

Research Achievements

Using the HPCI System
Including K computer



Manufacturing

By using K computer, the flow field around a propeller was observed, aiming for performance improvement of ship propellers

Environment

Innovation in weather forecasting brought about by big data assimilation using Himawari-8 satellite and K computer

Life Science

Exploring dynamic mechanism for reading genetic information from DNA by exhaustive calculation of nucleosome movement

Manufacturing

Exploratory realization of high-performance tires through reexamination of rubber materials using K computer



Japan's Supercomputers Create our Future



What is the K computer?

The K computer is a large-scale, high-performance supercomputer produced entirely in Japan, featuring not only high-speed computing but also ease of use.

Six and a half years have passed since the start of the shared use of the K computer. Its operation will end in the near future, and the K computer will be replaced by the post-K computer.

Evaluation of the K computer in the world

Supercomputer performance ranking

- **First place on TOP500** **First place in June and November 2011 (two consecutive terms)**
 - An international ranking of supercomputer performance evaluated on the basis of the speed of solving simultaneous linear equations using regular matrix calculations
- **First place on HPCG** **First place in November 2016 and June and November 2017 (three consecutive terms)**
 - An international ranking of processing speed determined by the conjugate gradient method, which is frequently used in industry and other actual applications
- **First place on Graph500** **First place in June 2014 and from July 2015 to November 2018 (eight consecutive terms)**
 - An international ranking of the speed of the breadth-first search for graphs used in big data processing

NOTE: The K computer is operated by the RIKEN Center for Computational Science and its shared use started in September 2012.
The "K computer" is a registered trademark of RIKEN.

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Using the HPCI System Including K computer

The advent of the K computer has led to rapid progress in computational science in Japan. Since the start of its operation, the K computer has provided the world's highest performance. The Research Organization for Information Science and Technology (RIST)* publishes Research Achievements every year with the aim of presenting to the public the achievements of research projects using the high-performance computing infrastructure (HPCI) centered on the K computer.

The sixth issue, Research Achievements 6, covers a wide range of research achievements including those of Sumitomo Rubber Industries, those of basic research with the potential to create breakthroughs and those related to meteorology and manufacturing that will be useful in our daily lives.

We hope this brochure will further promote the use of HPCI centered on the K computer and enhance public understanding of the research in the field of computational science. We sincerely appreciate the cooperation of all those who took part in the publication of this brochure.



関 昌弘

President

Masahiro SEKI, Ph.D.

Registered Institution for Facilities Use Promotion /
The Representative for HPCI Operation

Research Organization for Information Science and Technology

* Research Organization for Information Science and Technology (RIST)

In accordance with the Act on the Promotion of Public Utilization of the Specific Advanced Large Research Facilities, RIST has been in charge of user selection and usage support services, including the general contact point for user support, in its role as the Registered Institution for Facilities Use Promotion of K computer, since April 2012. From April 2017, RIST has also been in charge of various services such as general coordination for HPCI operation, project selection, the common contact point and user support, Access Point Tokyo, and promotion of the industrial use of HPCI as the representative for HPCI Operation commissioned by the Ministry of Education, Culture, Sports, Science and Technology (MEXT).

Propellers of merchant ships are up to 10 m in diameter. It is difficult to accurately measure the performance of such large propellers at sea. Therefore, we have been trying to simulate and analyze the flow around a propeller using the K computer. This study will improve ship efficiency and contribute to the trade activities in Japan.

By using K computer, the flow field around a propeller was observed, aiming for performance improvement of ship propellers

Resource	RIKEN K computer
Project Number	hp170069
User Report	https://www.hpci-office.jp/output/hp170069/outcome.pdf

Achievements

We simulated the flow around a propeller at several Reynolds numbers, which indicate various flow conditions. We acquired detailed flow field data and succeeded in visualizing the vortex structure near the propeller surface. The visualization as well as detailed data were not obtained in scale model experiments.

Future Perspectives

Simulating many types of propellers and ship hulls will lead to improved fuel consumption and safety. These will contribute to the economy of Japan, as a trading nation.

