Application Software and Usage Environment for the K computer

● Satoshi Itoh

The K computer is a super massively parallel computer consisting of about one million processing cores, so the development of an environment in which it is easy to use is important. To facilitate the use of the K computer, two application software development projects, called "grand challenge projects," are being carried out, one for nanoscience and one for life science. A number of program codes that are well-optimized for the K computer will be developed in these projects, and, after project completion, users of the K computer will be able to use these program codes on demand. Five science and technology fields have been specified for promoting use of the K computer and high-performance computing. Research and development related to accomplishing the strategic goals of the two projects are being pursued, and the establishment of a research system for computational science is expected. In this article, application software development and the usage environment for the K computer are presented.

1. Introduction

Science and technology need more than just computers to progress—they also need a computing environment. It goes without saying that optimal, high-performance software is an absolute necessity for making full use of the K computer's performance.[note)] In Japan, the standards in the research of such software are very high, and many software programs based on novel and creative algorithms have been developed over the years. Most of this high-performance software, however, has been confined to research applications; almost no high-performance software has been developed for a wide community of users, for use in industry, or for commercialization purposes as in Europe and the United States. In light of this situation, the development of the K computer is being accompanied by the establishment of two R&D software projects on a scale never before seen in Japan and the creation of a usage environment for making full use of the supercomputer's abilities. Research activities are thriving as a result of these projects. This paper describes the current state of these projects and the K computer's usage environment.

2. Two grand challenge projects

Simulation techniques are expected to play an important role in Japan's "green innovation" and "life innovation" growth strategies, and two "grand challenge" projects—one for nanoscience and the other for life science—are being promoted as part of this trend. The purpose of the grand challenge initiative is to 1) develop advanced software for various fields that can make full use of the capabilities of the K computer, 2) use

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.

that software to produce genuine breakthroughs by performing analysis on a scale not possible in past computational environments, and 3) enable that software to be used not just by developer groups but by a wide range of users. To this end, RIKEN is promoting an environment that will enable any general user to use that software on the K computer. The following describes the nanoscience and life-science grand challenge projects.

3. Nanoscience grand challenge project

Nanotechnology is both an infrastructure technology supporting an advanced information society and an essential technology for creating a sustainable society. Researchers seek to answer a number of questions using nanotechnology. For example, fuel-cell catalysts and high-performance magnets are considered to be the foundation of a future eco society, and they currently require noble metals to function, but why couldn't they use only base metals? What kind of molecular structure should a microcapsule have to achieve a drug delivery system (DDS) with absolutely no side effects? And what should the ultimate storage device be like to accommodate storage on the terabit level, which is already appearing on personal computers? The Next-Generation Integrated Nanoscience Simulation Software Research and Development project was established to answer such questions by using simulation techniques with the Institute for Molecular Science, National Institutes of Natural Sciences, as a research and development base (**Figure 1**).

In this project, 6 core applications and 38 additional software functions have been developed in 3 fields: next-generation functional nanomaterials for information technology, next-generation nano biomolecules, and next-generation energy. Of significance here is not the quantity of developed software but the new research community formed by this project. Participating in this project are not just researchers from the condensed-matter-science, molecular-science, and materials-science communities but also researchers from the computer-science community. The formation of this new community has made it possible to formulate original theories with respect to important problems in physical science and to evaluate those theories through computational science, and, at the same time, to develop innovative software from a computer-science approach. One outcome of this collaborative work between computational science and computer science is "nanomaterial simulations in real space based on first principles" using real-space density functional theory (RSDFT). This core application program performs detailed calculations of electron states in matter on the basis of the density functional theory on a scale in excess of 100 000 atoms (which is the number of atoms actually controlled in current advanced-device processes). The RIKEN Advanced Institute for Computational Science (RIKEN AICS) optimized this program for execution on the K computer in collaboration with its developers—Professor Atsushi Oshiyama of the University of Tokyo (computational science) and Associate Professor Daisuke Takahashi of the University of Tsukuba (computer science)—and achieved an effective performance of 3.08 PFLOPS using 442 368 cores.[1] This project has also developed electronic-structure calculation software for large-scale proteins based on the fragment molecular orbital (FMO) method developed originally in Japan and three-dimensional reference interaction site model (3D-RISM) software that incorporates solvation effects based on statistical mechanics. These two programs are expected to be used for high-speed, high-reliability screening in the development of pharmaceutical products—several drug manufacturers are already using them in product development.

