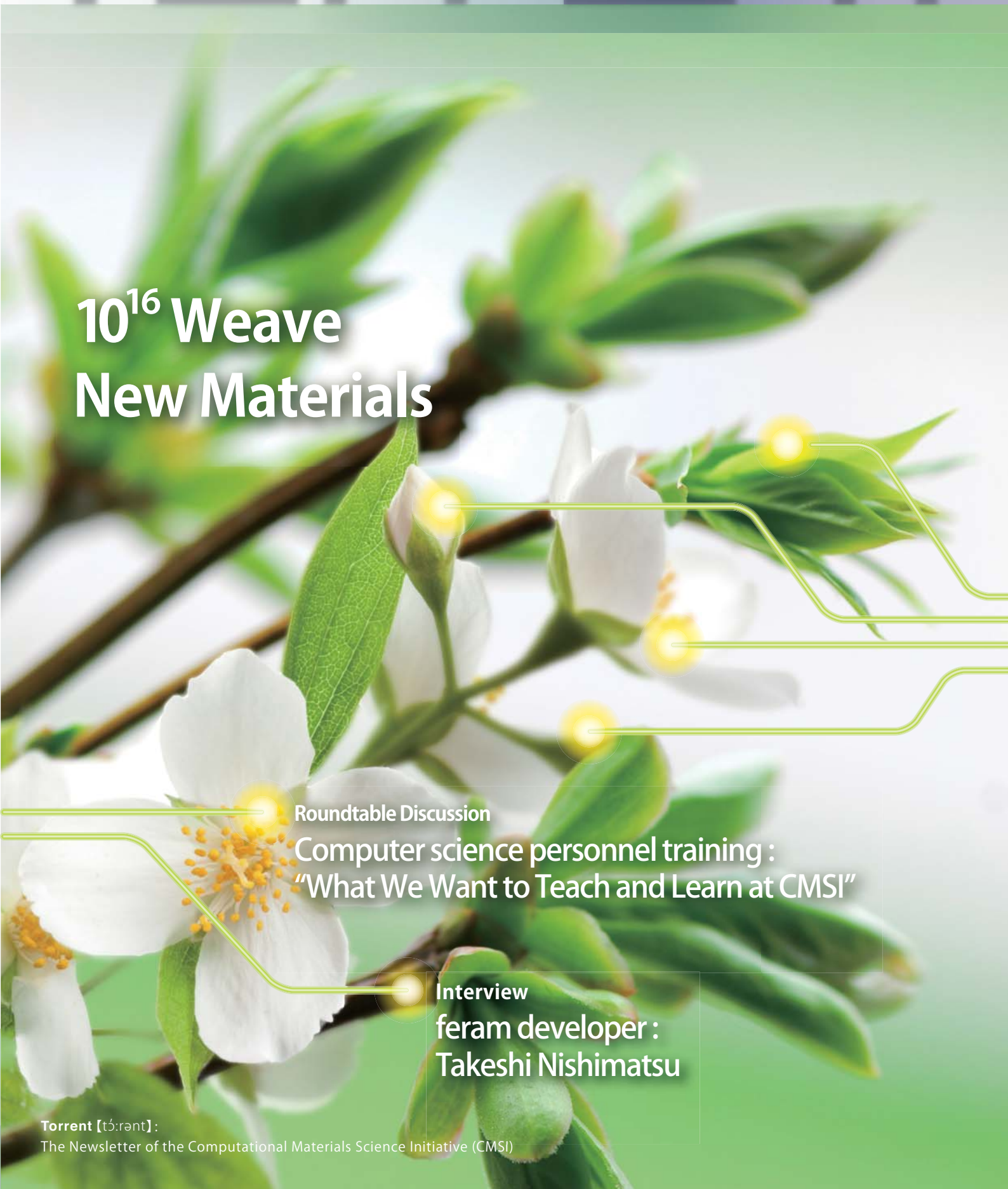
March 2012 NO.4

Torrent



10^{16} Weave New Materials

Roundtable Discussion

Computer science personnel training : "What We Want to Teach and Learn at CMSI"

Interview

feram developer : Takeshi Nishimatsu

Torrent [tɔ:rənt] :
The Newsletter of the Computational Materials Science Initiative (CMSI)

Torrent No.4 March 2012

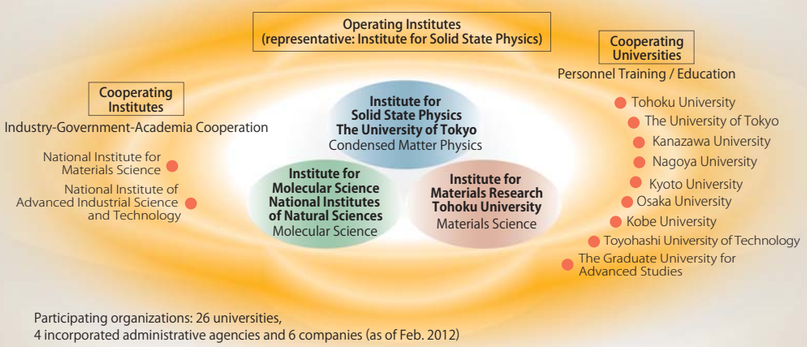
Cover: The image represents the research using the K Computer being about to flower right at this very moment.

The Computational Materials Science Initiative (CMSI) is a network-style organization made up of computational science researchers specializing in condensed matter physics, molecular science and materials science. CMSI was established through a grant for Field 2 "New Materials and Energy Creation" of the HPCI Strategic Program (SPIRE) of the Ministry of Education, Culture, Sports, Science and Technology. The Initiative is centered on three operating institutions — the Institute for Solid State Physics (The University of Tokyo), the Institute for Molecular Science (National Institutes of Natural Sciences) and the Institute for Materials Research (Tohoku University) and includes 11 cooperating institutes and personnel from universities, research institutions and companies involved in the field of computational materials science. It is an open community devoted to studying new research topics relating to computational materials science as well as providing collaboration and assistance for existing events and activities.

The goal of CMSI is to use supercomputers, among which the K Computer boasts the world's top performance, to create a new generation of materials science. Major research topics include determining the mechanism by which the functions of superconductors and molecules are manifested, developing next-generation technologies for energy generation and storage, producing breakthroughs that increase the speed of semiconductor devices, deducing the molecular control mechanisms of viruses and the like, and developing magnetic materials, structural materials and so on that offer equivalent performance without the need to use scarce elements. CMSI also provides computational resources for important new research topics that have been proposed, and support for further development.

The distinctive feature of CMSI activities is that one of their major objectives, in addition to state-of-the-art research and development, is the formation of a basic infrastructure for research and development that will lead to the next generation of computational materials science. For this purpose, CMSI holds seminars, symposiums, workshops, training sessions, collaboration with experimental researchers and company researchers, and other activities to build a network of people with an interest in computational materials science, especially young researchers. CMSI also provides support for organization-building and activities to promote the development and dissemination of computers and computer programs. In addition, CMSI promotes personnel training and education as well as public relations activities to promote the role of computational materials science in society and encourage understanding and interest.

The CMSI Newsletter "Torrent" was launched to provide a forum for interchange among students, teachers, researchers, companies and members of the general public, with a primary focus on covering the activities of young researchers. Its goal is to make people understand that the computational materials science is not a special esoteric field of science but one that is relevant to everyone. The Torrent staff will strive to make Torrent a medium that will create new encounters with a wide variety of people that will enhance and develop the discipline of computational materials science and its community.



