Research Team
- Complex Phenomena Unified Simulation Research Team

The research and development teams making up the computer science department, meanwhile, interface with the computational science teams to research and develop high-

Table 1
AICS Research Division.

Computational Science Provide a shared infrastructure to support a wide range of fields in making sophisticated use of the K computer by covering the major methodologies required by computational science.	Quantum	Computational Materials Science Research Team
		Computational Molecular Science Research Team
	Particle	Computational Biophysics Research Team
		Particle Simulator Research Team
	Continuous	Field Theory Research Team
	Discrete	Discrete Event Simulation Research Team (tentative)
	Complex	Computational Climate Science Research Team
		Complex Phenomena Unified Simulation Research Team

Common Area Branch Develop advanced techniques and technologies as a common research infrastructure in the computer and computational sciences, promote the computer and computational sciences, and help accelerate sophisticated use of the K computer.	HPC Programming Framework Research Team
	Advanced Visualization Research Team
	Data Assimilation Research Team (tentative)

Computer Science Solve issues surrounding the K computer by covering main elemental computer technologies.	System Software Research Team
	Programming Environment Research Team
	Processor Research Team
	Large-scale Parallel Numerical Computing Technology Research Team
	HPC Usability Research Team

performance computational techniques that make optimal use of next-generation supercomputers as well as computational techniques, software technologies, and computer systems to support next-generation and beyond computational science. These teams are summarized below.

- System Software Research Team
- Programming Environment Research Team
- Processor Research Team
- Large-scale Parallel Numerical Computing Technology Research Team
- HPC Usability Research Team

Three other research and development teams in this department (listed below) aim to develop advanced techniques and technologies as a common research infrastructure in the computer and computational sciences and to research visualization techniques, library development, and data assimilation to accelerate progress in the computer and computational sciences and to promote advanced use of the K computer.

- HPC Programming Framework Research Team
- Advanced Visualization Research Team
- Data Assimilation Research Team (tentative)

4. Need for cross-field collaboration and interdisciplinary computational science

It is important that an interdisciplinary computational science be established and continuously developed as a new scientific area to open up unexplored fields by using the K computer and applying computational science.

Interdisciplinary computational science has two shades of meaning with regard to "interdisciplinary." To begin with, advanced computational techniques are essential to making optimal use of large-scale, high-performance computer systems, and without the collaboration and cooperation of computer-science researchers, breakthroughs in computational science will be hard to come by. Next, with regard to the future of computational science, it is extremely important to think about the kinds of computer systems that will be needed to solve future problems in computational science. As a result, the ongoing research and development of computational techniques, computer systems, and computational science through the collaboration and cooperation of computational science and computer science is becoming a pressing issue.

It is a matter of urgency to establish an interdisciplinary computational science that, in addition to promoting convergence between the computational and computer sciences, can also handle the various fields of computational science in an interdisciplinary manner. Computational science, in which methodologies, modeling, common techniques, and numerical analysis form a common axis, is inherently capable of handling a variety of scientific fields in an interdisciplinary, comprehensive manner. Computational science is none other than an interdisciplinary field that can cut through highly fragmented research fields with the spear of "computational techniques." Computational science can mediate between various sciences and promote convergence and collaboration between fields.

The goal of AICS is to promote convergence and collaboration between the various fields in computational science and collaboration and cooperation between computational science and computer science under the concept of "interdisciplinary computational science." It aspires to enhance the results of infrastructure-related research and development and thereby support a wide range of fields in computational science and those of research and development of high-performance computational techniques that can make optimal use of the K computer.

5. Use of supercomputers

The use of supercomputers is not limited to academia—they can be applied to production in the corporate world and to real-world problems. In the field of drug development, the astounding leaps in supercomputer performance are enabling researchers to design drugs for cancer, lifestyle-related diseases, and other conditions. Drug-discovery technologies using simulation are suddenly accelerating. David Shaw, a former science advisor to the president of the United States, has developed a specialized supercomputer called Anton for developing drugs. Using Anton, he is dynamically simulating protein behavior on the millisecond level and attempting to make the discovery of drugs by computer simulation a reality. This development might be called the "Anton shock." It is, in actuality, part of a worldwide trend in which supercomputers are coming to be applied to all sorts of fields in addition to drug discovery. Indeed, the supercomputer is taking on an increasingly bigger role in increasing the international competitiveness of corporations as reflected by the increasing number of supercomputers owned by private companies. More than half (57%) of the supercomputers on the TOP500 list as of November 2011 are maintained by private companies.