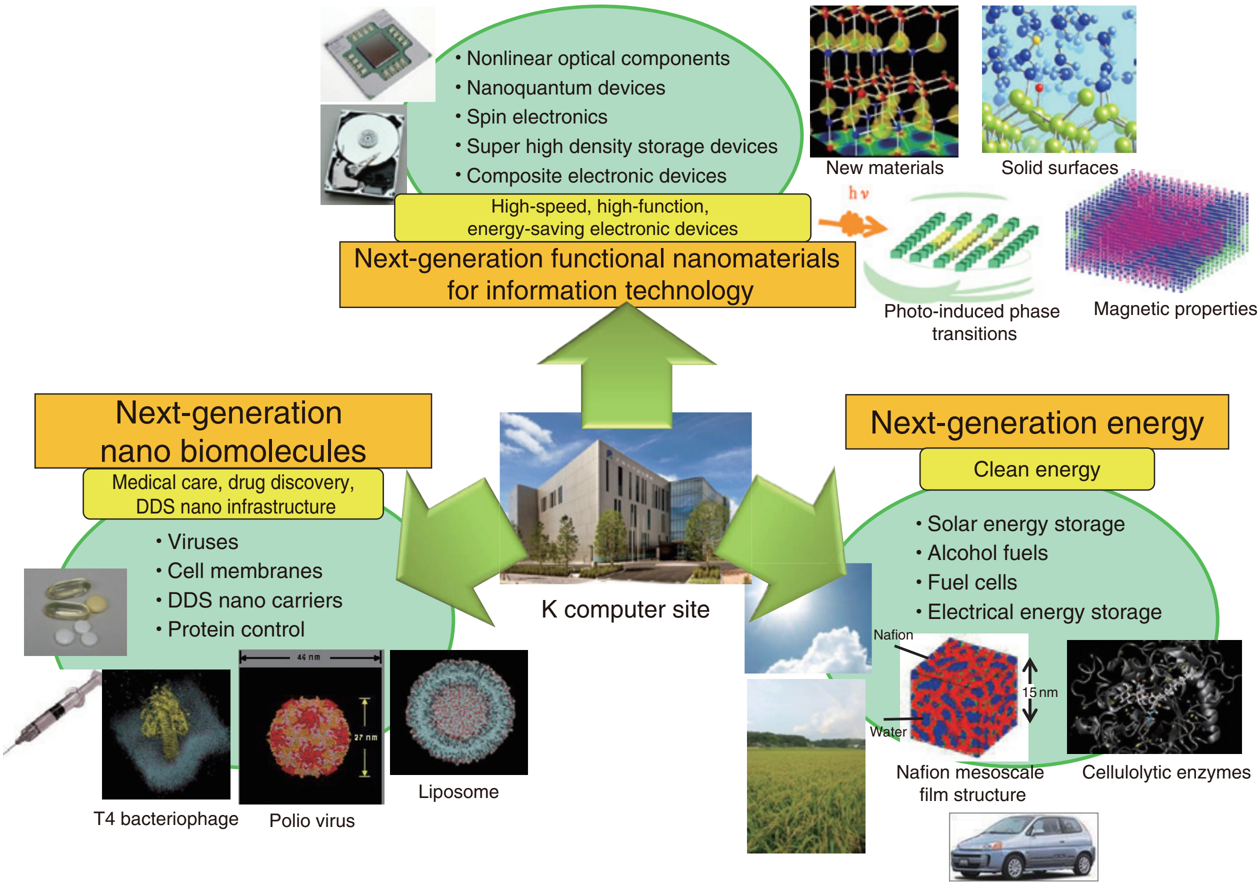

Figure 1
Next-Generation Integrated Nanoscience Simulation Software Research and Development (nanoscience grand challenge project).

4. Life-science grand challenge project

The "life innovation" growth strategy promoted by Japan is directly related to the desire of the Japanese people for a long and healthy life. The Next-Generation Integrated Simulation of Living Matter—Software Research and Development project, overseen by RIKEN since 2006, has the goal of providing a technology platform for this field (**Figure 2**). A key goal of this project is to understand biological phenomena through comprehensive and systematic application of software on diverse levels from multiple points of view. A living organism is made up of cells, which are in turn composed of genes, proteins, and other elements formed from atoms. These cells combine to form assemblies such as organs that demonstrate function. One example of a software application that treats the flow from genes to organs and living organisms is UT Heart, a virtual heart simulator developed by Professor Toshiaki Hisada of the University of Tokyo.[2] UT Heart achieves multi-scale, multi-physics simulation of the heart by modeling the heart from the molecular level, by performing motion analysis at the organ level on the basis of a mathematical model of myocardial cells and a homogenization method, and by establishing relationships between phenomena on different levels such as that between heart function and blood flow. It can also perform drug-response analysis, as in how the heart rate changes when

