Special Contribution
Supercomputing in Industrial Manufacturing

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1. Introduction

The K computer,[note)] Japan's supercomputer jointly developed by RIKEN and Fujitsu Ltd., achieved the world's best mark in the June and November 2011 performance ranking. It is equipped with 80 000 CPUs and 640 000 processor cores, and realized a performance of 10.5 petaflops in the LINPACK benchmark. A decade ago in the 2000s, the performance of the world's fastest supercomputer was in the order of teraflops. In comparison, the performance of supercomputers has taken great strides in the last 10 years to increase by about 1000 times.

Along with the dramatic performance improvement of supercomputers, there are also high expectations in the manufacturing sector for innovation of design processes and creation of new products by making sophisticated use of supercomputing. Obviously, taking advantage of supercomputing to improve product performance and reliability and reduce development costs and periods before other enterprises in the rest of the world will lead to the strengthening of Japan's industrial competitiveness. To that end, continuous development of supercomputers and strategic promotion of computational science and technology are essential.

note) English name of the supercomputer given by RIKEN in July 2010.

2. Trends in development of application software

In terms of the development of application software used in the manufacturing sector, Japan has been falling far behind the West. Application software in the field of computer-aided engineering (CAE) used in the industrial world is mostly made in Europe or the U.S. and software developed in Japan is rarely used. In the field of structural analysis, for example, software developed by NASA called NASTRAN is regarded as industrial-standard software. In fluid flow analysis, STAR-CD developed by the Imperial College London of the U.K. and Fluent developed by Creare Inc. of the U.S. are in wide use as standard software. Gaussian, which is quantum chemical calculation software that is widespread in the chemical engineering sector, was developed by Carnegie Mellon University of the U.S. and CHEMKIN, leading software for combustion calculations, was developed by Sandia National Laboratories of the U.S.

However, the situation is now coming to a turning point. The present supercomputers are equipped with tens of thousands or more CPUs and processor cores, which need to be run concurrently and efficiently in order to bring out their performance, but most application software that currently serves as the industry standard does not support such massively parallel computation. In addition, application programs alone are not enough to make the most of large-scale computation in the sites of manufacturing design. There are programs called preprocessors that automatically generate computational grids from computer-aided design (CAD) data handled by designers and postprocessors that assist designers in extracting information which is important from an engineering perspective out of an enormous amount of computation results and feed back the results to design. These preprocessors and postprocessors are required for the effectiveness of supercomputing to be brought out in the sites of manufacturing. As computer hardware rapidly progresses, application software and design systems that use it are seeing a paradigm shift as well.

3. Expected breakthroughs

Numerical simulation has long been in wide use for R&D and design of industrial products. However, there are limits to phenomena that can be predicted or to the prediction accuracy achievable with the conventional computers. Therefore, clarification of complicated microscopic phenomena or replacement of product prototyping by computer simulation has not been fully realized. By making use of the rapidly advancing supercomputers, part or all of product prototyping can be replaced by simulation and various design parameters, which were determined based on trial and error, can be theoretically optimized. Fundamental innovation of processes of drug discovery and material development is also anticipated. The following presents specific examples to describe the breakthroughs expected of supercomputing.

Figure 1 shows an example of large-scale fluid flow simulation used for reducing the air resistance of an automobile. Air resistance that acts on an automobile body increases in proportion to the square of the running speed. Accordingly, the effect of air resistance on fuel consumption is relatively small when running at a low speed but, in high-speed running at around 100 km/h, almost half of the fuel consumption

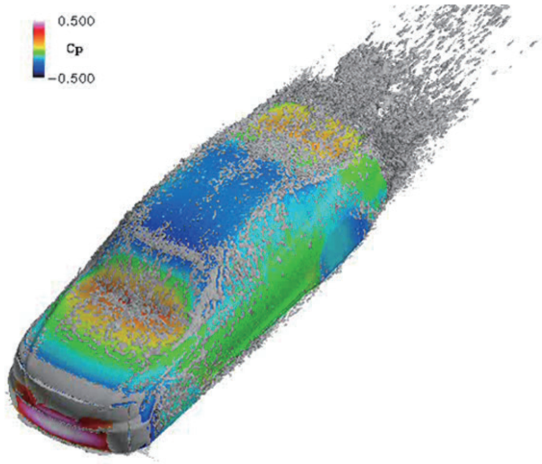


Figure 1
Detailed analysis of airflow around automobile.[1]

is accounted for by air resistance. For example, reducing the air resistance by 10% improves the fuel consumption of an automobile moving at high speed by approximately 4%.

