New Technologies of Applications Using Supercomputer

● Masahiro Watanabe ● Tamon Suwa ● Atsushi Furuya
● Kentaro Takai

In recent years, with the incredible increase of computing power, we can simulate accurately macro-scale phenomena based on the laws which govern micro-scale phenomena. For example, if we fully utilize the computing capability of the K computer, it is possible to simulate the behavior of a human heart and how it responds to medicine at the cellular level, and to calculate the efficiency of an electric motor by simulating the characteristics of its magnetic material. However, a problem arises because we must control more than tens of thousands of parallel processes properly in order to get high performance out of the recent supercomputers. For this reason, new computation techniques based on both the latest scientific findings and the understanding of supercomputer architecture are required. In this report, we introduce four applications as our approach to the problem described above.

1. Introduction

Fujitsu has been vigorously working on the development of supercomputers since the 1980s, mainly focusing on large scale integrations (LSIs), systems, software including operating systems and middleware and mathematical libraries. Meanwhile, the development of applications such as computer simulations has been left to external research institutions including universities and national laboratories and independent software vendors (ISVs). However, for effective utilization of massive large-scale parallel computers such as the K computer,[note)] a certain paradigm shift is required in application development as well. That is, as known by Amdahl's law, the ratio of the sequential fraction has a major impact on the scalability of a computer when a program is run in a parallel environment. As a result, the program itself ends up being unable to effectively use computation nodes even if they exist in abundance. The K computer has 640 000 cores and, to achieve a scalability of about 90%, the execution time for the sequential fraction must be reduced to about 1/5.8 millionths of the whole or less. Except for simulations using Monte Carlo methods or such like, the development of such a parallel program requires us to create new computation techniques based on thorough consideration of computer architecture. The key to doing that is to combine computer development technology and application technology.

Accordingly, since its initial development of the K computer, Fujitsu has embarked on research and development of applications as it aims to solve these challenges and achieve effective utilization, in a true sense, of super-large-scale computation systems like the K computer. For improved efficiency in these activities, Fujitsu has cooperated whenever

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.

possible with universities, enterprises and national research institutions already engaged in leading-edge research to move forward with the development of a super-large-scale parallel program.

This paper presents our approach to research and development in relation to four applications in which utilization of simulations in super-large-scale computation systems is expected to serve useful purposes.

2. Heart simulator

In biological phenomena, mechanical and electrochemical phenomena on multiple scales ranging from a micro scale of protein molecules through cells and tissues to a macro scale of organs and individuals mutually influence each other. The dramatic improvement in performance of computers in recent years has made simulation of such complicated biological phenomena possible. Advanced biological simulations using large-scale parallel computers exemplified by the K computer are expected to help people have an integrated understanding of molecular-level systems obtained through the development of biotechnology and macro-level life phenomena.

One of the organs attracting attention in this field of biological simulations is the heart. The role of the heart is to circulate blood containing energy sources (sugars etc.) and oxygen by using its pumping function that it achieves through contraction. It cannot achieve this pumping function without having coordination between multi-physics phenomena involving mechanics, biochemistry and electrophysiology which encompass multiple scales including molecules, cells, organs, and a living body, as shown in **Figure 1**. Heart simulations are a promising means of making clear the pulsation phenomenon and pathology of the heart. In addition, we believe that heart simulations are clinically effective as well. For example, heart simulations can assist doctors with diagnosis in cases where the most appropriate procedure is difficult to choose: heart valve replacement surgery, coronary artery bypass surgery, ventriculoplasty, or such like. This is because estimating the postoperative movement of the artificial valves, blood flow through artificial blood vessels, and