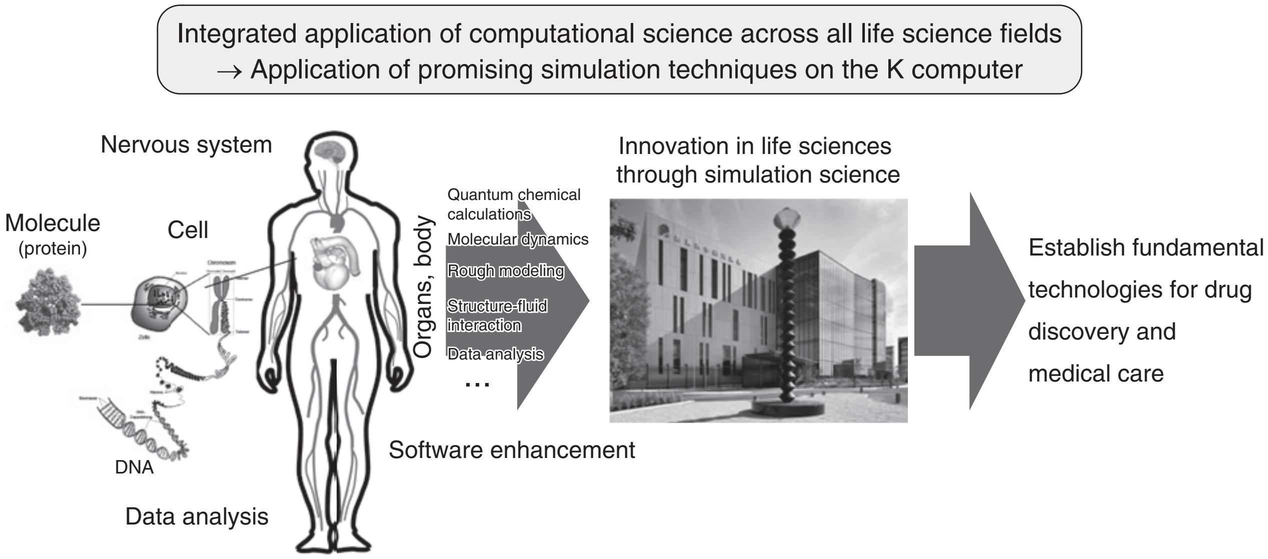

Figure 2
Next-Generation Integrated Simulation of Living Matter—Software Research and Development (life-science grand challenge project).

the ion concentration inside myocardial cells changes.

In drug development, compounds having a true medicinal effect while having no risk of toxicity or teratogenicity must be extracted from a large number of candidate compounds. Since compounds having specific-absorption characteristics with respect to protein related to the target disease can be expected to have a powerful medicinal effect, there is a need for high-speed docking simulation to search for and screen such compounds in drug discovery. There are two directions that can be taken here. One is high-speed docking simulation based on morphological homology analysis. In this project, a system called MEGADOCK has been developed to evaluate docking by adding physiochemical properties to structural information. The other direction is quantum-mechanical calculation taking the effects of surrounding solvents into account. Such calculations are needed to determine whether a detailed complex consisting of protein and chemical substances will form. A variety of molecular-simulation software applications (Platypus series) on various levels of approximation have been developed in this project. A large-scale data analysis system has also been developed to perform pathway analysis from a huge amount of genome information.

The expectations for advanced, cutting-edge medical care among the Japanese people are very high. The expected treatments include heavy particle radiotherapy and high-intensity focused ultrasound (HIFU) for tumors, both of which are non-invasive forms of treatment. This means a much lighter burden on the patient and enables treatment of body parts that have traditionally been difficult to operate on. On the other hand, these forms of treatment require highly detailed control, so high-accuracy analysis is essential. This project is researching and developing simulation software to support these advanced forms of treatment.

5. Five strategic fields

To promote research that can exploit the full performance of the K computer, fields that can be expected to produce noteworthy and beneficial results must be identified, research-and-development resources must be made more efficient, and large research communities must be promoted in contrast to individual or small research teams. To this end, the Japanese government established the five strategic fields listed below to complement the development of the K computer (**Figure 3**).