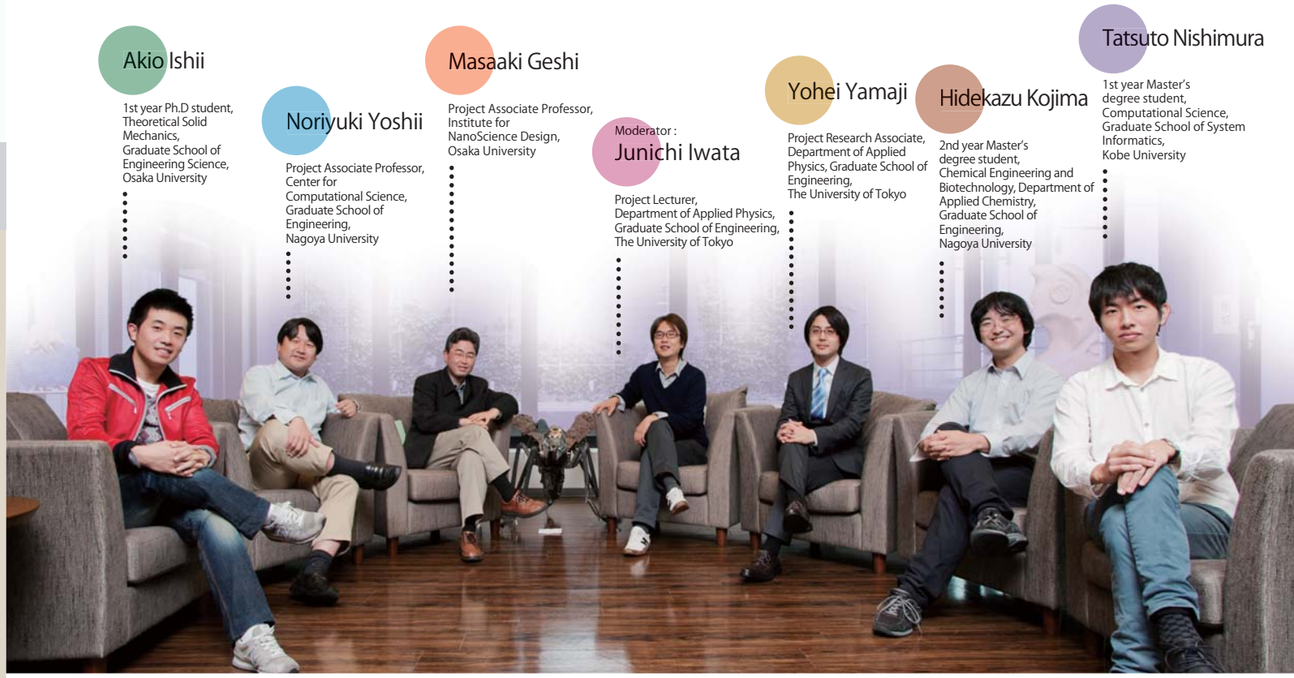
Participating organizations: 26 universities,
4 incorporated administrative agencies and 6 companies (as of Feb. 2012)

From left: Tetsuo Mori (Director, Materials Science Division), Naoki Kawashima (Director, Condensed Matter Physics Division), Shinji Tsuneyuki (CMSI Representative Director), and Kazuo Takatsuka (Director, Molecular Science Division) Photo : Shuichi Yuri

Roundtable Discussion

What We Want to Teach and Learn at CMSI

One of the most important roles of CMSI is to train computational science researchers. At the CMSI Divisions and institutions, new courses are starting up and teaching frameworks and systems are being discussed. We asked the teachers in charge of education and the graduate students to tell us what kind of instruction they were hoping for from their individual perspectives.



Starting with graduate school courses

Iwata (Moderator) : I don't have the experience to talk about CMSI education overall, but I'd like to begin from the explanation of a basic premise of today's discussion. It's clear that computers become increasingly complex and it's becoming difficult to write extensive program codes on the side of our primary work. So, we have to consider how to hone our skill at using such advanced computers while pursuing our researchs and how to make it easy for students to enter the field of computational materials science.

Instructors, what are you planning to do at CMSI from the next fiscal year?

Yoshii : Right now I'm in the process of formulating teaching plans. There are existing frameworks that can be adapted for CMSI projects with slight modification, and I'll utilize those. For example, this fiscal year we started supporting the Molecular Simulation School that had previously been held by the Molecular Simulation Society of Japan. In December, we will hold a Molecular Simulation School that will be organized by CMSI and the Institute for Molecular Science.

In the next fiscal year, we plan to create a credit transfer system using the existing systems between Nagoya University and the Graduate University for Advanced Studies. This will enable students to attend lectures on molecular simulation in the Advanced Molecular Physical Chemistry Course at

Junichi Iwata
Specializes in the first principle calculations and density functional calculations in the condensed matter physics. Currently using massively parallel computers to develop code for large-scale first-principles calculations.

Nagoya University and lectures on computational science at the Graduate University for Advanced Studies.

Iwata : Are you teaching at the Molecular Simulation School ?

Yoshii : Yes, I teach a class on parallelization. I start from the very basics, such as the structure of parallel computers, and cover up to OpenMP. I cram all of that into an hour and a half. Each time, there are about 100 students. I'm happy to see that molecular simulation has gotten this much exposure.

Kojima : I've attended the school twice, and I know a lot of people who have attended it.

Geshi : At Osaka University, there are Computational Materials Design (CMD®) workshops twice a year in which the density functional theory is mainly focused. The next one will be the 20th to be held. It's a five-day training camp style workshop. Students who attend can get graduate school credit at Osaka University, and it's also a required course for the continuing education program. But members of the general public who have no connection to any of those attend the workshop as well. There are four courses: a beginner's course, an advanced course that expands on the beginner's course, an expert course, and in 2010 a supercomputer course was also added. In the supercomputer course, a small group of students learn how to master supercomputers and the ways in which they can be used. Up to now, the course has been held using up to 8 nodes of the SX-9 in the Osaka University Cybermedia Center.

This workshop is popular with students who want to learn first principle calculations. Even if you're from the experimentation side and you feel self-conscious about knocking on the door of a research institute and asking to learn from them, you can feel free to ask any question you like.

Iwata : And you can get college credit by attending the workshop?

Geshi : Yes. The credits are approved as long as you receive the certificate of completion.

Also, to make it easy for people who have jobs, the courses are broadcast nationwide from 6:00 to 9:00 in the evening over a teleconferencing system. So you can study all the way through from basics to application.

Yamaji : The goal of CMSI instruction overall is to coordinate with all the other Educational Divisions. However, at the University of Tokyo there is not yet an adequate framework for delivering courses. For this reason, at the outset, we plan to begin in FY 2012 with 1st and 2nd year Master's degree courses taught on-campus together with Prof. Iwata. The courses will deal with linear algebra, the Monte Carlo method, partial differential equations and other mathematical topics relating to time evolution. In addition, students will write their own programs from scratch, starting from the simple things, and have students train up through parallelization using MPI and OpenMP. We'll prepare a PC cluster environment that allows students to freely use up to 120 processors in parallel.

Masaaki Geshi
Specializes in first-principles calculations and density functional theory (DFT) calculations. Designs new materials that are synthesized at high temperature and high pressure. In terms of large-scale computing, parallelizes the Order N tight-binding approach using MPI and conducts experiments using approximately 2 million atoms.

Noriyuki Yoshii
Uses molecular dynamics calculations to study the interaction between biomembranes and drugs, as well as drug membrane permeation phenomena.

Yoshii : How many students do you anticipate being in each class?

Iwata : We've reserved a study room that can accommodate 80 students. But we only expect about a half of the number.

Yamaji : Ultimately, we're planning to receive courses from the other CMSI Educational Divisions and transmit our courses to the others. At present, there is no credit transfer system between the Divisons, so we plan to start with places nearby like Tokyo Institute of Technology and Ochanomizu University and accumulate experience, as well as cooperating with Prof. Geshi and Prof. Yoshii to deliver courses.

Interchange with computer science is also education

Iwata : As students, what kinds of things are you hoping for the courses?