Takeharu Fujisawa

Japan Marine United Corporation
Technical Research Center
Hydrodynamics Research Group

Outline of Research

Simulation realized by K computer as an alternative to difficult experiments

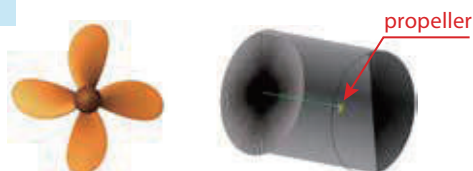
Propellers are equipped on most ships, and their performance directly affects the ship's fuel efficiency or speed. However, it is virtually impossible to conduct accurate and detailed experiments on actual ships. The length of the ship is up to 300 m and the diameter of the propeller is up to 10 m, so it is too large for experimentation. Furthermore, accurate measurements are difficult due to winds, waves, and currents at sea. Therefore, experiments are conducted in a towing tank using scale models. Propeller models are usually 200–250 mm in diameter. Nevertheless, when these experiments are carried out, it is difficult to accurately measure the velocities and pressure of flow around a propeller because of its high speed rotation. Flow field information can be measured by several limited methods, such as LDV (Laser Doppler Velocimetry) or PIV (Particle Imaging Velocimetry), or oil flow pattern observation technique on the propeller surface. Large-scale computing using the K computer has made it possible to analyze the flow field around the propeller in detail under conditions with several Reynolds numbers as model experiments (Fig.1). In the simulation, the space around the propeller is divided into 800 million grids, and the pressure and

velocities in each grid are calculated in milliseconds time marching method. It is necessary to solve equations over and over again for each variable of this huge number of grids. Such large-scale simulation would not be realized without the K computer's high performance.

The results of this study will help to reduce export/import costs in Japan

In this simulation, we succeeded in visualizing the fine vortex structures on the propeller surface that could not be resolved by scale model experiments. We found that the large-scale simulation based on CFD (Computational Fluid Dynamics) can be an alternative to towing tank experiments (Fig. 2). Ships must operate at a certain performance level for many days continuously at sea. Hence, even only 1% improvement of ship efficiency will result in a huge energy saving and reduction of greenhouse gas emissions, which will benefit Japan. It will also contribute to the reduction of the enormous export/import costs of Japan as an island country. More than 200 years have passed since the invention of propellers as the ship propulsor, but many aspects of propellers still remain to be clarified. Through the large-scale computing using the K computer and the post-K computer, we will further explore the frontiers of this field.

Fig.1 Propeller shape and calculation domain



We used a 4-bladed propeller. Eight hundred million grids are used in the simulation.

Fig.2 Flow and vortex structures on propeller surface for Reynolds number of 1.1×10^6



The left figure shows the results of an experiment in which colored oil was applied to the surface of a scale model. The center and right figures are results of the simulation using the K computer. The pink droplets show the fine vortex structures on the propeller surface.

Although we watch weather reports on TV, phenomena occurring in a short period of time or in a specific limited area, such as sudden localized torrential rain, cannot yet be predicted. Our research team aims to realize much more rapid and accurate weather forecasting by combining the observation data from an advanced weather radar and the geostationary meteorological Himawari-8 satellite with a simulation using the K computer.

Innovation in weather forecasting brought about by big data assimilation using Himawari-8 satellite and K computer

Resource	RIKEN K computer and FX10 at University of Tokyo
Project Number	hp170178
User Report	https://www.hpci-office.jp/output/hp170178/outcome.pdf

Achievements

By combining the observation data from an advanced weather radar with a simulation using the K computer, our research team developed a method of predicting sudden localized torrential rain that previously had been unpredictable.

By analyzing the meteorological data from Himawari-8 using the K computer, the time interval between updates of weather forecast simulations was decreased from one hour to 10 minutes.

Future Perspectives

Our research team is developing a new numerical weather forecast system that is compatible with the high-resolution simulation and can rapidly predict the risks of flood and landslide disasters.