Airflow around an automobile body contains eddies of different sizes including large eddies of about 1 m and very small ones of 1 mm or smaller, and the airflow around an automobile is determined as a result of their mutual interaction. With the conventional computers, it was impossible to calculate the motion of small eddies in airflow due to the restrictions of computation speed and memory capacity. By using the most advanced supercomputer, however, large-scale fluid flow simulation with a computational grid containing up to about one trillion points is possible, and this allows the interaction of all eddies around an automobile to be clarified. Controlling eddies based on this knowledge is expected to break through the limitations of air resistance reduction. In addition, such simulation allows aerodynamic force to be predicted as accurately as can be done in a wind tunnel test. This will make it possible to partially or entirely replace wind tunnel tests, which are now conducted by using prototype vehicles and clay models, with numerical simulation.

While numerical simulation has been used also for determining various design parameters, optimization of numerous design parameters requires possibly an enormous number of cases to be simulated. The computation time required for it has posed a bottleneck and optimum design that uses numerical simulation has not been put to practical use. Meanwhile, the present supercomputers are composed of tens of thousands or more CPUs and are capable of computing many cases simultaneously, which brings high expectations for the realization of optimum designs by making use of supercomputers.

Figure 2 shows an example of a significant reduction of noise generated from a cooling fan for computer servers achieved by optimization using numerical simulation.[2] The heat released by CPUs is increasing year by year and the rotation speeds of fans to remove this heat are increasing as well. The intensity of the noise generated by a fan theoretically increases in proportion to the fifth to sixth power of the rotation speed of the fan, and noise rapidly increases along with the increase in the rotation speed. For this reason, although reducing the noise of cooling fans is an important technological challenge, reducing noise by empirical methods had reached the limits.