Ishii : We have to study a lot if we want to be able to do parallel computing well enough to enable our knowledge to stand up to actual use in research. We all want to use parallel computing for practical research, but how should we approach that?

Yoshii : There are two sides in CMSI. One is the people who develop the codes for the K Computer, the fastest computer in the world. The other is the people who want to use the K Computer to do actual research. I think we have to teach the users and the code-writers differently.

Yamaji : The issue is practical application. Even when you talk about parallel computing, if you're using the Monte Carlo method, for up to 100 parallel computers or so you don't need any specialist study.

Yoshii : If there's existing code, then you can use that. But particularly in the case of molecular dynamics (MD), you can't clearly sort things into "OK, for this calculation we can use such-and-such a routine." If you don't have any code, you have to begin your research by writing the code.

Iwata : There are many program libraries in which the most commonly used calculations are collected. One way would be to have your own programs linked to those libraries.

Yoshii : It's definitely true that some parts of the programs we've written are ridiculously slow. If one replaces those sections by a numerical librariy, sometimes performance suddenly picks up.

Yohei Yamaji
Earned his degree through analytical research of copper-oxide superconductors and other strongly-correlated electron systems. Currently conducts numerical calculations for many-body electron systems. Expected to be involved in code development for parallel computing with 10,000 – 100,000 processors in the future.

Molecular Simulation School (CMSI/TCCI, the Institute for Molecular Science, the Molecular Simulation Society of Japan)

Geshi : It's difficult to sit down and really focus on numerical techniques, but there are certain things that you should know. What about the idea of getting information from specialists in numerics? It seems like CMSI should take the lead in that kind of interchange.

Iwata : On the theory that interchange will turn into education.

Geshi : There's an advantage in using the code for people like us, but conducting joint research with us also provides advantages to the people who create the code. I think we need a place where research "needs" could be matched with research "seeds" and the joint researches could be expanded into the development of new algorithms and so on.

Kojima : I'm interested in writing programs and gaining an understanding of the principles. If possible, I'd like to write programs myself. Right now I'm working on one-dimensional reactions, but there's room to expand this, to three dimensions and so on. If that happens, I guess I'll have to write the program myself.

Yamaji : I hope students will be interested enough to do that.

Geshi : The Institute of Industrial Science at the University of Tokyo invites specialists from Hitachi to conduct intensive training courses in which students write programs in half a term.

Nishimura : Are the courses on parallelization designed for graduate students?

Yoshii : The credit exchange program is for graduate schools. But even at the undergraduate level, the physical chemistry laboratory instruction includes an introduction to molecular simulation.

Geshi : The current workshops are for graduate level and above, and even for working people they're for people with a Master's degree or above. The purpose is user training, so we have to encourage the use of simulations by showing how helpful they can be to undergraduates and members of the general public, and gather more people who want to do full-fledged computational science.

Yamaji : I'm all in favor of providing instruction from the undergraduate level onward. But the fourth year students have to conduct experiments, and they have to study statistical mechanics and quantum mechanics as well. So the question is how to incorporate numerical calculations and how to motivate them.

Geshi : People from companies have clear motivation. There are even some who look to first-principles calculations to provide them with direction in their own research. And these days people in a management

role can't get by without a knowledge of first-principles calculations.

Many paths to large-scale computing

Iwata : I'd like to ask you, students. What type of research are you planning to do from now on?

Kojima : I want to go on to the next stage of higher education and continue doing research of proton transfer reactions in solutions. Right now I'm working on intramolecular reactions, but I'd like to expand this to reactions between molecules and three-dimensional reactions. In intermolecular reactions, we have to deal with numerous molecules, so it gets even more difficult.

Iwata : You have not only the problem of the cost of computations, but also have the fact that the methodology has not yet been established. So you have to do everything: develop the theory, create the program and so on.

Yoshii : That's like what Mr. Ishii is working on, analysis of carbon diffusion in solids.

Ishii : The technique itself is in place, but there's no immediate need for large-scale computing. My laboratory's style is apparently to use small systems and keep the amount of calculations to a minimum to perform "smart" analysis of phenomena. We have a parallel computer of 20 processors with 8 cores each to perform parallel computing.

Akio Ishii
Affiliated with a condensed matter physics laboratory. Currently studying MD acceleration using a statistical-mechanical approach and its application to the analysis of solid interiors.

Iwata : Mr. Nishimura is developing programs with the prospect of parallel computing in mind.

Nishimura : In the PC cluster in our laboratory, I use only one core, and it's now at the stage where we can use it for parallel computing from this point on. So at present we're only using one node, but in the future I want to make them into programs designed for large-scale parallel computing that can run on the K Computer.

Iwata : In other words, your goal is not only parallelization using existing computing methods, you're thinking about it from the algorithm level onward?

Nishimura : That's right. I only started learning parallelization after I joined the laboratory.

Iwata : Mr.Nishimura, since you have an information systems background, I'd assumed you were using the parallel computers more than that.

Nishimura : We have a training course for third year students in which we connect four Macs together in parallel. So there are some undergraduate students who have a basic knowledge of parallelization. A computer science major was created a year ago, and I've just started studying parallel computing as well.

Tatsuto Nishimura
Studied information systems in his undergraduate days, but joined a quantum chemistry laboratory. Currently studying the development and implementation of algorithms for numerical calculation of two-electron integrals, as well as parallelization.

Yamaji : Are the fields of algorithms and code development highly regarded?

Nishimura : My laboratory focuses on chemistry, and it's difficult for someone with an information systems background to come into the laboratory and suddenly be told to start doing chemistry. Leaving aside the question of whether or not you'll receive recognition for it, it's still computing. Computing doesn't exist in a vacuum; it only has meaning once it's linked to something else. So I think it's important to carefully study fields of application.

Iwata : So you're studying chemistry.

Nishimura : I'm taking a course in the theory of quantum mechanics, and I'm having a hard time. But I started on the path of computational science because I wanted to use supercomputers, so that's fun. I'd love it if there were a type of hands-on training that used large-scale supercomputers.

Geshi : Do you want to use the K Computer?

Nishimura : You bet. I love the fact that computing speeds keep getting faster and faster.

Iwata : Mr.Kojima, you're going to be performing large-scale computing. Have you ever written programs?

Kojima : I've written simple MD programs in Fortran.

Yoshii : Have you had any instruction in parallelization?

Kojima : Not a bit. I studied using books in my laboratory.

Hidekazu Kojima
Conducts MD simulations of intramolecular proton transfer reactions in solutions. As protons are light in weight, they must be treated as quantum particles, and methods for accomplishing this are currently under development.

Iwata : Mr.Ishii, you said you're able to get along fine with the present scale of computing, but do you write programs yourself?

Ishii : At our laboratory, we have a main MD program, and we modify that to match our own research.

Yoshii : Regarding what you said about using statistical mechanics to accelerate simulation, is that like the multicanonical method?

Ishii : Yes, it's similar to that. My original motivation was that I wanted to analyze real-world phenomena, and it won't be in proportion unless I'm able to increase the time scale. So I want to figure out some way of increasing the time scale.

Iwata : So rather than learning how to become a computer whiz, you want to improve the method. Where are the hurdles in terms of sampling?

Ishii : Sampling is similar to MD.

Geshi : If that's the case, then if you run that program on a faster computer outside the laboratory, it might be so fast that it would astonish you. I'm sure there will be barriers, but it's also important to see the outside world.

Yamaji : I know you students are all busy just trying to do the job that's right in front of you, but you should at least preserve the feeling that it's also good to see what's on the other side of the wall once in awhile. Pointing that out to students may also be part of our job.

Courses you can access anytime, anywhere

Yoshii : Mr. Ishii, what was the educational system that enabled you to arrive at the main research topics in your laboratory? In the past, the attitude was that even if only those students who had managed to pull themselves up by their own bootstraps remained, that would be OK. But that's too inefficient.