Takemasa Miyoshi

RIKEN Center for Computational Science

Outline of Research

Predicting torrential rain via “big data assimilation”

Torrential rain has been occurring frequently throughout Japan in recent years. Torrential rain is very heavy rainfall that is caused by rapidly growing cumulonimbi and falls over a limited area. It can disrupt normal city functions and even threaten human lives. However, it had been difficult to predict such sudden localized torrential rain because the conventional weather forecasting simulation retrieves data from rough grids of $2 \times 2 \text{ km}^2$ mesh size only once every hour. Therefore, our research team attempted to predict torrential rain using a phased-array weather radar that can observe the atmosphere in a grid of $100 \times 100 \text{ m}^2$ mesh size every 30 seconds and process the observation data with the K computer. This is a method of “big data assimilation”. Because the amount of data dealt with in this method is overwhelmingly large compared with that in the conventional weather forecasting system, it would not have been realized without the K computer’s high computational capability.

In this study, the changes in the atmosphere that occur during 30 minutes before the torrential rain were calculated by assimilating big data from the phased array weather radar. As a result,

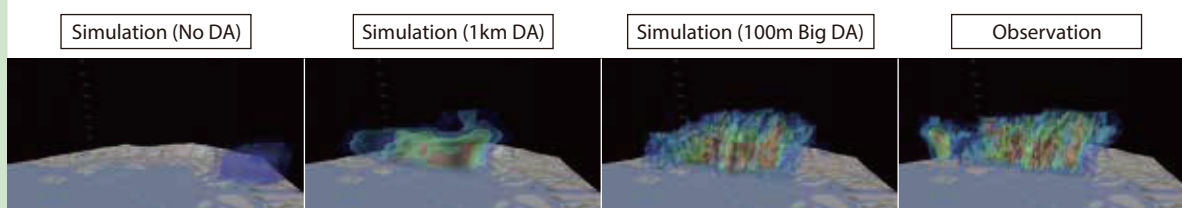
cumulonimbi similar to those that actually brought the heavy rain were replicated in the simulation using the K computer (Fig. 1).

Preventing weather disasters by means of weather prediction updated every 10 minutes

This year, our research team further advanced our study. We demonstrated that more accurate weather prediction can be realized by using the K computer to perform a simulation with cloud image data obtained every 10 minutes from the latest geostationary meteorological Himawari-8 satellite (Fig. 2). In order to predict the risk of flood and landslide disasters caused by heavy rain, it is necessary to retrieve and calculate the ever-changing meteorological data within a short span of time and perform calculations. Conventionally, weather prediction has been updated approximately every one hour. However, it can be updated every 10 minutes using the big data from Himawari-8. The combination of high-accuracy simulation using supercomputers, such as the K computer, and meteorological big data will bring about innovation in weather forecasting and help people protect themselves from weather disasters such as typhoons and heavy rain.

Fig. 1

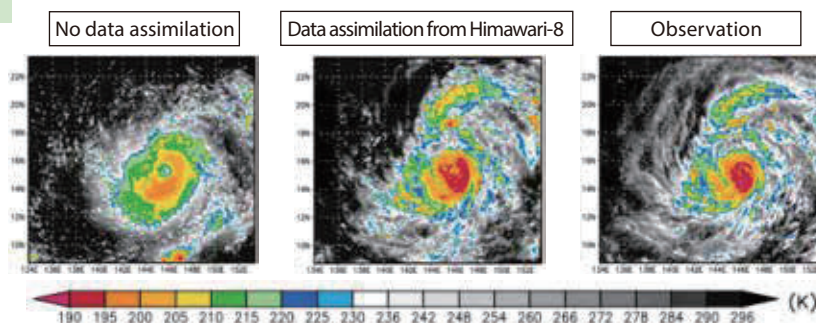
Data of torrential rain observed near Kobe City on the morning of 11 September 2014 (right) and results of simulation using K computer




Cumulonimbi similar to those that actually brought heavy rain were replicated in the simulation performed with data assimilation (DA) on a grid of $100 \times 100 \text{ m}^2$ mesh size using the K computer.

Fig. 2

Actual observation data from Himawari-8 (right) and results of simulation using K computer



By means of big data assimilation, the structure of a typhoon (outer rain band and central region) is modified to make it more similar to the actual observation data.



DNA, which contains the genetic information of an organism, is wrapped around a protein called "histone". The structure consisting of DNA and histones is called a nucleosome, which is arranged like beads on a string in a cell nucleus. Our research team is working to reveal the real nature of the dynamic movement of DNA and nucleosomes in a cell by calculating more than 60 patterns of interaction between five hundred thousand atoms (~30 million atoms in total) using a supercomputer.