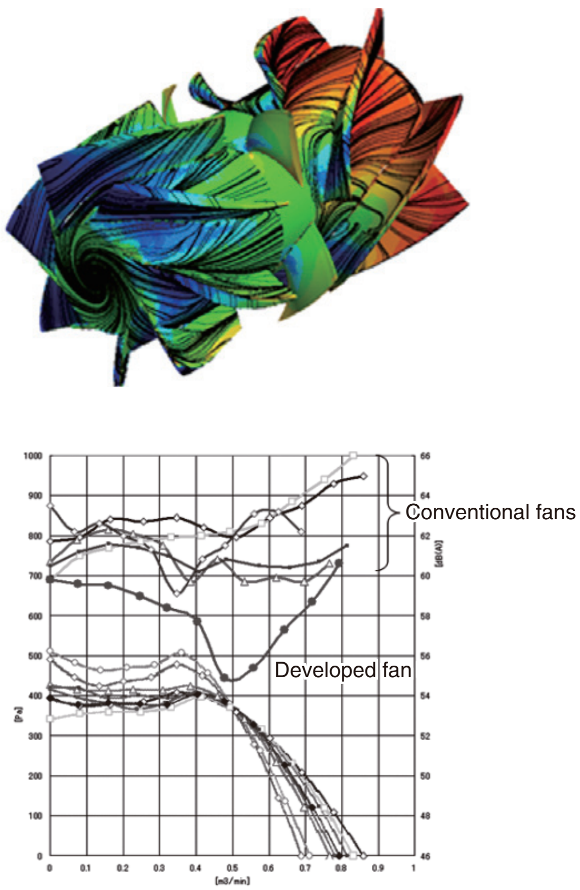
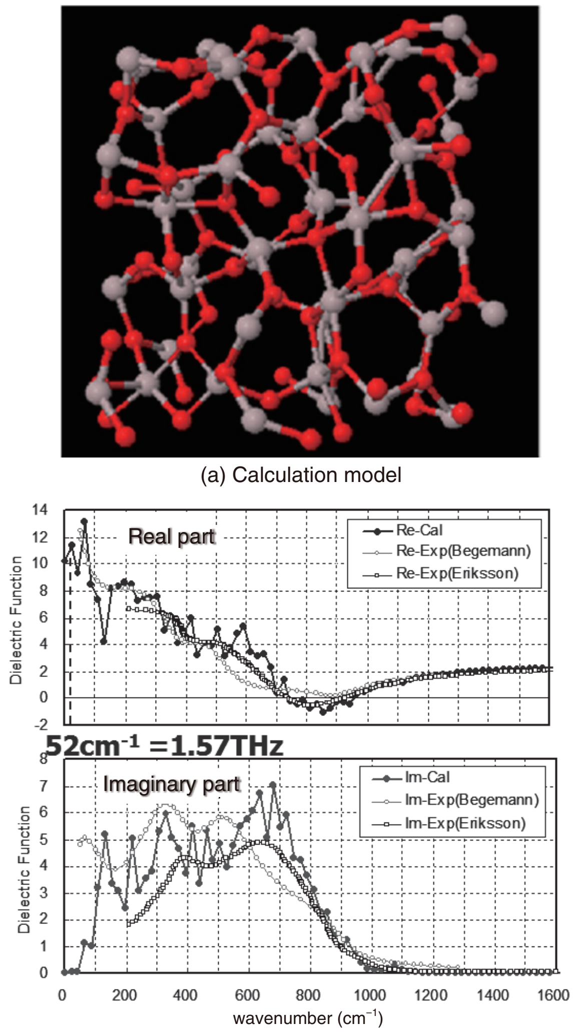


Figure 2
Example of reduction of fan noise.[2]

The shape of the blades of a cooling fan is determined by combining a few tens of parameters. With the processing capacity of the conventional computers, it was impossible to predict the performance and noise of each of the numerous parameter combinations to search for the optimum one. By using supercomputers, however, a parameter study of hundreds of cases can be conducted in a few hours, and this allows for optimization by numerical simulation. In the case presented here, a noise reduction of 6 dB or more has been achieved.

Simulation using supercomputers is giving rise to high expectations for investigation of materials and development of new materials as well as fluid flow design and structural design. In particular, nanomaterials and nanostructures have the potential to bring various technological innovations to future manufacturing and they will provide an important field of research. As the scale of a device is reduced, it becomes insufficient to characterize it as a continuum and the characteristics and functions of materials must be evaluated in view of its electronic state. However, it is difficult to experimentally evaluate with accuracy the characteristics of nanoscale structures and functions of nanodevices. For this reason, there are high expectations that nanosimulations conducted on the basis of quantum mechanics (first-principle calculation), which can evaluate functions and characteristics based on the electronic state of materials, will be useful as an investigation and development tool for new materials.

As an example, **Figure 3** shows the result of predicting the dielectric constant of candidate materials for a next-generation gate insulating film for semiconductors by using a large-scale first-principle calculation.[3),4)] Along with the miniaturization of semiconductors, gate lengths are increasingly being reduced and the leakage current generated by the tunnel effect causes power consumption and heat generation of semiconductors to increase. Accordingly, the development of a gate insulating film with a high dielectric constant (high-k gate film) is a key issue. In this simulation, the dielectric constant of alumina (Al_2O_3), a material with an amorphous structure and a candidate for use in a high-k gate film, is predicted by a first-principle calculation and the result is compared with the actual measurement. The simulation has proved that such calculation is capable of quantitatively predicting a dielectric constant. In this way, first-principle calculations are beginning to be actually used by enterprises for R&D of next-generation materials, as one field expected to significantly advance.