Ishii : We only discuss things when it's necessary. The rest of the time, we pursue research on our own. The idea is that students should teach each other how to use the program.

Kojima : We get handed out research papers written by the research accosiate, and they give us a little instruction in how to use the program.

Geshi : At CMSI, we're in the process of putting together a curriculum. Assuming that students will write programs, would you like to hear more practical lectures, lectures on specific numerical algorithms, lectures on computer architecture and so on?

Ishii, Nishimura, Kojima : Yes!

Geshi : How about if we expanded the on-demand classes that you can access anywhere, and expand them to other fields besides chemistry?

Ishii : I'd also like to see the classes in video format that you could access anytime.

Geshi : The Osaka University program has video recordings, so you can hear the lecture either live or at a later time.

Yamaji : With that kind of system, it's inconvenient if you can only view the videos if you're registered. It would be best if they were offered free of charge, but I'm also concerned about the issue of copyright.

Geshi : At Osaka University, students who are registered for the class can access the content using their ID and password. Partly because of the copyright issue, the lectures are streaming only.

Up to now, the classes have been presented once and then taken down. But that means the accumulated expertise is only available to your own students. I think at the very least it should be preserved for the community in Japan.

Iwata : Courses that you can access right away just be clicking on them are convenient, but you can't get college credit for them.

Ishii : That's OK — provided that, in addition, you can ask questions easily and get a response.

Iwata : Maybe it would be good to make a CMSI version of "Tell Me Goo," the Q&A function of the Japanese search engine, goo.

Geshi : It might be possible to get support from groups of Division Researchers and so on. But to get answers to questions, you'd need to come to class at least.

Iwata : We've heard a variety of opinions. It's clear that the needs for utilization of advanced computers in researches will be greater and greater. We need to provide instruction in a way that doesn't require students to take much time away from their core tasks. We'd also like to propose dissemination systems to provide the courses on parallelization, tuning and programming tools to wider audiences not only within CMSI.

(Recorded December 8, 2011 at the CMSI Kobe Branch)

Photos：Shuich Yuri

Computational Materials Design (CMD®) Workshop © http://ann.phys.sci.osaka-u.ac.jp/CMD/index.html

From the Front Lines of Application Development

Interview with Takeshi Nishimatsu, developer of feram

Interviewee :
Takeshi Nishimatsu
Assistant Professor, Institute for Materials Research, Tohoku University

Interviewer :
Yoshimi Kubota
2nd year Ph.D candidate, Department of Earth and Planetary Science, School of Science, The University of Tokyo

Ferroelectrics hold intriguing possibilities as materials for electronic devices. FeRAM memory, which utilizes these ferroelectrics, is expected to be used in state-of-the-art PCs and other digital equipments. The application program "feram," developed by Dr. Nishimatsu, simulates the thin film capacitors used in FeRAM and other applications. Dr. Nishimatsu's unique idea has made it possible to conduct high-speed simulations once thought to be difficult to achieve.

High hopes for FeRAM nonvolatile memory

Have you ever heard the term "ferroelectrics?" If you apply an electric field to an insulator from the outside, the material itself develops a charge bias (becomes polarized). Materials that have this property are called dielectrics. Some of these materials exhibit polarization that is an order of magnitude larger than the others, and they are known as ferroelectrics. Not only ferroelectrics produce large polarization, but also the spontaneous polarization remains even if no external electric field is applied. Furthermore, if a reverse electric field is applied, the charge bias within the ferroelectrics is reversed. Materials that are known to be ferroelectrics include ceramics such as barium titanate and lead zirconate titanate (PZT). Barium titanate was discovered in 1942 in the United States and at roughly the same time in former Soviet Union and Japan in 1944. Since that time, it has attracted a great deal of attention in the material field for its high electric permittivity, and considerable research has been conducted in an effort to develop practical applications.

In recent years, particular attention has focused on computer memory as an example of applications for FeRAM. As PCs become ever smaller and faster, they need new types of memory. The development of FeRAM (ferroelectric random access memory), made by combining layers of PZT and other ferroelectric thin films, is one example. As FeRAM uses ferroelectrics, it is possible to create memory from which information does not disappear when the power is turned off (nonvolatile memory). If a computer is equipped with FeRAM, application programs, which are used before shut down, can be restarted up as soon as the power is turned on, making computer operation faster, more convenient and more energy conservable.

However, some problems must be resolved before FeRAM can be used as computer memory. Currently there are some examples of the practical application of FeRAM, such as in IC cards. However, the downsizing is not enough to enable FeRAM to be employed to create giga-bit memory chips for practical use as computer memory. For example, "dead layers" that resist polarization are produced between the electrode and the ferroelectric thin film, and these are said to affect capacitor performance, making material design difficult. But the thickness of the tiny thin film measures only several tens of nm, so it is difficult to observe directly and hard to determine exactly what phenomenon is occurring. For this reason, the use of computer simulations is expected to play a major role in research in this area.

Calculating dipole behavior

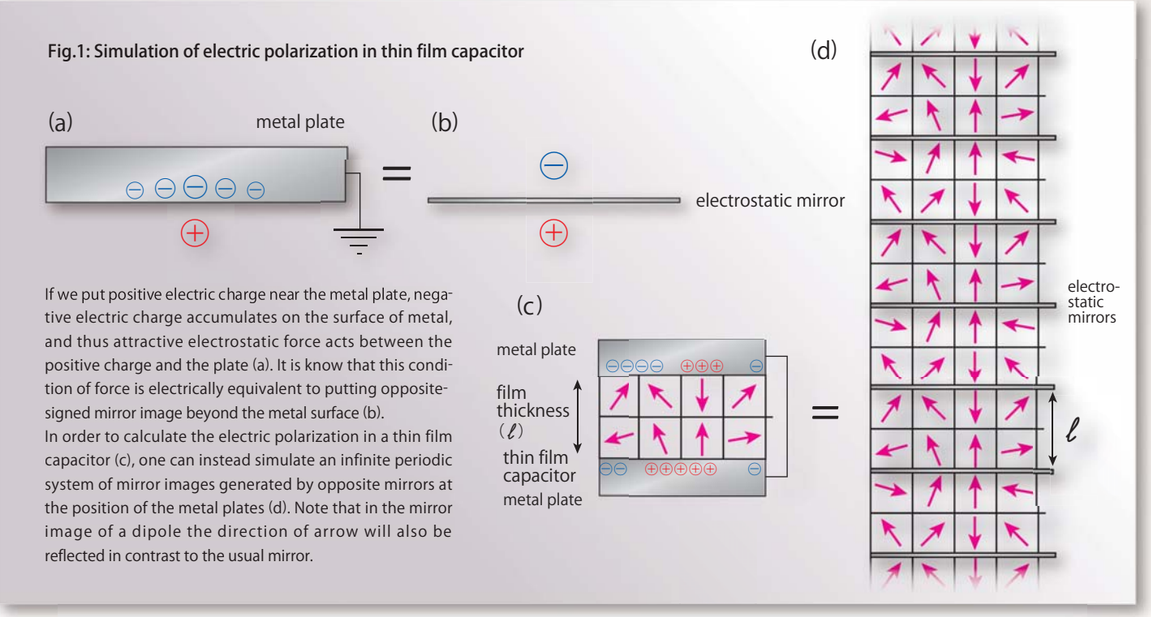
feram, the application program developed by Dr. Nishimatsu, is a molecular dynamics program capable of realistically simulating thin film sizes on the order of several tens of nm. feram is available worldwide as free software, and people are free to use, modify and redistribute the program. Currently, if I google the word "feram", its homepage ranks in top 10. The software package has been downloaded more than 900 times. "I've also benefitted from free software, so I released feram so that anyone can easily reproduce simulations to check the results of my research," says Dr. Nishimatsu. "I named it feram, like FeRAM, to make it easy for people to find on the Internet. I'd like both memory developers and researchers to use feram."