Exploring dynamic mechanism of reading genetic information from DNA by exhaustive calculation of nucleosome movement

Resource	CRAY XC40 at Kyoto University
Project Number	hp170066
User Report	https://www.hpci-office.jp/output/hp170066/outcome.pdf

Achievements

Through exhaustive analysis of the movement of all atoms in a nucleosome, our research team succeeded in accurately simulating the interaction between two adjacent nucleosomes that are closely related to gene functions.

We found that the positional relationship between two nucleosomes is determined by the strong electrostatic interaction between the H4 tail of one nucleosome and the DNA of the other nucleosome.

Future Perspectives

Clarifying the mechanism of gene expression from DNA at the atomic level will lead to the development of drugs for cancers associated with abnormal gene expression.



Hisashi Ishida

National Institutes for Quantum and
Radiological Science and Technology
Institute for Quantum Life Science

Outline of Research

Histones wrapped by DNA are the key to reading genetic information

DNA contains all the genetic information of an organism. Human DNA, which is about 2 m long, is wrapped around histones and stored in a cell nucleus ~0.01 mm in diameter. Nucleosomes, which consist of histones and DNA, undergo dynamic structural changes in the cell nucleus. To read genetic information from DNA, two adjacent nucleosomes must be positioned at a certain distance from each other so that transcription factors, which are essential for reading genetic information, can access DNA.

The objective of this study is to clarify the interaction between two adjacent nucleosomes.

We focused on the tail-like end of histones called the "histone tail". Although histones are folded protein-forming clumps, their tails move freely and interact with adjacent nucleosomes. However, the details regarding the function of histone tails and their role in the interaction with adjacent nucleosomes have not yet been clarified.

Calculating more than 60 patterns of interaction between nucleosomes to clarify DNA movement inside cells

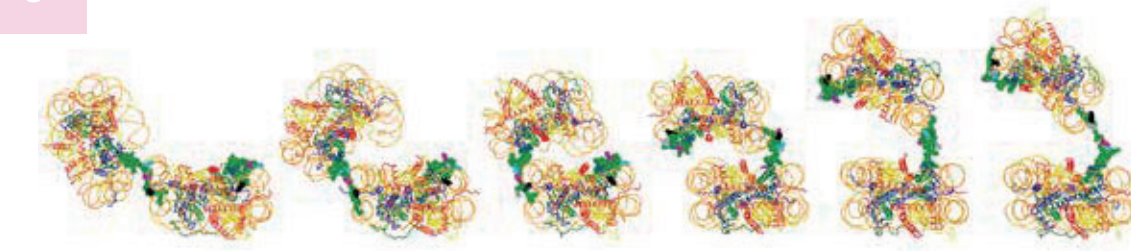
Using a supercomputer, we attempted to simulate how two adjacent nucleosomes are positioned at a certain distance from each other. To model an event inside a cell, it is necessary to consider not only the interaction between the atoms that make up nucleosomes but also the interaction between those atoms and a large number of water molecules. Approximately five hundred thousand atoms are involved. Also, among the four types of histone, H1 to H4, the tail of H4 (H4 tail) is considered

to be the most closely involved in the interaction. Therefore, 63 patterns of different structures of the H4 tail were considered in the simulation. Thus, we calculated the behavior of ~30 million atoms (five hundred thousand atoms \times 63 patterns) using a supercomputer and proposed a reasonable model that agrees with experimental results (Fig. 1).


In the simulation, the structural changes were examined exhaustively while changing the distances between the centroids of adjacent nucleosomes. The interaction force at each distance was also calculated. As a result, it was found that the interaction force between nucleosomes is determined by the strong electrostatic interaction between the H4 tail of one nucleosome and the DNA of the other nucleosome.

The DNA and nucleosomes appear to be stationary when observed by X-ray analysis or electron microscopy. However, they are actually moving in the cell nucleus as the cell reads the genetic information and their movement is dynamically regulated. At present, the behavior of all atoms in DNA and nucleosomes under such conditions can be tracked only by simulation. A model closer to reality can be constructed by comparing the findings from the simulation with the experimental results, leading to the clarification of the mechanism behind genetically related diseases as well as the development of new drugs. With the aim of understanding the real nature of DNA and nucleosomes, we will make further efforts to improve the sampling efficiency and to realize more complex simulations.