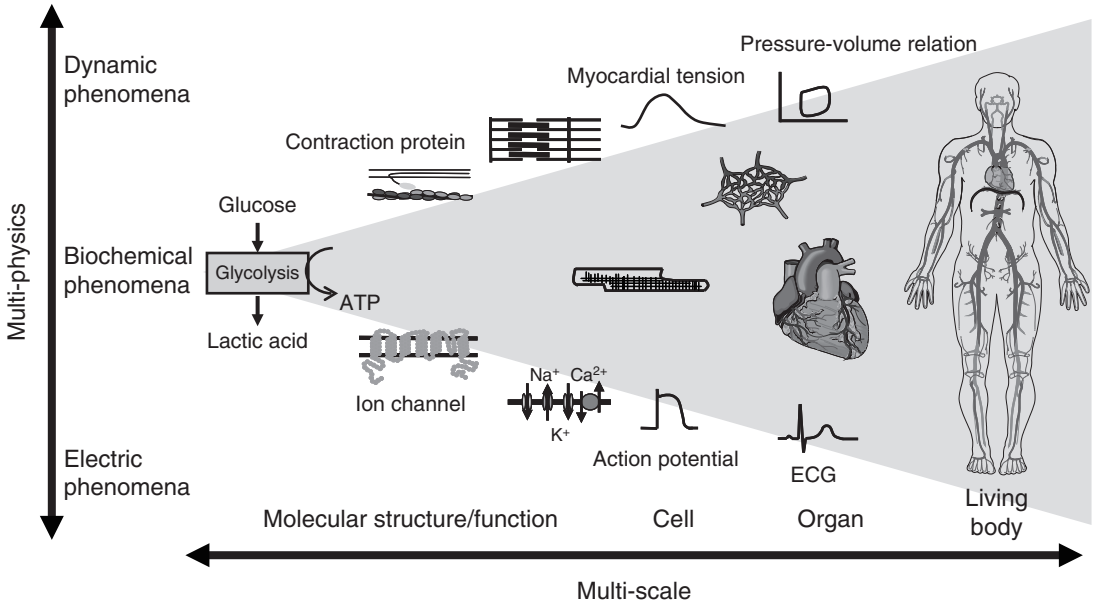


Figure 1
Cardiocirculation consisting of multi-scale and multi-physics phenomena.

volume of blood ejected can be used together with the existing diagnostic information such as blood pressure electrocardiogram (ECG), computed tomography (CT) and magnetic resonance imaging (MRI) to quantitatively evaluate the effect of procedures.

We are cooperating with Prof. Toshiaki Hisada, Prof. Seiryo Sugiura and other members of their team at the Graduate School of Frontier Sciences, the University of Tokyo to work on the research and development of the heart simulator (UT-Heart), which is based on the finite element method and achieves seamless coupled calculation including a scale of cardiac myocytes and macro pulsation, and its speedup.[1] It is intended to realize *tailor-made medical treatment* that uses data, reconstructed in a three-dimensional way, on cross-sectional images of the heart of individual patients obtained by CT and MRI to select the most appropriate treatment method for each patient. The following briefly describes the two types of heart simulators we are developing.

2.1 Heart simulator based on macro constitutive laws

When an electrical impulse is propagated from the pacemaker cell (sinoatrial node) located at the top of the right atrium to the surrounding cardiac myocytes, calcium ions are released from the sarcoplasmic reticulum of the individual cells to increase the intracellular calcium ion concentration. If the calcium ion is connected to a part of an actin filament, a bond between actin and the myosin filament is permitted (forming of a cross-bridge) and the rotation of the head of the myosin filament makes the actin filament slide. As a result of these processes, the myocyte contracts. Such contraction of cardiac myocytes occurs in the entire heart in a coordinated manner, and in this way the heart pulsates. Our heart simulator performs coupled calculations of:

- Propagation of electrical excitation of cells
- Increase in intracellular calcium ion concentration
- Actin-myosin filament state transition
- Contraction of cardiac muscles
- Flow of blood

Then, the pulsation of the heart and pumping process of blood is realized on the computer. In the excitation propagation analysis, the time series of a membrane potential and concentration of calcium ions are calculated by the finite element model for the heart in which the ion channel mathematical model, known as electrophysiology, and organs inside or outside of cells are combined. Mechanical analysis simulates the myocardial strain and flow of blood caused by the contractile force which is derived from the calcium ion concentration in cardiac myocytes calculated in the excitation propagation analysis.

The heart simulator based on macro constitutive laws takes into account the alignment of myocardial fibers and reproduces the high pumping ability (i.e., ejection fraction) of the heart that reaches 55% in volume despite the fact that the contraction of myocardial fibers is around 10%. **Figure 2** shows a virtual ECG output by the heart simulator. After comparing the lead II ECG and measurement results, we found they coincide fairly well with each other.

