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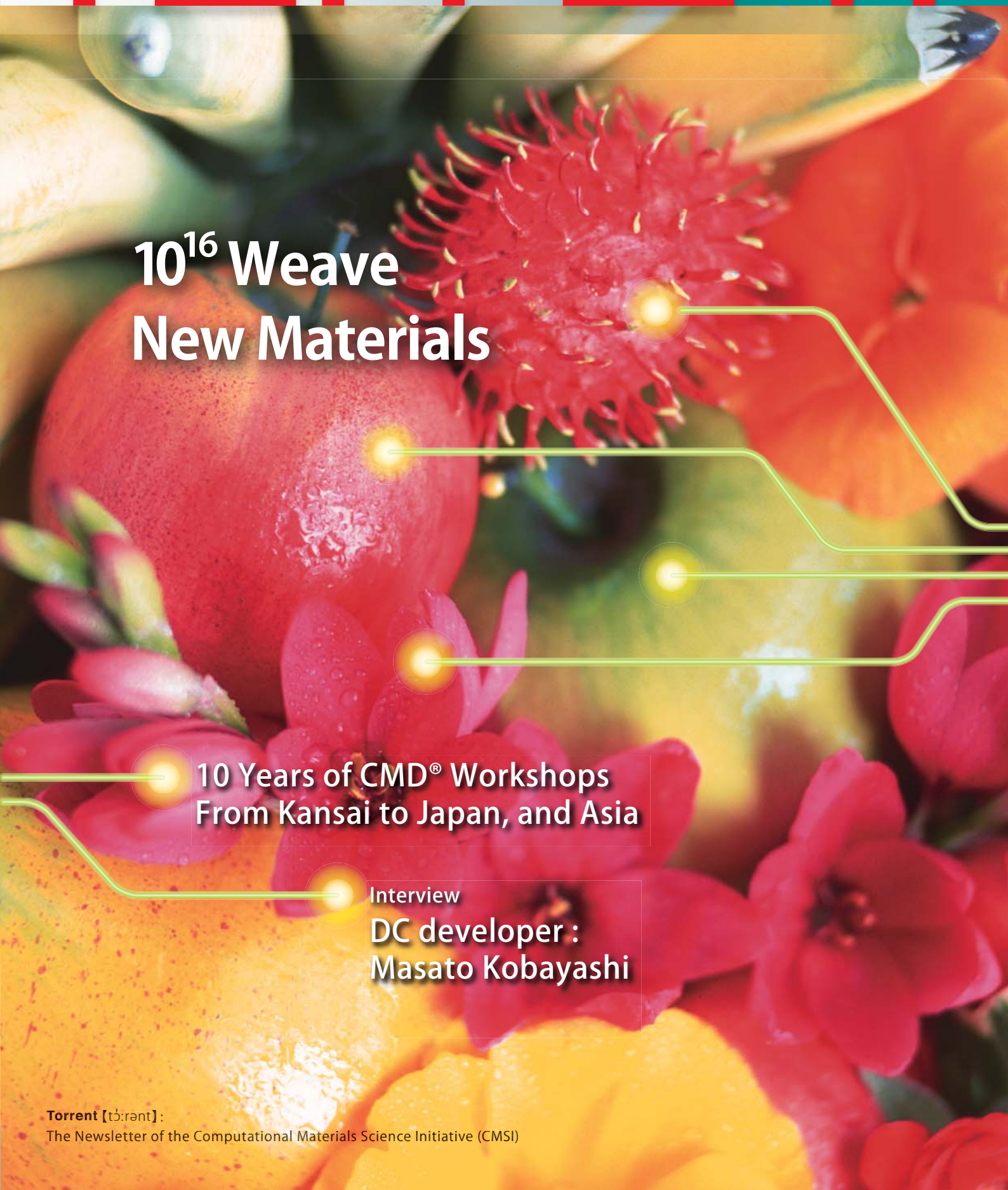
Torrent



10^{16} Weave New Materials

10 Years of CMD® Workshops From Kansai to Japan, and Asia

Interview

DC developer : Masato Kobayashi

Torrent 【tɔ́:rənt】:
The Newsletter of the Computational Materials Science Initiative (CMSI)

10 Years of CMD® Workshops

From Kansai to Japan, and Asia

from JAPAN to ASIA

Tamio Oguchi

Professor
Nanoscience and Nanotechnology Center
Institute of Scientific and
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Osaka University

Participants and lecturers of the 20th CMD® Workshop. Prof. Geshi (far left in front), Prof. Ono (third from the left in front), Prof. Akai (fifth from the left), and Prof. Oguchi (second from the right).

The 20th Computational Materials Design (CMD®) Workshop was held at the International Institute for Advanced Studies (IIAS) in Kizugawa, Kyoto Prefecture, for five days, from Tuesday, March 6 to Saturday, March 10, 2012. The CMD® Workshops have been held twice a year, and this year marks the 10th anniversary of the establishment of the workshop. In this special report, we introduce the CMD® activities over the past ten years, including the history leading to collaboration with the Computational Materials Science Initiative (CMSI) and survey future prospects.

* CMD® is the trademark of CMD Consortium.