How does feram simulate ferroelectric thin films? It is easiest to explain using the concept of the dipole. Electrons, which have a negative charge, cannot move freely within dielectrics. In that case, how is it possible for such substances to have an electric bias? If a dielectric substance is placed under an electric field, the positions of the atoms in the crystal are displaced slightly, producing an electric bias within a tiny area. This can be thought of as the positive and negative point charges being separated by a tiny distance. This state is called an electric dipole (or simply dipole). The movement of these dipoles determines the electric bias of the substance as a whole.

In the first stage of ferroelectric thin film simulation, the properties of the ferroelectrics are determined by means of first-principles calculations. In the case of barium titanate, the subject of calculations is a unit lattice cube, with each side measuring 0.4 nm and made up of one titanium atom, one barium atom and three oxygen atoms. First-principles calculations can be used to determine the lattice constant, elastic constant and lattice vibration (phonon properties) comparatively easily and with a high degree of precision.

Next, the relationship between the energy and the degree of displacement of the atoms is investigated. The distinguishing characteristic of ferroelectrics is that spontaneous polarization occurs, meaning that the atoms are displaced. When the atoms in the unit lattice are displaced, the energy in the lattice overall changes. Dr. Nishimatsu modified the free software first-principles program ABINIT to develop a program that can determine various parameters in such a way that energy is at a minimum with respect to the displacement of atoms. These parameters are constructed as effective Hamiltonians required for molecular dynamics calculations in feram. "25 parameters are determined in first-principles calculations," says Dr. Nishimatsu. "It's difficult to determine so many, so I modified ABINIT to make it easy to have them calculated automatically."

Fig.1: Simulation of electric polarization in thin film capacitor



If we put positive electric charge near the metal plate, negative electric charge accumulates on the surface of metal, and thus attractive electrostatic force acts between the positive charge and the plate (a). It is know that this condition of force is electrically equivalent to putting opposite-signed mirror image beyond the metal surface (b).
In order to calculate the electric polarization in a thin film capacitor (c), one can instead simulate an infinite periodic system of mirror images generated by opposite mirrors at the position of the metal plates (d). Note that in the mirror image of a dipole the direction of arrow will also be reflected in contrast to the usual mirror.

Takeshi Nishimatsu

Dr. Nishimatsu has a wealth of research experience in foreign countries such as the United States and India. While studying in India, he came up with the idea of "opposite mirrors" for feram. "The idea for the opposite mirrors came to me the day before I went hiking in Shiv Ganga, a holy place near Bangalore, when I was having a discussion with Prof. Waghmare, my academic advisor. I stayed up all night thinking about it, so climbing the mountain the next day totally wore me out." He laughed. "But I guess you could say I achieved enlightenment in India." It's quite an interesting coincidence.

Dr. Nishimatsu says this is one area of research in which he has poured his heart and soul.

Using the 25 parameters determined with first-principles calculations, molecular dynamics calculations are performed using feram. With feram, the key is how to express the interaction between dipoles. Dipoles exert force on each other in inverse proportion to the cube of the distance between them. The dipoles are placed in each unit cell of a lattice called a supercell, a cube with each side consisting of several tens of cells, and the force acting between the dipoles is calculated in order to simulate the movement of dipoles over time. The distinguishing characteristic of feram is that conditions such as temperature and external electric fields that are difficult to incorporate into first-principles calculations can be varied in the simulation.

feram makes fast Fourier transform possible

Dr. Nishimatsu says that the nature of the force acting between dipoles is anisotropic long-range force. As the effect is greater in dipoles that are farther away from one another, tiny changes in form on the part of the objects being simulated change the movement of the dipole as a whole. A particularly important issue is how to treat the edges of the objects. Even if, from a broad perspective, the boundary between the object and the other space appears to be clearly visible, from the narrow perspective, electrons exhibit complex behavior near this boundary. As the boundary between the object and the surrounding space cannot be clearly determined, it is difficult to simulate. This problem of the boundary is itself an intriguing topic for research, but it becomes a troublesome problem when, as in the case of the present objective, we want to know the behavior of fairly large systems. Moreover, because the interaction between dipoles is long-range force, the fact that the results of calculation will be different for infinite systems and (finite) systems that have edges is also a problem.

Finiteness of the systems also poses disadvantages in terms of calculation methods. It would take an extremely large amount of time to calculate the long-range force between dipoles on a realistic scale. Even for a thickness of some tens of nm, when converted into dipole layers, this becomes large-scale calculations for more than 100 layers.

"The edge problem and the problem of calculation speed were headaches. But one day, in the course of discussions with Prof. Waghmare, I hit upon an outstanding idea that could solve them both," says Dr. Nishimatsu, speaking excitedly.

What was this idea? The structure of a thin film capacitor is that of a thin film of ferroelectrics placed between two metal plates. If the ferroelectric thin film becomes spontaneously polarized, an electric charge appears on the surface of the thin film. If the two metal plates are connected with an electric wire, the electrons in the metal can move freely, so a charge that is the opposite of that in the thin film will appear on the surface of the metal plates. It is as if the ferroelectric thin film is sandwiched between two mirrors: the two metal plates function as opposite mirrors, and infinite images of the ferroelectrics appear beyond the opposite mirrors (Fig.1). In other words, the thin film is the only area being calculated, but an infinite series of mirror images are displayed above and below the thin film.

"When I came up with the idea for the opposite mirror, I thought, Eureka!" says Dr. Nishimatsu. "Using feram to perform calculations considering the thin film as an infinite, periodic structure makes it possible to use fast Fourier transform. And, as a result, much faster calculations can be achieved than was possible up to now. Only my feram program uses fast Fourier transform to perform simulations of ferroelectric thin film capacitors."

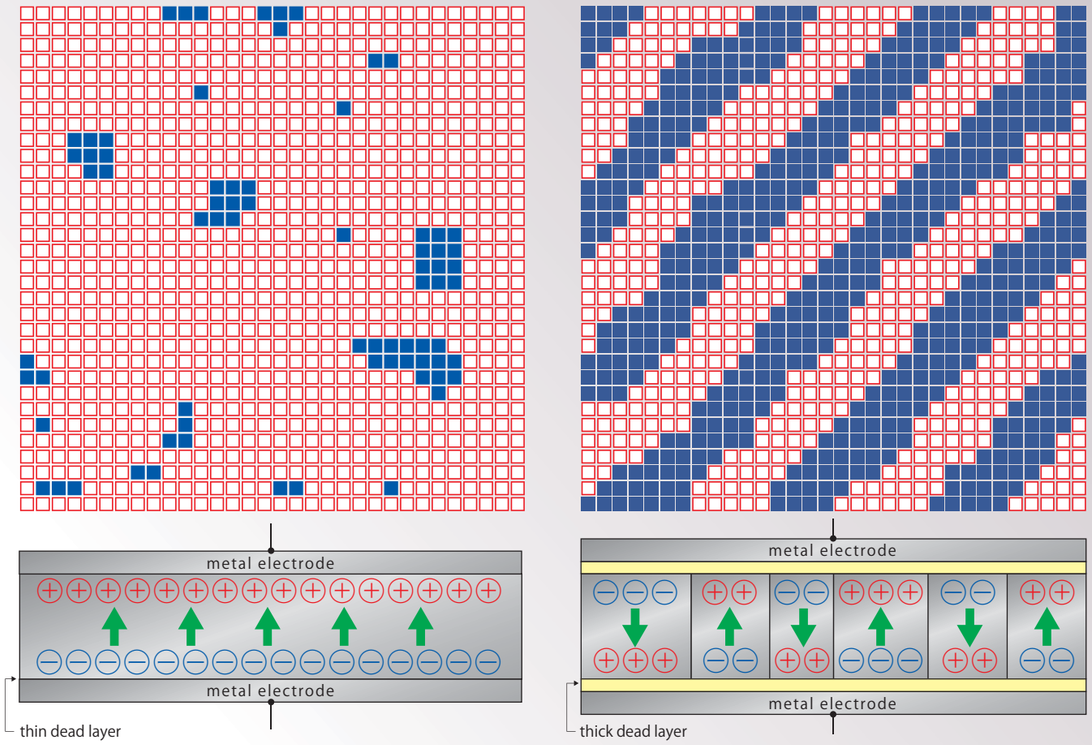
Already, Dr. Nishimatsu's research has clarified the adverse impact of dead layers (Fig.2) on the performance of ferroelectric capacitors and the manner in which these adverse effects are manifested, by calculating hysteresis loops — which indicate how the charge bias of thin films will change in response to changes in electric fields applied externally — when dead layers are present.