2.2 Multi-scale heart simulator

The multi-scale heart simulator realizes coupled calculation analysis encompassing a scale of cardiac myocytes and a macro scale at the organ scale. It applies the results of state-of-the-art medical measurements, cardiac myocytes mathematically modeled based on nonlinear finite element theory (numerical cardiac myocytes) and a multi-scale technique called the homogenization method adapted with the focus on the periodicity in the arrangement of cardiac myocytes in the actual heart. We are moving ahead with research and development mainly in view of applying our work in the field of internal medicine. For numerical cardiac

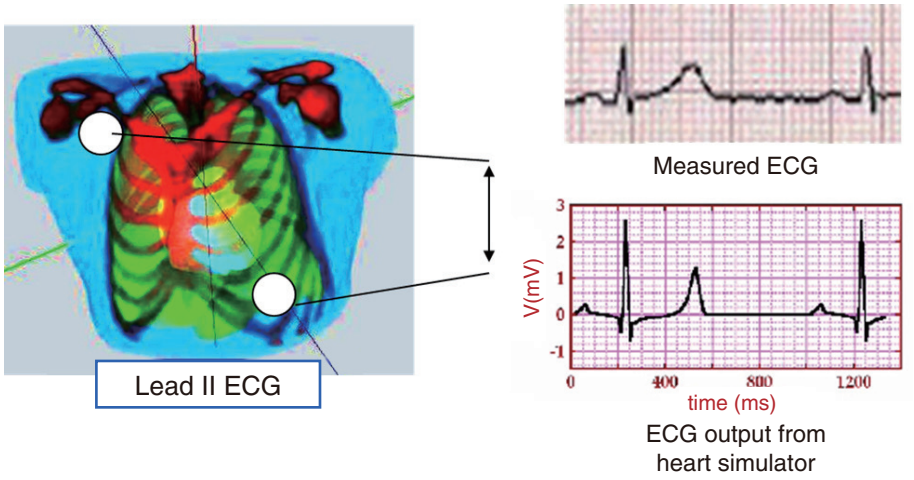
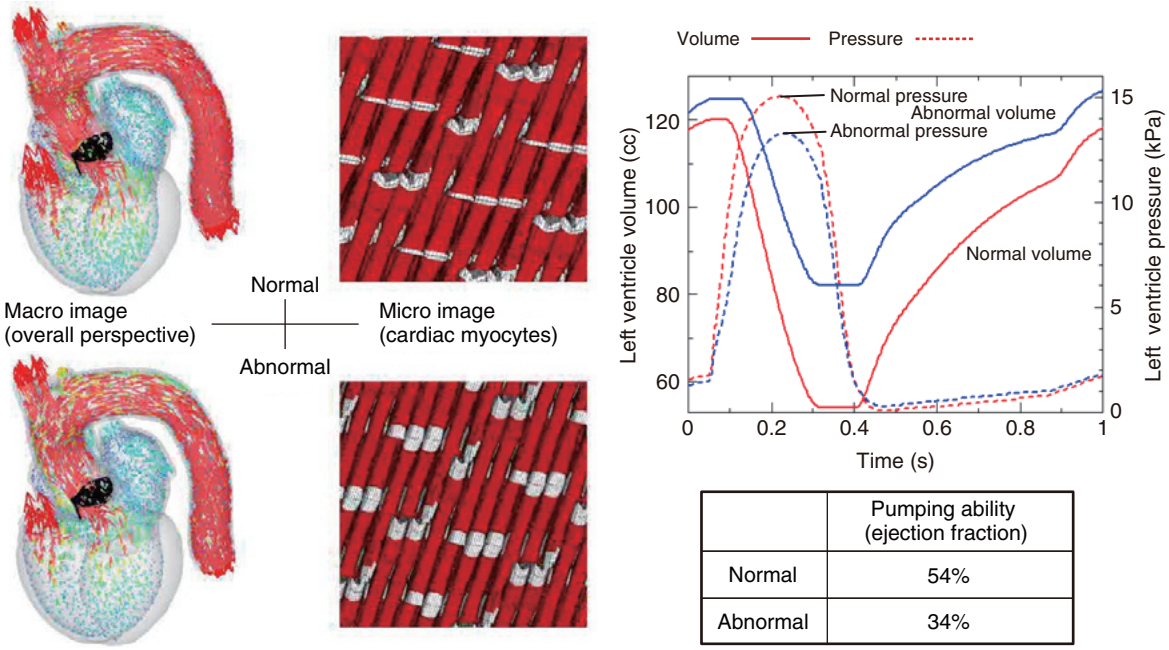


Figure 2
Lead II ECG from simulator (bottom right) and real one (top right).