Fig. 1 Positional relationship of two adjacent nucleosomes obtained by calculation



The simulation revealed that there is a strong interaction between the positively charged H4 tail (green) of one nucleosome and the negatively charged DNA of the neighboring nucleosome so that the H4 tail forms a bridge between the nucleosomes. As a result, two nucleosomes are energetically stable and arranged in various conformations. The figure shows typical conformations.



As the number of vehicles increases worldwide, the improvement of fuel efficiency through the use of high-performance tires has become a common global issue. Our research team aims to develop safer and environmentally friendly tires through the research on rubber materials at the molecular level on the basis of large-scale molecular dynamics calculation using the K computer.

Exploratory realization of high-performance tires through reexamination of rubber materials using K computer

Resource	RIKEN K computer
Project Number	hp170063
User Report	https://www.hpci-office.jp/output/hp170063/outcome.pdf (To be published in April 2020)

Achievements

On the basis of the simulation of rubber materials using the K computer, we developed tires with wear resistances 51% higher than those of conventional products.

As a result of simulating four patterns of bonding between the particles of silica and the coupling agent added to rubber materials, we found that tire materials with even higher wear resistances can be developed by increasing the number of chemical bonding points on the silica surface.

Future Perspectives

The simulation of the friction performance of tires has not been realized even with the K computer because of the enormous amount of calculation required. In the future, we will perform such a simulation using the post-K computer and help address global environmental issues through the development of tires that provide better roadability and fuel efficiency.



Masaya Tsunoda

Sumitomo Rubber Industries, Ltd.
Research & Development HQ.

Outline of Research

Conflicting requirements in tire development

The rolling resistance of tires is an important factor that can affect a vehicle's fuel efficiency by nearly 20%. Generally, rolling resistance can be decreased by reducing the energy loss of tires, but the tire grip will then be decreased, leading to a decrease in turning performance and the loss of the braking effect. On the contrary, as the tire grip increases, the fuel efficiency will decrease. The challenge in tire development is to find the optimum balance among these conflicting requirements.

Successful research achievements

Since the start of shared use of the K computer, we have used it continuously in our research on rubber materials with the aim of developing tires that reduce fuel consumption and have a high grip and long life. While a vehicle is moving, tires are continuously changing their shape owing to forces applied from the road. The fracture phenomena occurring on the surface of and inside a tire can be replicated by simulating the movement of molecules inside the tire using the K computer. By the method called large-scale molecular dynamics calculation, we realized significant improvement in wear performance in the development of the tire "ENASAVE NEXT II", the wear resistance of which is 51% higher than those of conventional products.

Before the introduction of simulation using supercomputers, such as the K computer, in tire development, skilled engineers determined the composition and amount of materials to be mixed on the basis of their experience and previously manufactured products through a process of trial and error. Therefore, the level of achievement of development objectives in terms of material physical properties was often affected by the skill of

engineers. Also, because materials were developed without an understanding of the mechanism of interaction between molecules, new ideas rarely arose during the development process. The advantage of simulation using the K computer is that we can freely change the amount and composition of the materials that make up a tire, as well as the bonding state between micron-sized particles. In real experiments, it is difficult to form a material with a predicted structure. It is also difficult to understand the strain and stress generated in a material, the intermolecular interaction, and the state of entanglement of polymer chains. Much information has been obtained through model experiments based on the simulation using the K computer with ultrahigh performance.

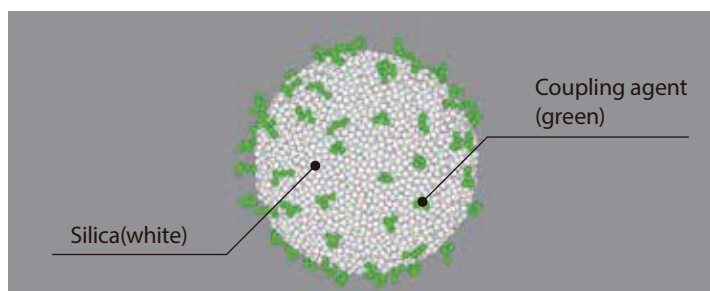
Simulating fracture phenomena in rubber at molecular level

This year, we further advanced our study and simulated how the bonding state at the molecular level of silica and the coupling agent, which are added to enhance the strength of rubber, affects tire wear (**Fig. 1**). The formation of voids as a result of physical adsorption/desorption at the molecular level or the breakage of molecular chains, as well as the enlargement of those voids, contributes to tire wear. Silica is added to rubber to enhance tire strength, and the coupling agent acts as a bridge between silica and the main ingredient of tires, namely, rubber polymers.