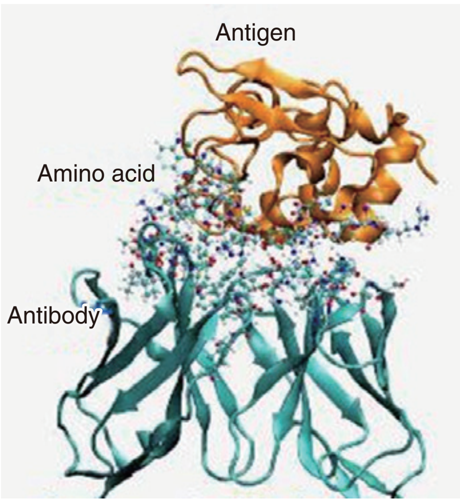
(a) Calculation model

(b) Dielectric constant

Figure 3
Calculation model and dielectric constant of amorphous Al_2O_3 predicted by first-principle calculation.[3),4)]

In the field of life science, especially drug discovery, simulation using supercomputers is giving rise to great hopes. For example, development is under way for an antibody drug that is effective against the types of cancers with high incidences in Japan (cancers of the lung, colon, stomach, liver, pancreas, prostate and mammary gland) and progressive cancer that has recurred or metastasized and produces few side effects. The aim is to create artificial antibodies that target cancer cells only and it is attracting attention as a revolutionary drug with few side effects as compared with treatment with the existing anticancer agents. The number of low-molecular compounds that make candidates for drugs is said to theoretically amount to 10 to the power of 30 or more and, for many years screening by means of computers has been conducted as a preliminary step in investigating candidate compounds. Screening candidate compounds requires a simulation that assumes an in vivo environment with a drug administered to a patient. However, most of the conventional simulation techniques only accommodate a vacuum environment due to the limitations on the computation technique and speed, and a problem with the reliability of the simulations has been pointed out.

This problem is being solved thanks to the improved performance of supercomputers and the advancement of computational science and technology. That is, it is now possible to calculate the motion of all atoms constituting a protein in a water solution by using one of several analysis methods, such as molecular dynamics (MD), with the surrounding water molecules simulated and predict with high accuracy the structural changes in the protein and binding affinity between the protein and a compound.[5),6)] Use of such simulation technology makes it possible to accurately identify the complicated interaction between an antigen (cancer cell) and antibody via a low-molecular compound that makes a candidate for the drug. In addition, by running in parallel many independent simulations using a large-scale automatic parallel algorithm, free energy change in the binding and dissociation processes of the protein and low-molecular compound can now be calculated. **Figure 4** shows a simulation of how antigens and antibodies are bound to each other in water via an amino acid; this simulation makes it possible to accurately predict the interaction between the antigens and antibodies while incorporating the effect of the surrounding water molecules. With the conventional computers, this simulation took 10 days for one case but the latest supercomputers are capable of computing a few different types in one day. There are now hopes that it will be possible to use computer simulations to develop an effective anticancer agent with few side effects.



Source: Systems Biology and Medicine Laboratory, Research Center for Advanced Science and Technology, The University of Tokyo

Figure 4
Example of molecular dynamics calculation of antigen-antibody reaction.

Other expected achievements of supercomputing include playing a major role in the establishment of a safe and secure society in the future. The Great East Japan Earthquake that occurred on March 11, 2011 had a magnitude of 9.0 and an intensity far beyond that assumed in the design of buildings and facilities. The earthquake and tsunami caused extensive damage to the Tohoku Region (the northeastern region of Japan's main island) and other areas. The four atomic power plants located on the coast of the region were seriously damaged. All of the 11 reactors that were in operation when the earthquake struck had their control rods inserted and were brought to an emergency stop. Among them, four of the six reactors in the Fukushima Daiichi Nuclear Power Plant lost their cooling functions and reached a serious condition. In particular, very highly radioactive materials were detected in the turbine building but the process of their generation was not immediately identified, and this caused a major obstacle in recovering the cooling functions.