1) Field 1: Life Sciences and Drug Discovery (strategic institution: RIKEN)
2) Field 2: New Materials and Energy Creation (strategic institutions: Institute for Solid State Physics, University of Tokyo; Institute for Molecular Science, National Institutes of Natural Sciences; Institute for Materials Research, Tohoku University)
3) Field 3: Projection of Global Change for Mitigating Natural Disasters (strategic institution: Japan Agency for Marine-Earth Science and Technology)
4) Field 4: Next-generation *Monozukuri* (strategic institutions: Institute of Industrial Science, University of Tokyo; Japan Aerospace Exploration Agency; Japan Atomic Energy Agency)
5) Field 5: The Origin of Matter and the Universe (strategic institutions: University of Tsukuba; High Energy Accelerator Research Organization; National Astronomical Observatory of Japan)

Strategic field 1 was established to research biological phenomena through the analysis of intra-cell molecular dynamics and to research and develop high-accuracy docking-simulation techniques in relation to drug discovery. Quantum-mechanical docking simulations have so far focused on the evaluation of binding energies, but it should be

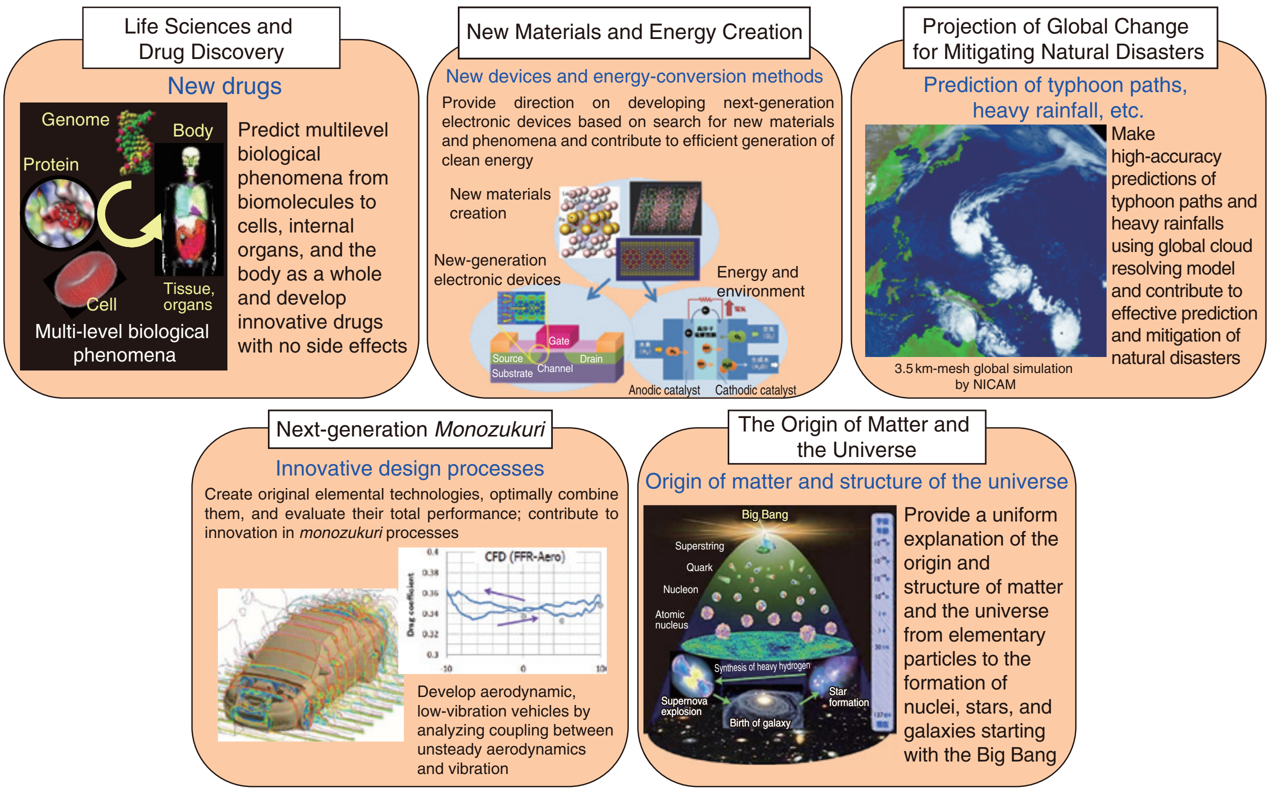

Image credits: Osaka University, RIKEN, Institute for Molecular Science, The University of Tokyo, Japan Agency for Marine-Earth Science and Technology, The University of Tsukuba