In the simulation, we virtually generated four types of tire rubber materials using the K computer, applied strain to the materials, and collected the data on material strain, generated stress, and the volume of generated voids. The four patterns examined were as follows: two patterns with a small or large number of coupling agent particles bonded to silica particles and two patterns with a long chain, assuming that a

Fig.1

Diagram of model generated using K computer, showing coupling agent bonded to silica particles

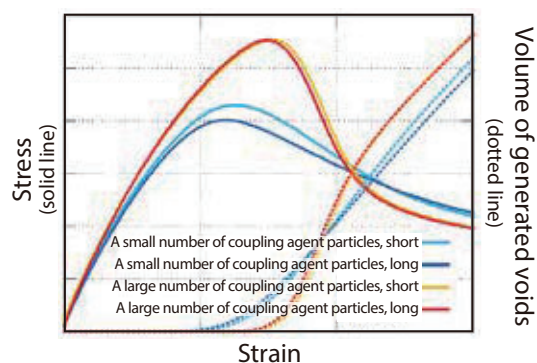


The amount of coupling agent per silica particle is small in the example shown in this figure.

Outline of Research

long coupling agent is used, or short bonds in which silica particles and polymers are directly bonded by a single particle of the coupling agent. As a result, we found that the number of bonds between silica and the coupling agent has a greater effect on the wear performance and strength of tire materials than the length of bonds formed by the coupling agent (**Fig.2**).

Fig.2 Stress with respect to elongational strain and changes in total volume of voids



The solid lines show the stress with respect to elongational strain and the dotted lines show the changes in the total volume of voids. The patterns with a large number of bonds with the coupling agent (red and orange lines) have a higher resistance to applied forces and fewer voids that cause tire wear.

Such large-scale calculation of molecular movement at the nanometer scale is impossible with the supercomputer we own. It would not have been realized without the K computer's computational capability, which is ~1,000 times that of our supercomputer. The reaction between silica and the coupling agent varies depending on the time spent on blending them together in a certain temperature range during the rubber mixing process. To shorten the development period, it would be very helpful if we could decide, during the early stages of material

development, whether the tire performance can be improved by manipulating the manufacturing process or by adding other compounding agents. Referring to the simulation results, we will carry out experiments using actual materials and make use of the research achievements in material development.

Using large experimental facilities to realize efficient tire development

In addition to the simulation using the K computer, we are also analyzing the structure of actual tire materials at the large synchrotron radiation facility, SPring-8, which is located in Sayo-gun, Hyogo Prefecture, and the high-intensity proton accelerator facility, J-PARC, located in Tokai-mura, Ibaraki Prefecture. The molecular-level data regarding tire materials obtained at those facilities are input to the K computer and used in the simulation. Materials are developed on the basis of the simulation results, and then the structure of materials is analyzed again. The repetition of these processes has led to a dramatic increase in the efficiency of tire development. Now, global warming due to the increase in CO₂ emissions has become a major issue as the number of vehicles continues to increase worldwide, it is very important to improve the fuel efficiency of vehicles. We would like to help address global environmental issues through the development of high-performance tires.



This photo was taken at Sumitomo Rubber Industries, Ltd. Tyre Technical Center.

Expectation for simulation of friction performance using post-K computer

Tires are the only parts of a vehicle that come in contact with the ground. Therefore, in addition to rolling resistance and wear resistance, tires should have good friction performance so that they grip the ground well and turn or stop as the driver intends. The rolling resistance and wear resistance have been simulated using our own supercomputer and the K computer. However, the simulation of friction performance, such that its results can be used for material development, has not yet been realized. This is because a longer-time and larger-scale simulation of tire deformation is required to analyze friction phenomena.