	Pumping ability (ejection fraction)
Normal	54%
Abnormal	34%

Figure 3
Influence of abnormal cell adhesion protein (vinculin) on blood ejection and pressure.

myocytes, proteins responsible for intracellular organization or intercellular or interfilament junction are incorporated in the model. As an example, the result of a simulation assuming a disorder with congenitally weak adhesion between cardiac myocytes is shown in **Figure 3**. The reproduction of the clinical condition in which pumping grows weaker can be confirmed.

As described above, the human heart is a massive, multi-scale and multi-physics complex. Our heart simulator, which is designed to reproduce the whole heart system according to the principles by which it operates, needs to handle an enormous amount of data for the respective scales and phenomena. The processes of coupling them grow to be huge and its execution would require a tremendous amount of time with the extension of the existing

computation techniques. Accordingly, speeding up the processes is a significant challenge to tackle in order to put this heart simulator to practical use in the field of cutting-edge medicine. We are aiming at speeding it up so that this calculation can be completed in approximately two days by using the more than 80 000 CPUs of the K computer through the development of massively parallel computation techniques and high-speed solvers. In **Figure 4** the speedup of strong scaling in the multi-scale simulation on the T2K Open Supercomputer (of the University of Tokyo) is depicted. This figure reveals good scalability that is demonstrated with 89.3% of the ideal value achieved in computation that uses 6144 cores.

In order to promptly realize diagnostic support and medical treatment support to the 150 000 patients (nationwide estimate) suffering from cardiac disease, we are developing the input data processing technology capable of accurately reproducing physiological and anatomical information and the geometry of the heart of each patient. At the same time, we are improving the accuracy and efficiency of the heart simulators presented in this section. Our target is to realize a tailor-made medical treatment system by combining these technologies.

3. Particle-based simulator

A particle-based method is a computation technique for representing the target of analysis as a set of particles. The smoothed particle hydrodynamics (SPH) method[2] and the moving particle semi-implicit (MPS) method,[3] which are techniques for discretizing continuous materials such as fluids (water, air, etc.) and elastic materials (rubber, gel, etc.) by using particles, are well known as representative examples. A technique of conducting a simulation by using naturally granular materials including pebbles and pellets as particles can be seen as a type of particle-based method. This section describes the techniques we used with the focus on the SPH method[4] we are developing.

In particle-based simulation, continuous materials are represented by a distribution of particles. Each particle has physical quantities including position, velocity, density and stress as variables and the actual behavior of the object is simulated by calculating their temporal changes. For the computation, each particle has an influence only on particles within a certain range (called the smoothing length h) from itself

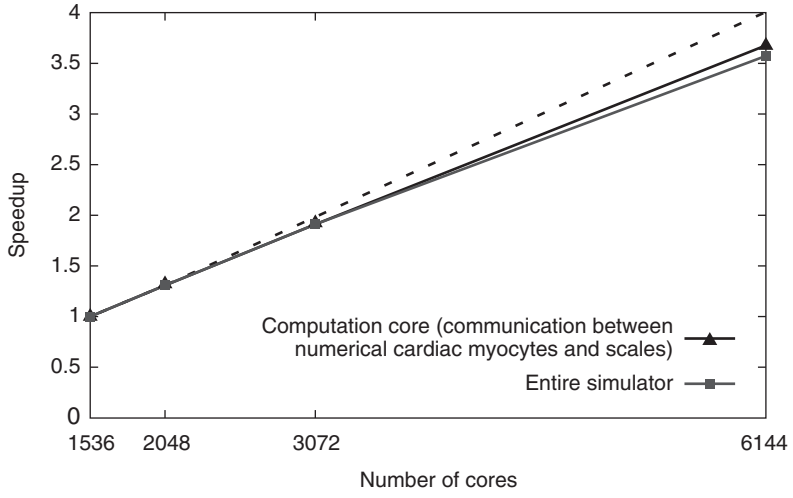


Figure 4
Speedup of multi-scale heart simulator.

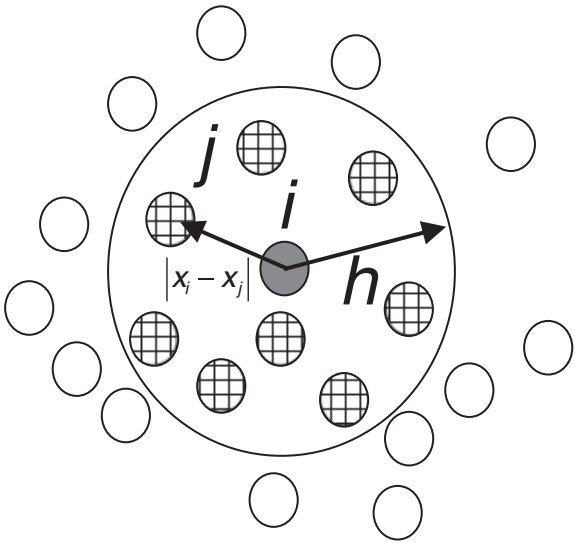


Figure 5
Smoothing length *h* and neighboring particles *j* (hatched) of particle *i* (gray).