In the future, Dr. Nishimatsu wants to study new ways to expand the potential of supercomputers. Modylas and RSDFT, which have been introduced previously in this series, improved internodal communication to achieve large-scale computing using as many nodes as possible. In contrast, feram uses only a single node. "In material development, it's important to draw a phase diagram," says Dr. Nishimatsu. "The large capacity of a supercomputer (capacity computing) can be used to determine how properties change as a result of changes in temperature and external electric fields. By varying the conditions and performing numerous calculations for a single node, you can accumulate the statistical data needed to draw a phase diagram. I want to use feram to develop new uses for supercomputers."

feram seems poised to discover new and expanded potential for supercomputers.

Application Spec Sheet [feram]	
Code Name	feram
Method / Algorithm	Molecular dynamics method based on first-principles effective Hamiltonian
Overview / Features of Code	Dipole-dipole interaction is calculated using fast Fourier transform, so calculations are conducted at high speed. Not only bulk simulations but also simulations of ferroelectric thin film capacitors are possible. The use of GNU Autotools makes it easy to perform compiling and development on individual machines.
Materials for Simulation	Perovskite-type ferroelectric
Development Leader	Takeshi Nishimatsu
Developers / Developing Institutions	Kawazoe Laboratory, Institute for Materials Research, Tohoku University
Development Period	Began in 2005 under the direction of Professor Umesh V. Waghmare while visiting in Bangalore, India.
Development language and number of lines of source code	Fortran / 3500 lines / Object-oriented programming (OOP) is used.
Operating Environment	SR11000, FX1, GNU/Linux, GNU Fortran, Intel Fortran etc.
Parallelization Method	OpenMP, automatic parallelization using a compiler
Status of parallelization	Runs quickly on one node of the SR11000
Software Release	Made publicly available as free software at http://loto.sourceforge.net/feram/
Related / Competing Applications	Similar programs are being developed independently by 2–3 groups overseas; the phase-field method is also a rival.

Fig.2: Distribution of electric polarization in thin film capacitor



Upper panels are horizontal slices of ferroelectric thin film capacitors. Red □ and blue ■ denote upward and downward polarization, respectively. Lower panels are the edge views. When the dead layers are thin enough, uniform and large polarization appears spontaneously (left). On the other hand, if the dead layers are too thick, the amplitude of spontaneous polarization becomes smaller by the cancelation of polarization due to the domain structure (right).

Yoshimi Kubota

◆ Interviewer's Postscript

Electric dipoles are invisible to the eye, so they're not easy to understand. Dr. Nishimatsu explained their action to me using magnets as stand-ins for electric dipoles. He also showed me an experiment in which a piezoelectric element, one type of ferroelectric device, becomes a speaker that emits sound when voltage is applied to it, and becomes a vibration sensor in which an LED blinks when you hit it. Dr. Nishimatsu's use of techniques like this to give an idea of the properties of ferroelectrics made this a very enjoyable interview.

Truong Vinh Truong Duy
Research Center for Integrated Science,
Japan Advanced Institute of Science and Technology (JAIST)

During November 12-18, 2011, I attended the SC11 conference in Seattle, WA, the United States of America.

SC, formerly Supercomputing, is the international conference for high performance computing, networking, storage, and analysis. Established in 1988, it has built and brought together a diverse community to facilitate information exchange and address challenges in virtually every area of computing. SC11 attracted about 11,000 attendees, 350+ paper submissions with an acceptance rate of 20%, 23 workshops, and 349 exhibitors including 33 universities.

I attended the conference to showcase our research activities in OpenMX, Green Cloud, etc. and exchange ideas with other SC11 attendees as an exhibitor of JAIST. We set up a research-content-rich booth there, with LCD screens displaying 3D simulations, posters introducing O(N) large-scale first-principles calculations, and so on. As a CMSI researcher, I also participated in several sessions of interest to catch up with recent advances in the HPC area, such as Gordon Bell Prize Finalists, HPC Challenge Award, Top500, GPU computing and DFT, and performance analysis and tuning.

The K Computer shined at the conference with 3 major achievements: Gordon Bell Prize for the Peak Performance, first place in all benchmarks of the HPC Challenge Award, and the top spot in the Top500.

SC11 was not perfect, as it featured too many overlapped sessions. Also, it was commercialized to a certain extent that many attendees may not think it was truly a scientific conference. However, I think SC11 was worth attending because it made it possible to showcase our research to a diverse community. I learned a lot from the new developments and breakthroughs presented in high quality papers in the area I have been involved in, and have new ideas about what I should do next. GPU computing has been applied successfully to accelerate DFT and QCD calculations and will likely become more popular. A few petascale applications debuted, and exascale supercomputers are expected to appear within the next 10 years, most likely a hybrid design of multicore CPUs and GPUs or an integrated chip using ARM architecture. In addition, I obtained up-to-date knowledge on the next release of MPI with more support for hybrid programming and nonblocking collectives. These observations will guide me on how to develop algorithms that are scalable and compatible with future computing systems.

The booth of Japan Advanced Institute of Science and Technology (JAIST) at SC11.

The future of supercomputing is "super phones?"

Photo : Truong Vinh Truong Duy

The 2011 Gordon Bell Prize, Peak Performance Award

The research paper "Simulation of Electronic States of Silicon Nanowire" using the K Computer won the Peak Performance Award of the 2011 Gordon Bell Prize.

They performed a first-principles calculation of nanowire of 100,000 silicon atoms using the Real-Space Density Functional Theory (RSDFT), which was featured in Torrent No.3, and achieved 3.08 petaflops (43.6% of peak performance). The Peak Performance Award is since the Earth Simulator (1st generation) in 2004.


Photo provided by RIKEN: The 2nd from the left on the front row is the RSDFT developer, Junichi Iwata.

Profiles of Division Researchers

This section presents profiles of the Division Researchers who adopted in research at CMSI between September 1, 2011 and February 29, 2012.

Tsutomu Kawatsu

Molecular Science Division Researcher
Fukui Institute for Fundamental Chemistry
Kyoto University

Majored in theory of the biophysical chemistry at the Nagoya University and received a Doctorate of Science. Currently pursuing a research into bridge-mediated excitation energy transfer at Fukui Institute for Fundamental Chemistry, Kyoto University.

Motivation for applying for the posion
Accurate, large-scale sampling is needed for numerical calculations in natural science. I wanted to obtain techniques for using large-scale parallel computers for this purpose.

Mission / Role
My mission and role is to increase the speed of the gradient calculations used in first-principles molecular dynamics for the path integral approach, and to pursue development relating calculations in order to conduct high-efficiency sampling using first-principles molecular dynamics.

Ambition
My goal is to establish a sampling simulation method that can treat quantum chemical properties in a statistical manner, while achieving a balance between speed and accuracy.