Figure 3
Five strategic fields.

possible to pursue actual docking processes by evaluating free energies that incorporate the effects of surrounding solvents. At present, the aim is to apply highly parallel processing to quantitative in silico screening. This field also includes hierarchical integrated simulation for predictive medicine in relation to myocardial infarction, cerebral infarction, cardiovascular disease, and other conditions. Researchers are now simulating the formation of clots in blood vessels and analyzing related processes such as the breaking loose of clots by blood flow. Such processes are difficult to observe directly by experimental means, which is why quantitative analysis by simulation is an important endeavor. Another important research theme in this field is the large-scale analysis of biological data as in the next-generation DNA sequencers using techniques from the field of information science.

Under the slogan of "turning the wellspring of basic science into a torrent of technologies for manipulating material functions and energy-conversion processes," strategic field 2 aims to make a full assault on challenging problems in condensed matter physics, molecular chemistry, and materials science. This assault includes the research of new quantum phases in systems of strong electron correlation, the development of advanced devices such as silicon nanowire field-effect transistors, the design of new functions for soft nanomaterials that include biological molecules, and the development of new energy-creation technologies using solar light. Japan has traditionally been strong in this field in terms of industrial competitiveness, and many corporate researchers are participating in this research as a result. The development of human resources is also a prime objective in this field, and a variety of activities are being promoted for this reason, including seminars and training sessions on Japan-developed nanoscience software.

In strategic field 3, the research theme is technology for predicting global change to prevent and mitigate natural disasters. The focus here is on weather, climate, and environmental predictions in the midst of global warming as in predicting the properties of typhoons and hurricanes occurring throughout the world and predicting localized, heavy rainfall. Researchers in this field also aim to improve the accuracy of tsunami predictions and the accuracy of earthquake/tsunami predictions using more detailed earthquake hazard maps. In this field, Japan has already made major contributions to predicting warming trends on a global scale through the use of the Earth Simulator, but from here on, it will pursue with urgency the use of the K computer in this field, particularly for disaster prevention and mitigation.

Strategic field 4 was established to research and develop technology for driving innovation in *monozukuri* (Japanese art of manufacturing and engineering). Simulation techniques have already become indispensable to the development of automobiles and semiconductor devices, but most simulations in those industries use commercial software packages that cannot be run on highly parallel computing systems. The question arises, however, as to whether running software supporting highly parallel processing developed by universities or other parties on the K computer can truly revolutionize *monozukuri*. An industry-academia joint system in the form of research committees and consortiums has been established to examine this question. The specific objectives of research and development in this strategic field are 1) to create a technology-innovation support system to achieve drastically more efficient, smaller, and quieter social infrastructures and consumer products through product innovation, 2) to create a next-generation design system to dramatically accelerate the value-creation and product-to-market process with an eye toward future society through process innovation, and 3) to create a safe and secure society through a next-generation safety/soundness evaluation system that can significantly improve the reliability of large-scale plants.

Finally, strategic field 5 concerns fundamental science, that is, elementary particles from the time of the early universe to the formation of galaxies, as well as nuclear physics and astronomy. Researchers in this field have already accumulated a string of impressive results by introducing dedicated computers at an early stage, but even more discoveries are expected using the K computer. This field also includes R&D themes related to mathematical science, which is viewed as a common infrastructure technology.

The activities in each of these five strategic fields are not simply concerned with achieving superior academic results by making optimal use of the K computer. Much energy is also spent in community-formation activities such as industry-academia interaction and human-resource development, which helps to return research results to society and build up the industrial competitiveness of Japan.

6. Conclusion

Japan's K computer is a computing resource open to all researchers and engineers in industry, government, and academia. The purpose in getting the industrial world, in particular, to use the K computer is not simply to get it to use computers but to solve problems affecting the work of industry. To this end, there is an urgent need to provide a user-friendly usage environment and an extensive support system. In collaboration with registered institutions, the RIKEN AICS plans to provide users with a user-friendly K computer when shared use commences in the fall of 2012.

As the world's top computational environment, the K computer will provide researchers and engineers in Japan with a powerful tool for becoming leaders in their fields.

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Satoshi Itoh
RIKEN
Dr. Itoh is engaged in promoting the K computer for industrial use.