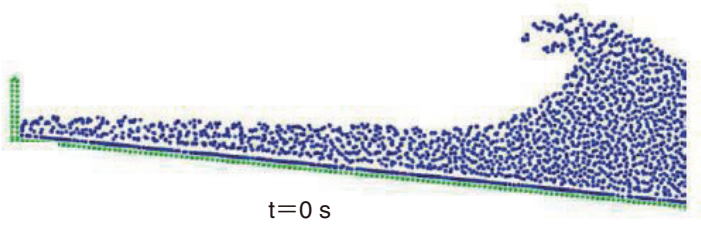
(neighboring particles) and vice versa. For example, particle *i* shown in gray in **Figure 5** has an influence only on particles *j* (hatched) and vice versa. By searching for these neighboring particles as required, a high degree of freedom can be given to the spatial distribution of particles, which allows us to avoid mesh failure that can occur in the finite element method and other techniques. This shows the characteristics of particle-based methods makes them suitable for handling large deformations and free surfaces.

Each particle only uses information on neighboring particles, which means that particle-based methods characteristically suit massive parallel computation. Parallel computations can be executed by spatially dividing the calculation area in an appropriate way and assigning each sub-area to each processor. Our particle-based resolver can achieve a scalability of 90% when the particle distribution is nearly uniform.

On the other hand, particle-based methods have only a short history of industrial application and have challenges including the facts that the number of actual application examples is still small and that guaranteeing the accuracy in a mathematically precise way is still insufficient. We believe these challenges will be solved in the future. As an approach to finding a solution, we are attempting to uncover user needs and are engaged in joint research with universities for increasing the number of application examples and obtaining mathematical backing of the theory.

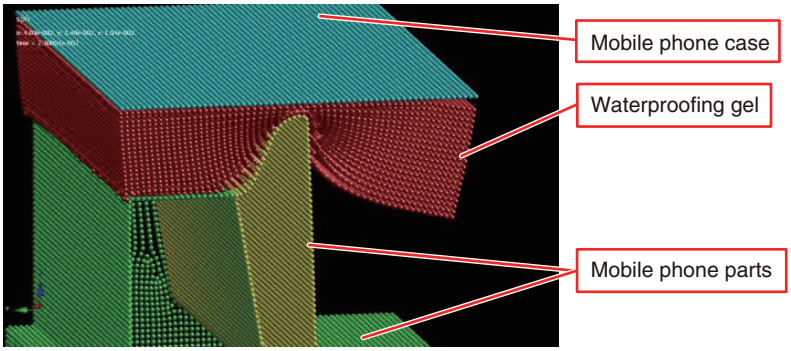
Particle-based methods can be applied in a variety of fields. The first one to mention is the field of disaster prevention including tsunami analysis. For example, in the processes of flooding of urban areas by a tsunami and wave-breaking on a seawall of high waves caused by a typhoon, the fluid (seawater) has a free surface that can deform in a complicated manner, which makes it suitable to be handled by the particle-based method. **Figure 6 (a)** shows an example of computation simulating the process of high waves breaking on a seawall. Tsunami analysis requires a large area to be handled in a simulation and, to calculate a harbor of around 1 km square with particle intervals of 1 m, for example, a PC cluster takes a few to a few tens of days. A supercomputer is expected to be able to complete computation of the same scale or even with the area expanded to a few kilometers square in about one hour. One problem posed in such large-scale computation is that the particle distribution (seawater distribution) is not uniform and an ideal parallelization efficiency is difficult to achieve. To address this issue, we are developing a computation technique that can keep the parallelization efficiency as high as possible for distribution with high nonuniformity. For example, we take a phenomenon in which particles move greatly in the direction in which the tsunami travels, but not as much in the orthogonal direction, to focus on specific characteristics and improve the efficiency of the simulation.