Truong Vinh Truong Duy

Condensed Matter Physics Division Researcher
Research Center for Integrated Science, Japan Advanced Institute of Science and Technology (JAIST)

Majored in Information Science at Japan Advanced Institute of Science and Technology and received his Ph.D. (Information Science). Engaged in research into High Performance Computing and Green, Grid, Cloud Computing Technologies at Japan Advanced Institute of Science and Technology. Country of Origin: Hochiminh City, Vietnam.

Motivation for applying for the posion
I wished to apply my skills of information science to computational materials science in an interdisciplinary research project.

Mission / Role
To develop efficient petascale hybrid parallelization of extreme-scale applications for fully exploiting state-of-the-art supercomputers.

Ambition
I wish to become a good role model in interdisciplinary research that crosses traditional boundaries between Information Science to Computational Materials Science.

Guo Zhi-Xin

Condensed Matter Physics Division Researcher
Department of Applied Physics, The University of Tokyo

Majored in computational physics at Fudan University in China for my Ph.D degree. Engaged research into the application and development the Real-Space DFT code.

Motivation for applying for the posion
I wanted to expand my research field from the thermal conductance to the electronic conductance, and also expand the research method from the classical molecular dynamics to the first principles.

Mission / Role
To calculate the electronic structure of C/Si materials in use of the Real-Space DFT code, and also make some contribution on the development of Real-Space DFT.

Ambition
My ambition is to develop an efficient code for conductance calculations and apply it to obtain new results for transport properties of nanometer-scale devices, and also to make many friends in Japan.

Mission of Division Researchers

Category A
Development of state-of-the-art elemental technologies and algorithms
Example: development of matrix diagonalization, matrix inversion, FFT and other parallelized algorithms.

Category B
Development, release and dissemination of applications common to multiple fields
Example: electrical conductivity calculation, matrix diagonalization programs, quantum Monte Carlo method.

Category C
Advancement of the field through the support of multiple research topics
Example: Application advancement that includes parallelization.

Category D
Development and management of portal site / Application release and dissemination
Example: portal site development and administration, license management.

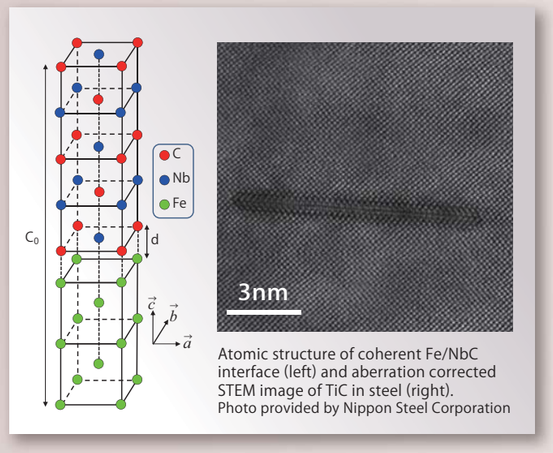
"Interface and Structural Control" — CMSI Symposium on Industry-Government-Academia Cooperation

December 7, 2011 Venue: Institute for Materials Research, Tohoku University

This CMSI Symposium on Industry-Government-Academia Cooperation was held jointly with the 2nd Computational Materials Research Initiative Symposium on December 6 and 7, 2011. The CMSI Symposium was held on the afternoon of the second day. The symposium began with case studies of the use of computational materials research at companies in accordance with the symposium's theme "Interface and Structural Control."

Hideaki Sawada of Nippon Steel Corporation gave a presentation entitled "Structure and energy of steel precipitate interfaces." He presented the results of a simulation study of precipitates, which are an important factor determining steel strength. The interface energy between the matrix phase and the precipitate determines how the size of the niobium carbide (NbC) and other precipitates produced in matrix phase steel will grow, and under what conditions. Tiny nanosize-level NbC has the same lattice position as the matrix layer of the steel (figure below), but as the precipitates mature, they come to be only partially aligned (semi-coherent interface), and this changes the interface energy between the matrix phase and the precipitate. A number of atoms on the order of several thousand to several tens of thousands must be taken into consideration in order to calculate this semi-coherent interface energy, and this was difficult to do using conventional first-principles calculation. Accordingly, Dr. Sawada used OpenMX, developed by Taisuke Ozaki of the Japan Advanced Institute of Science and Technology, to conduct parallel computing. This program uses the Order-N method, which employs a Krylov subspace, to make it possible to calculate polyatomic systems efficiently. The used computer was the TSUBAME2 at Tokyo Institute of Technology. As a result of the study, the energy and atomic positions of the semi-coherent interface were determined. In the future, Dr. Sawada plans to perform calculations that also take into account strain produced near the interface to predict the size of the precipitate that shifts from coherent to semi-coherent, in order to develop higher strength steel.

Next, there were presentations by Kaoru Nakamura of the Central Research Institute of Electric Power Industry on a study entitled "Creep damage simulation in heat-resistant steel interfaces," and Hiroshi Kaido of Sumitomo Metal Industries, Ltd. on a study entitled "Evaluation of dislocation dynamics calculations and mechanical characteristics based on a phase-field model." The content of these presentations gave a real sense that computational science is being incorporated into materials development.



Atomic structure of coherent Fe/NbC interface (left) and aberration corrected STEM image of TiC in steel (right).
Photo provided by Nippon Steel Corporation

Two trends in industry-government-academia cooperation

These presentations were followed by a panel discussion on the theme of "Expectations for Industry-Government-Academia Cooperation." In addition to the three presenters, the panelists were Masanori Kohyama (National Institute of Advanced Industrial Science and Technology), Hiroshi Otani (Kyushu Institute of Technology) and Ying Chen (Tohoku University). Tooru Matsumiya of Nippon Steel Corporation served as moderator.

The panel discussion began with each of the panelists describing their experience with industry-government-academia cooperation. Then the main topic of discussion was posed to the panelists: what type of industry-government-academia cooperation would you like to see from the standpoint of computational materials science and industry promotion?


Hideaki Sawada, presenting the results of simulation study. He works on large-scale ab initio calculation aiming to improve the steel strength based on the first principles.

"I have the impression that academics think that, for the industry side, the objective of industry-government-academia cooperation is to pursue the ultimate outputs, but I'd like universities to get the basics right," said Dr. Sawada. "I want to convert those basics into concepts based on specific needs and have this lead to materials development."

"If academics clearly determine the scope of application for software and so on, it would be helpful to people on the industry side who use that software," said Mr. Nakamura, indicating that one trend in industry-government-academia cooperation was for academia to build the foundation and for companies to employ their capabilities for application.

In additional, Prof. Chen is thinking about another trend in industry-government-academia cooperation. "If issues that need resolution from an industry perspective and experimental data are provided to us, it would be very helpful for academics when we are considering where to put the focus of our research."

Dr. Kohyama spoke about his hopes for the exchange of information. "What problems arise at manufacturing sites, and where are the issues that computational science can help resolve? If these were disclosed at seminars and the like and there were a venue for the frank exchange of information, it would enable calculations using fresh research topics."

Seeking measures to link industry, government and academia

So what kinds of specific things should be pursued? The need for personnel interchange and the introduction of internships has already been mentioned previously. "We had student interns to calculate the atomic states of elements in the periodic table using first-principles calculations, and determine through calculation why there is a tradeoff between strength and corrosion resistance, said Mr. Kaido. "Calculations that lead to useful properties are difficult to do at the university, so the students found this very rewarding."

"I'm thinking about doing the opposite as well," said Prof. Chen. "I hope companies send young researchers to the universities to pursue research for joint projects with us together. It would result in both collaboration and personnel training. I think there should be such a system."

When Dr. Matsumiya responded, saying "What companies will need in the future, for instance, the Materials Strategy Committee is trying to make and show a roadmap." the view was expressed that this would differ depending on the industry, and that it was sometimes difficult for small companies to keep their expertise confidential.