In Japan, the importance of computational science and simulation in industry has not necessarily been recognized to a sufficient degree, and, as a result, the use of private supercomputers has been limited to only some business fields and major corporations. However, the appearance of the K computer is making a big change to this situation. In fields like *monozukuri*, material development, and energy, in which Japan has traditionally demonstrated much strength, the use of supercomputers has jumped, and various initiatives have begun to widen Japan's international lead in these fields. There are great expectations surrounding these efforts.

6. Collaboration and cooperation with strategic institutions

A major goal of the K computer project is to have supercomputers used in a wide range of fields in computational science and technology. To this end, the Kobe complex centered about the K computer must provide attractive facilities to researchers, which means that a mechanism and environment conducive to the proactive use of the K computer as a research and development platform and to the attainment of outstanding results must be constructed. The complex must be more than simply a computation center—it must be an R&D base that promotes learning in computational science and computer science and the creation of new fields.

Strategic institutions will be responsible for implementing the strategic programs for the five previously mentioned fields of fundamental research selected by the Japanese government. Each institution will each be asked to

- Produce world-class research results in their strategic field through effective and strategic use of the K computer and the computational resources in that field, and
- Construct a system centered about that institution to promote and drive research beyond the K computer project.

At the same time, the role of AICS will be to

- Maintain, manage, and enhance the K computer and enable strategic-program users and others to use the supercomputer in an effective and efficient manner
- With an eye to effective use of the K computer and future developments in computational science and technology, research and develop shared-infrastructure issues, research the convergence of fields, open up new fields that hold future promise, and provide a leadership role in computational science and computer science
- As an interdisciplinary research institute, help build a stronger computational science and technology community and contribute

to a comprehensive future vision of computational science and technology.

Each strategic field will be provided research space at AICS, and plans are being made for accommodating a number of researchers on a full-time basis and many researchers and students for short-term stays and visits. Close interaction between these researchers and students and the research teams at AICS is expected to promote not only research in each of the strategic fields but also research that extends beyond traditional research boundaries and research that straddles computational science and computer science.

7. AICS and HPCI Consortium

Since its reevaluation in FY2009, Japan's next-generation supercomputer project has been reorganized to construct and promote the use of an HPCI centered about the K computer to support diverse user needs.

Leading this construction of the HPCI is the HPCI Consortium, whose members include user communities involved in Japan's computational science and computer science and institutions providing computational resources.

The basic philosophy of the HPCI Consortium can be summarized as follows:

- Be open to all users wishing to use the HPCI
- Engage in cooperative activities with the aim of producing world-class results and recirculating those results back to society with a focus on promoting computational science and technology in Japan
- Build and operate an HPCI system that interconnects computational resources throughout the country as a foundation for supporting the above activities into the future

With the above in mind, the HPCI Consortium will pursue the following activities:

- Setting up and operating an HPCI system
- Consolidating opinions of the computational science and technology communities and making proposals accordingly (including proposals on the operating policies and facility planning of institutions providing computational resources from the viewpoint of world-class standards)
- Promoting computational science and technology (nurturing and expanding computational science and technology and application techniques, creating new fields and user communities, and developing personnel)
- Studying future supercomputing

8. Conclusion

Simulations performed on the K computer will drive progress in science and technology and play an important role in solving difficult problems that we face as a society. Simulations should not only be able to reproduce and explain phenomena but should also be able to predict phenomena. The K computer is making this possible. In addition to problems in the natural sciences, we can envision simulations of the future to boldly take on pressing social problems. The role of simulations will become increasingly larger, and the results that they provide will undoubtedly greatly affect society. In this sense, we scientists and researchers at AICS shoulder much responsibility, which calls for some humility on our part.

Compared to nature, which is extremely complex and diverse, our simulations have a long way to go. Nevertheless, when it comes to solving clearly defined problems, simulations exhibit a level of power in no way inferior to experiments. Simulations, in the end, can see things that experiments and theory cannot. They constitute a new research technique different from experiments and theory and have the potential of making scientific breakthroughs. If we can raise the reliability of simulations and humbly approach the actual mechanisms of nature, simulations will become all the more attractive as a research tool.

We hope to produce exciting results using the K computer. I think that the ranking of the K computer as the top-performing supercomputer in June 2011 could not help but be encouraging news to the people of Japan in the wake of the devastating Great East Japan Earthquake earlier in the year. I would like to make the K computer—the No. 1 supercomputer in the world—a catalyst for the restoration of Japan. Its true value will be put to the test in the years ahead.