As another application, a particle-based method has been used to analyze a waterproofing gel used in mobile phones. **Figure 6 (b)**



t=0 s

(a) Analysis of overtopping of seawall



(b) Large deformation analysis of waterproofing gel used in mobile phones

Figure 6
Examples of particle method simulations.

shows an example of computation handling the deformation of waterproofing gel caused by mobile phone parts. It has been confirmed that the gel fills the gap between the parts and the pressure of a certain level or higher is applied to the entire surface of the parts.

As a development for the future, we are also working on enhancing the functions of this simulation so that it can be used for various industrial applications based on the fact that particle-based methods are characterized by their relatively high flexibility in incorporating various physical processes. Applications we currently aim at include:

1) Techniques for molding in a liquid phase such as casting and molten metal forging (implementation of solidification, shrinking and residual stress)
2) Processes of plastic kneading and agitation (implementation of visco-elastic material)

4. Magnetic simulator

Based on the improvement of the computational capacity of computers and advancement of simulation technologies, magnetic simulations using the finite element method are being applied to the design of electrical devices that use magnetic materials such as motors and transformers. However, because the present finite element method does not take into account hysteresis characteristics observed in magnetic substances, the energy loss cannot be calculated with sufficient accuracy. Accordingly, calculating the loss with the hysteresis characteristics of magnetic materials is important for further improving the efficiency and reducing the size of electrical devices.

Hysteresis characteristics of magnetic materials can be affected by various physical mechanisms such as the magnetic domain structure, magnetic anisotropy and magnetostriction of the magnetic materials. To deal with this, we are studying the possibility of using hysteresis models of an electrical steel sheet and ferrite by applying the method of micromagnetics.[5] This section describes a large-

scale simulation conducted by calculating the coupling loss with a hysteresis model based on micromagnetics with the finite element method.

Micromagnetics is a method of calculating the magnetization state according to the Landau-Lifshitz-Gilbert (LLG) equation shown in expression 1). We use a magnetic single domain particle as the fundamental model for calculation based on this equation.[5)]

$$\frac{dM}{dt} = -\gamma M \times H - \frac{\alpha\gamma}{M} M \times (M \times H) \quad (1)$$

Here, M is the magnetization, H is the effective magnetic field, γ is the gyromagnetic ratio and α is the damping constant. The magnetic field corresponding to the physical phenomena to be considered for the effective magnetic field H must be calculated. With an electrical sheet, magnetic anisotropy, an applied field and a classical eddy current field are generally introduced. A magnetic field caused by an anomalous eddy current due to magnetic domain wall motion can be introduced as shown in expression 2).

$$h_{ano} = \frac{H_{ano}}{H_k} = -\frac{c_{ano} \sigma L^2}{H_k} \frac{\Delta M}{\Delta t} \frac{H_{app}}{H_{app}} \quad (2)$$

Here h_{ano} is the effective magnetic field normalized with respect to the anisotropy field H_k.

The result of calculations performed with the hysteresis characteristics of non-oriented electrical steel sheets (35A350) used for motors is shown in **Figure 7**. The calculations (solid