Even in such a situation, more reliable safety assessment of buildings and structures can be achieved if the heights of the waves caused by a tsunami, for example, can be predicted with high accuracy. In addition, the ability to predict multi-scale, multi-physics phenomena such as seismic wave propagation in the earth's crust and ground, vibration response of concrete buildings, vibration response of containment and reactor vessels and fluid-flow-structure coupled vibration of the fuel rods and the surrounding coolant will make it possible to accurately assess the margin of safety of buildings, devices and parts against the input of seismic waves assumed in design.

4. Strategic promotion of supercomputing

As described above, the use of supercomputers has raised expectations for various breakthroughs in the manufacturing sector. For Japan to exercise long-term leadership in this sector, however, continuous development of supercomputers and strategic promotion of computational science and technology are required.

While the peak performance of computers is rapidly improving year by year, bringing out the performance of computers in actual application software is conversely becoming difficult and this trend is expected to further intensify in the future. The reasons for this include the fact that the number of processor cores of a computer is increasing and the ability to transfer data from memory to a CPU is being relatively degraded in comparison with the performance improvement of CPUs. Since 2005, the operating frequencies of CPUs and memory have barely increased and the performance improvement of computers has been realized entirely by increasing the number of processor cores. For example, the K computer is equipped with 640 000 processor cores and application software cannot bring out the computer performance unless these processor cores can be run concurrently. Ingenuity is also required to minimize the number of accesses to memory and make efficient use of data once transferred from memory to a CPU.

In this way, future development of application software must be carried out while giving due consideration to the characteristics of computer hardware. Meanwhile, the development of computer hardware must also be conducted based on a thorough understanding of how each piece of application software performs computation and communication. Furthermore, the development of technology for making the most of large-scale massively parallel computation in the sites of design and R&D is important as well.

Japan, the U.S. and China, a country which has recently been catching up in the development of computer hardware, are the only countries with technology that allows processors for supercomputers to be independently developed. By making use of this capability to promote technological development for supercomputing based on integrated development of hardware, application software and utilization technology, Japan will be able to exert long-term leadership.

In manufacturing, the development of fundamental application software is essential but that alone is not enough to put it to practical use in product design. To make the most of advanced computational science simulations for manufacturing design, a next-generation CAE system must be established that is equipped with a preprocessing process allowing rapid computation by using design data, a postprocessing process to efficiently feed back the computation results to design, and functions to assist optimization of design. To take fluid flow simulation as an example, direct computation using a computational grid containing tens of billions of points is expected to become possible at a practical level in a few years but, without a system that allows users to conduct analysis while not being aware of the large-scale computational grid, the computation will be useless in design. Such a system cannot be realized by extending the existing preprocessing and postprocessing. The preprocessing information accessible to users is CAD data or relatively small computational grids and the postprocessing information should be information of a highly consolidated flow field. All of the processing between them must be realized by massively parallel computation. That is, a paradigm shift in the entire design system by fluid flow simulation is required. In addition, it is also important to have greater user-friendliness as a design system by providing databases of material constants and such like or allowing examples of large-scale analysis to be reused.

5. Conclusion

Innovation of manufacturing by making use of supercomputing is giving rise to great expectations. At present, however, many enterprises only use numerical simulations with a few CPUs at the most. One reason is that the effects that can be actually produced in product development by using massively parallel computation with supercomputers have not been verified. Another factor hindering the dissemination of supercomputing is that considerable investment is required for individual enterprises to introduce computer facilities and application software themselves and make them usable in sites of R&D and design.

As one measure for overcoming these hurdles, cloud computing is attracting a great deal of attention. While cloud computing has not made much progress in Japan, it has already become popular in the West. Cloud computing allows users to use computer resources on an as-needed basis simply by connecting to networks without having to put in place or maintain large computer facilities. In addition to computer resources, if kinds of application software use services (software as a service: SaaS) and also analysis services become well developed, enterprises currently not using CAE, let alone supercomputers, will come to use simulation, which as a result is expected to lead to further advancement in the supercomputing technology of Japan.

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