While a vehicle is moving, tires vibrate with a frequency of 10,000 cycles per second (10,000 Hz) owing to unevenness of the road. During this time, tire rubber expands and contracts like an accordion, but there is a time lag between the strain signal and the stress signal because of the viscosity of materials. The greater the time lag, the higher the friction performance of tires. However, even with the K computer's high performance, it has been difficult to perform the calculation of the phenomena occurring at 10,000 Hz, which are "long-time" phenomena in the field of simulation, in a large-scale simulation model.

Also, when a vehicle turns, the direction of forces applied to tires changes in accordance with the steering operation, causing friction between the tires and the ground. In the large-scale molecular dynamics calculation of tire materials using the current K computer, only the molecular movement in a region of approximately $300 \times 300 \text{ nm}^2$ (a nanometer is one-billionth of a meter) can be simulated. However, friction performance is largely affected by the state of dispersion of silica and unevenness of the road. Therefore, to analyze friction performance, it is necessary to simulate tire deformation at a micrometer scale, which is 1,000 times larger than the nanometer scale.

The shared use of the post-K computer will start around 2021. The post-K computer is expected to have an application performance up to 100 times that of the current K computer, enabling the ultralarge-scale and long-time calculations such as that described above. With the support of RIST, we are now preparing the software for the simulation to be run on the post-K computer. Be on the lookout for the "next-generation tires" that we will develop with the power of the post-K computer.

Back Issues

Back issues of Research Achievements are available at Research Achievements on the HPCI portal site. Those issues are downloadable.

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



Volume I
Issued: March 2015



Volume II
Issued: July 2015



Volume III
Issued: June 2016



Volume IV
Issued: May 2017



Volume V
Issued: May 2018

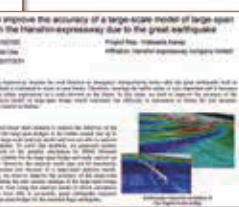
Achievements

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Research Achievements Using the HPCI System Including K computer 6

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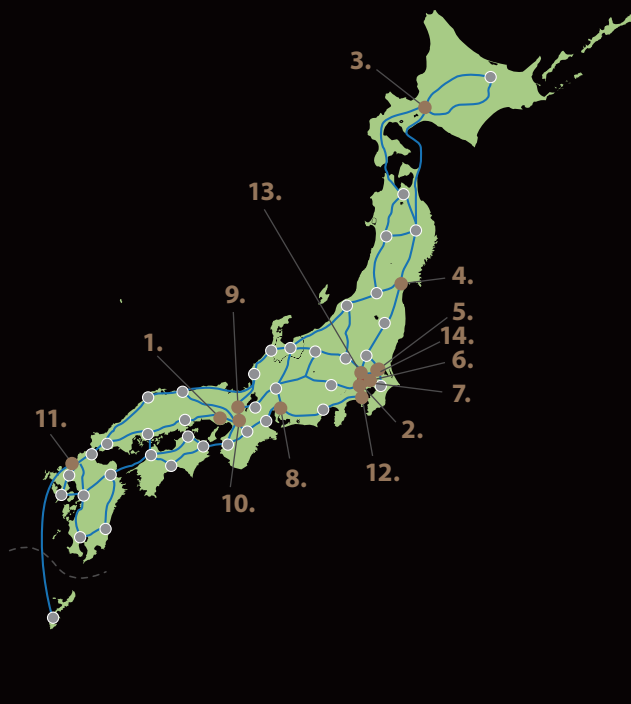
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High-Performance Computing Infrastructure (HPCI) including the K computer

The HPCI is an infrastructure built by the Ministry of Education, Culture, Sports, Science and Technology (MEXT) to create an innovative shared computational environment that meets various user needs. In the HPCI, which has been in service since 2012, the K computer is connected to other supercomputers at major universities and research institutes throughout Japan via a high-speed network, and a highly convenient environment is developed in which users can gain access to multiple supercomputers and storages.

The HPCI partners consist of the following 14 institutes as of April 2019.

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4. Cyberscience Center, Tohoku University
5. Center for Computational Sciences, University of Tsukuba
6. Information Technology Center, The University of Tokyo
7. Global Scientific Information and Computing Center, Tokyo Institute of Technology
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High
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Photos courtesy of RIKEN, Kyoto University,
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