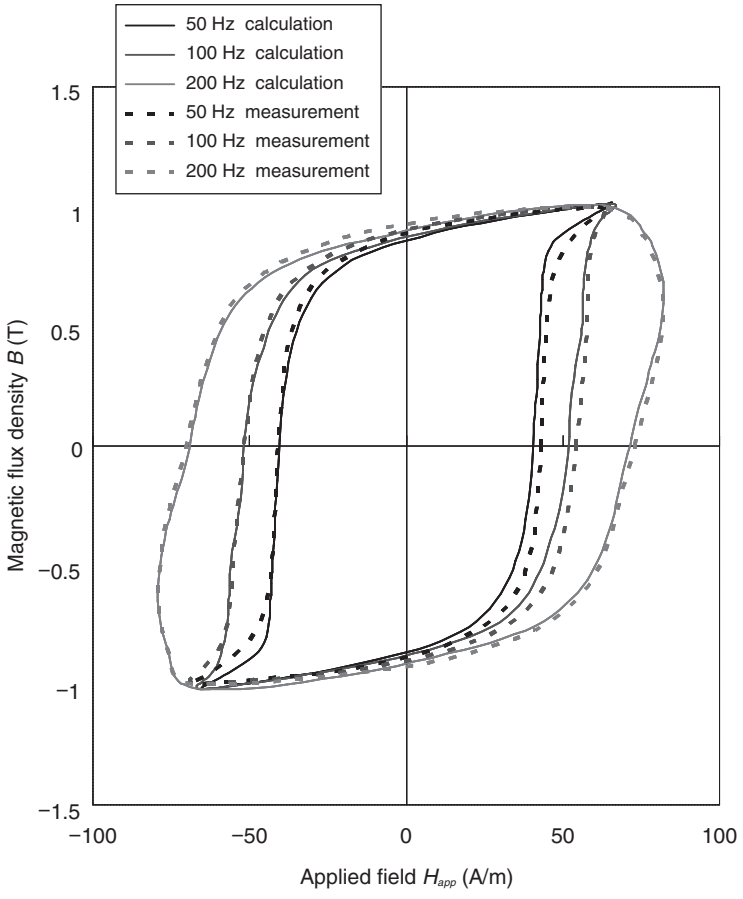


Figure 7
Hysteresis loops of non-oriented electrical steel sheets (solid lines: calculations, dashed lines: measurements).

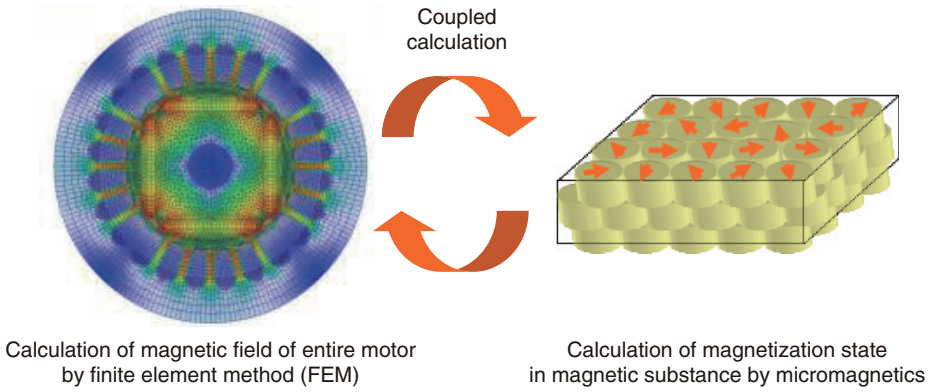


Figure 8
Analysis by coupling micromagnetics and finite element method (FEM).

lines) coincide very well with the measurements (dashed lines) at all frequencies and the frequency dependency of the hysteresis characteristics of non-oriented electrical steel sheets has been confirmed to be sufficiently reproducible by the method of micromagnetics.

To use the method of micromagnetics in calculating the loss of electric devices, micromagnetics must be coupled with the finite element method (**Figure 8**). The magnetic field distribution in an entire motor is calculated by using the finite element method and micromagnetics is used to calculate the hysteresis characteristics of the individual elements. Analysis of the entire motor including hysteresis characteristics becomes possible by considering the magnetic field characteristics in the mesh as uniform and applying the homogenization method. The application of micromagnetics significantly increases the computational complexity. For example, 3D analysis of a motor used in electric vehicles requires approximately 7 million elements, which takes about one month for computation if a PC cluster is used, and analysis as verification before design is difficult to carry out. Calculation in micromagnetics, on the other hand, can be independently processed for each element and features high scalability and very low communication complexity with reference to the computational complexity. For example, a parallelization efficiency of nearly 60% has been achieved with a PC cluster. For that reason, use of the 1000 cores of a massively parallel computer is expected to reduce the time required to a practical level of about one day.

5. Tight binding method

Computer simulations in the field of nanotechnology need material modeling, in which atoms are arranged one by one on a computer, and numerical calculation methods based on physical laws in order to investigate the behavior of atoms. First-principles calculations based on quantum theory and classical molecular dynamics calculations using a spring model for approximating an interatomic bond are well known methods to clarify the properties of materials on a nanometer scale (1 nm = 1 billionth of a meter), which corresponds to the size of atoms. The former only allows us to calculate small numbers of atoms due to the large amount of computational work (a few hundred atoms with a little over ten parallel processes). And the latter, which features little computational work, allows us to calculate larger numbers of atoms (a few tens of thousands of atoms with a little over ten parallel processes). One of the techniques capable of handling calculations on a scale between those of the above two methods is the tight binding method (TB

method)[6] (**Figure 9**). While it is approximately based on quantum theory, the TB method has a possibility of conducting simulations on a scale close to the size of the actual devices. Accordingly, we are focusing on developing a TB code and are making use of the localization of the electronic degree of freedom[7] to work on research and development for executing in a parallel way most of the computation. Our goal is to be able to simulate entire devices within a practicable time period by proving the parallelized TB code.