Prof. Otani said that companies and universities look at things from a different perspective. He said that universities have to disclose the results of their research, and that at present it was difficult to create a system for personnel interchange between companies and universities for this reason. He pointed out that regional universities in particular are restricted by intellectual property agreements with companies in the degree to which they can exchange information. "The problem regarding intellectual property is a result of the fact that they are dealing with only a single company. If multiple companies were involved and the knowledge were understood to be a common foundation, it would become easy to disclose it." In this way, he expressed high hopes for projects in which multiple companies participated.


Panelist, Ying Chen. Specializes in first-principles calculation of properties of materials such as metals, magnets and nuclear fuels.

Members of the audience also participated in a spirited debate and proposed a number of ideas. One computational materials researcher gave a real-world example. "I'm always concerned about how the things I and my colleagues are working on can be applied in an industrial setting. For this reason, we created a project that we call the Industry-Academic Collaborative Creation Basic Infrastructure Research Center. We've gotten the involvement of many people from the industrial world as well. Calculations relating to the complex structure of steel as in the presentation a few minutes ago were achieved by exchanging ideas with people from the corporate world and breaking the problem down. Although we may have a limited degree of confidentiality imposed on us, I think this is a viable form for achievable industry-academia collaboration." Another said, "Once I inherited a research project from my more experienced colleague, who said 'My generation can't do this – you do it.' It is seminars and academic meetings, where people from industry, government and academia gather, that these kinds of connections are possible. I think computational science will soon reach that stage. The Iron and Steel Institute of Japan is conducting an ongoing education program with a great deal of enthusiasm." Another person proposed that multi-disciplinary workshops be held that links mechanical engineering with materials development.

We felt that, although each entity involved in industry-government-academia cooperation has a different perspective and is in a different phase of grappling with the issues, it is essential for there to be a common recognition of the importance of finding out how the issues that they are dealing with can lead to solutions that will benefit society.

Kazuhito Shida (Tohoku University) contributed to this report.

CMSIカレンダー

For more information, see the CMSI website (http://cms-initiative.jp)

● 3rd CMSI Symposium on Industry-Government-Academia Cooperation (Current state of industrial applications for computer simulations in the electronic materials field and future prospects)
Date : February 10, 2012
Venue : Akihabara Conference Center

●CMD® Workshop
Date : February 16 - 19, 2012
Venue : Mahidol University (Bangkok, Thailand)

●International Workshop on Quantum Chemistry Massively Parallel Programming Now in Supercomputer
Date : February 28, 2012
Venue : Komaba Faculty House, The University of Tokyo

●2nd AICS International Symposium
Date : March 1 - 2, 2012
Venue : Advanced Institute for Computational Science

●Open Symposium of Integrated Nanoscience
Date : March 5 - 6, 2012
Venue : Nichii Gakkan, Kobe

●CMD® Workshop
Date : March 6 - 10, 2012
Venue : International Institute for Advanced Studies (Kyoto)

●5th Young Researcher Technical Workshop
Date : March 12 - 14, 2012
Venue : Hotel Suiyotei, Atami

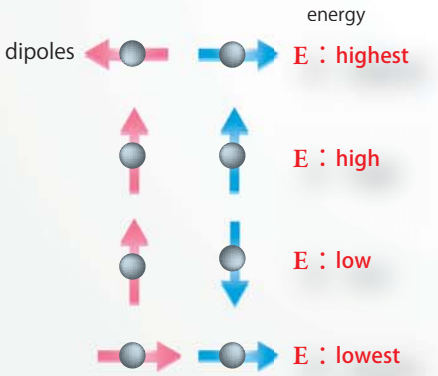
●K Computer Symposium 2012 / Joint Workshop of 5 Fields in Strategic Program
Date : June 14 -15, 2012
Venue : Kobe University and Advanced Institute for Computational Science

●MASP – transient international workshop
Date : June 25 - July 13, 2012
Venue : Institute for Solid State Physics, The University of Tokyo

●CCP2012
Date : October 14-18, 2012
Venue : Kobe

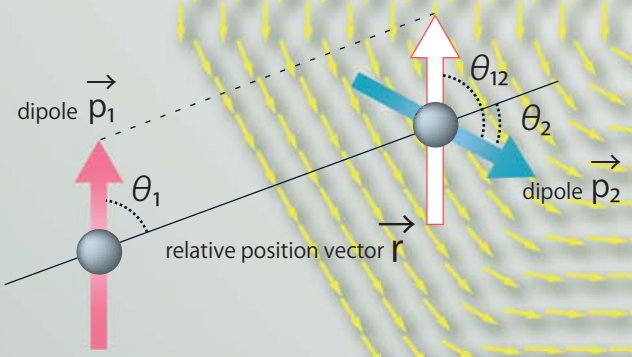
Dipoles and Ferroelectrics

In this issue, our "From the Front Lines of Application Development" section features feram. Let's take a closer look at dipoles and ferroelectrics, the key concepts for feram.



Overall, insulators are generally electrically neutral. Sometimes, however, bias is produced locally in the charge distribution due to external electric field or distortion in the crystal. This phenomenon is called "electric polarization." Conceptually, the electric polarization can be depicted in the form of tiny arrows. An arrow pointing from negative charge to positive charge with length representing the product of the amount of the electric charge and the distance between the charges is called an "electric dipole," or simply a "dipole."

$$E = \frac{\vec{p}_1 \cdot \vec{p}_2}{|\vec{r}|^3} - \frac{3(\vec{p}_1 \cdot \vec{r})(\vec{p}_2 \cdot \vec{r})}{|\vec{r}|^5} \sim \frac{\cos\theta_{12} - 3\cos\theta_1 \cos\theta_2}{r^3}$$



What is dipole interaction?

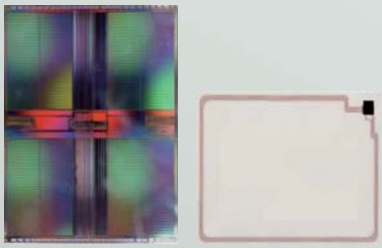
The interaction (E) exerted between two dipoles is based on the mutual attractive and repulsive forces acting between the charges that make up the dipole. The combination of these forces in the form of a dipole is expressed by a complex equation like the one shown above. This dipolar interaction is characterized by the fact that the effect extends to a comparatively long distance, and the fact that the strength is dependent not only on the orientation of the dipoles with respect to one another (θ_{12}) but also their relative positions (θ_1, θ_2).

Properties of dipole interaction

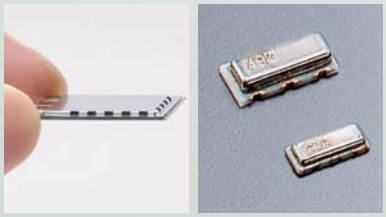
For example, when two dipoles are placed in parallel, the energy becomes lower (in other words, stable) when they are pointing opposite directions from one another. Conversely, when they are placed in series, the energy is lower when they are pointing the same direction. Because of this property, which is called "anisotropy," the stable structure when three or more dipoles are grouped together becomes complex in general. When the dipoles are arranged on a triangular lattice for example, a vortex-like structure is known to appear as shown in the left figure.

Applications of ferroelectrics

Materials whose electric polarization is aligned in a single direction even when there is no external electric field, and that are capable of switching this orientation in response to an electric field, are referred to as ferroelectrics. Ferroelectrics has an increasingly wide range of applications. They are used as piezoelectric speakers in cell phones and IC recorders, as ceramic resonators in oscillating circuits that are stable but low cost, and in IC cards and IC tags in the form of FeRAM memory.



4MB FeRAM chip (left) and IC card inlet (right).
Pictures provided by Fujitsu Semiconductor Ltd.



Piezoelectric speaker (left) and ceramic resonators (right).
Pictures provided by Murata Manufacturing Co., Ltd.

Torrent : The Newsletter of the Computational Materials Science Initiative (CMSI) No.4, March 2012

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