This subsection presents examples of calculation using the code under development. The calculated materials are silicon (Si), carbon (C) and 3C-silicon carbide (3C-SiC), which is one of the polytypes. In visible sizes, these materials have indirect transition characteristics and light emission hardly occurs. In nanoscale sizes, however, they are known to show higher emission intensity because of the quantum effect. For that reason, optical semiconductor devices that take advantage of this characteristic have attracted great attention from both industry and academia. Here, we attempted to clarify the physical properties of these materials by using the TB method capable of calculating relatively large sizes in short time periods while taking the quantum effect into consideration. Specifically, we prepared a model in which a cluster of up to about 3000 atoms (nanocluster) was made into a sphere and estimated the size dependency of light wavelengths corresponding to energy gaps of the nanoclusters (**Figure 10**). We found that the Si clusters with a diameter of 1 nm, the 3C-SiC clusters with a diameter of less than 2 nm, and the C clusters with a diameter of less than 2 nm have energy gaps corresponding to blue visible light, ultraviolet light, and far-ultraviolet light, respectively. Simulations of about 3000 atoms at room temperature were successfully performed in a few hours by using a 512-core machine.

In the future, we intend to carry out research and development on larger nanostructures. We

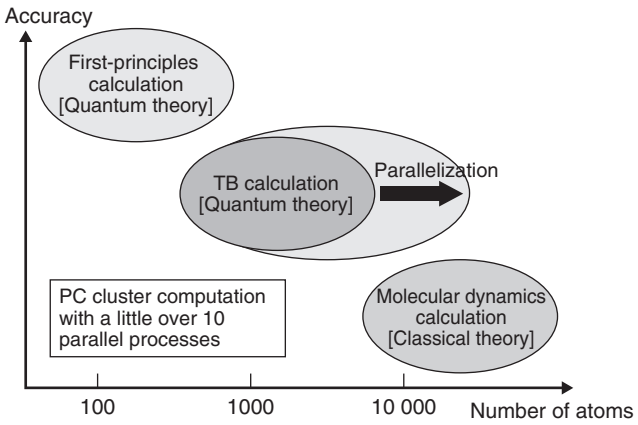


Figure 9
Computable numbers of atoms and accuracy for each calculation method.

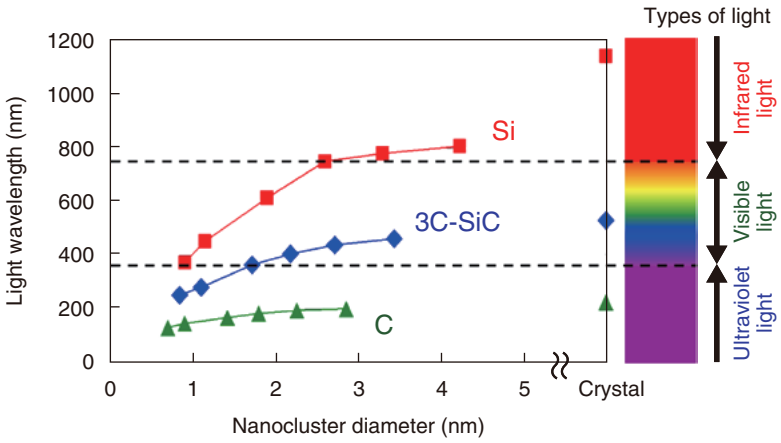


Figure 10
Size dependency of light wavelengths corresponding to energy gaps in Si, 3C-SiC, and C clusters at 300 K.

will also expand and enhance the functionality of applications as we aim to have supercomputers more effectively used in the field of materials development and promote the development of new materials.

6. Conclusion

This paper has presented the massive parallel simulation that we are developing. The computing capability of computers is certain to improve further in the future and it is easy to imagine that simulation technology using massive parallel computation will be called for more than ever. To realize a computer that can contribute to society in a true sense, we are committed to developing application technology.

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Masahiro Watanabe
Fujitsu Ltd.

Mr. Watanabe is currently engaged in research and development of heart simulator.

Atsushi Furuya
Fujitsu Ltd.

Mr. Furuya is currently engaged in research and development of magnetic field simulator.

Tamon Suwa
Fujitsu Ltd.

Mr. Suwa is currently engaged in research and development of particle-based simulator.

Kentaro Takai
Fujitsu Ltd.

Mr. Takai is currently engaged in research and development of tight binding method.