The CMD® Workshops are planned by CMD Consortium.

The Birth of the CMD® Workshop

The entity that became the parent organization for the CMD® Workshops was the specialist training projects at IIAS. In 2001-2002, the first of these projects, "Bio-Informatics," had been held successfully. The project dealt with new topics of research that could not be covered in the existing graduate schools. Specialists and professors were invited, and seminars and workshops were held for young students using a training camp style. There was an active effort to not merely ensure that the students acquired the target knowledge but rather to create opportunities for bidirectional interchange with the instructors, with the aim of using the synergy to train a group of specialists who would become the future leaders in these areas.

At the time, Osaka University had many researchers specializing in first-principles calculations: Profs. Hisazumi Akai, Hiroshi Yoshida, Hideaki Kasai, Naoshi Suzuki and Kikuo Cho. This background was employed skillfully, resulting in the adoption in 2001 of the "Development of methods for computational nano-materials design" computer-based project of the Japan Science and Technology Corporation (JST) (now the Japan Science and Technology Agency). Through the support from this project, the CMD® Workshop was born in September 2002 as the second IIAS specialist training project.

Computational Materials Design (CMD®) is the theoretical design of new materials and structures in an effort to achieve certain functionalities or properties — in other words, "quantum design." Specifically, CMD® involves the use of computing power to conduct calculations based on the basic theory of condensed-matter physics. The computer is the basic tool for quantum design. The purpose of the CMD® Workshops is to provide the basic knowledge and techniques needed to enable quantum design.

The lectures in the first CMD® Workshop were held primarily at IIAS, and the hands-on computer training sessions used the ITBL facility of the Kansai Research Institute of the Japan Atomic Energy Research Institute (JAERI) (now Japan Atomic Energy Agency). Totally 22 participants comprised five graduate students, four university and technical college staffs, 12 private company researchers, and one from a public research organization. For four nights and five days, the lectures continued until around 9 pm every night, with the kind of fulfilling content only possible in a learning camp environment.

Collaboration with CMSI

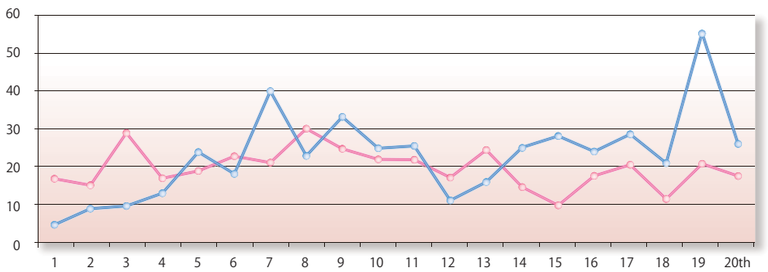
Subsequently, the CMD® Workshops received support not only from IIAS but also from the New Energy and Industrial Technology Development Organization (NEDO) Materials Nanotechnology Program, the Special Coordination Funds for Promoting Science and Technology, Grant-in-Aid for Scientific Research on Priority Areas, the Program for Training Personnel in Fields to be Promoted and so on, enabling the workshops to be held on an ongoing basis. Figure 1 shows the statistics on the number of students and working people attending the workshops from the first through the 20th workshop. The total number of participants of these 20 workshops came to 858 (461 students and 397 working people).

The large number of participants from private companies was notable from the very

beginning, underscoring how few of these types of workshops are held. In October 2004, a Continuing Education Program specially designed for working people was established at Osaka University.

Beginning with the 6th CMD® Workshop, it became mandatory to attend the CMD® Workshop as part of the Continuing Education Program. In addition, credits for this program were accepted as completion of graduate school coursework. Beginning in 2009, these workshops became the Graduate-level Career-up Programs for Nanoscience and Nanotechnology (http://www.sigma.es.osaka-u.ac.jp/pub/nano/). Prof. Kasai's laboratory was in charge of the secretariat of the workshop from the beginning to this time. Moreover, since the 18th workshop held in October 2011, the CMD® Workshop has also been positioned as one of the activities sponsored by CMSI. There are several reasons for this. When the object of quantum design is on a material with unitcell that includes many atoms or is on a large scale system such as a nanoparticle. large-scale computing is needed, and technology to develop code that can be executed on such a computer is needed. CMSI was established in September 2010 with the aim of conducting large-scale computing on the K Computer, and so both organizations overlap each other in this context. Their goals also include training people talented for quantum design.

Fig. 1 Number of participants in the CMD® Workshops. students working people



Efforts to accommodate a wide range of participants

The lectures and hands-on training in the first two CMD® Workshops were held in a single class, a system that was equivalent to the content of the subsequent Beginner's Course. However, the experience and practical skill level of the participants ranged widely, and this created a number of difficulties in the operation of the actual workshop. From the third workshop, a two-course system was introduced, with participants attending courses based on their experience. Several workshops were conducted with the participants attending either the Beginner's Course or the Advanced Course. Subsequently an Expert Course was also added. Moreover, to meet the needs of the various participants, a new Supercomputer Course was added beginning with the 17th Workshop (for details, see "CMD®20 Supercomputer Course" on the next page).

In practice, participants come to the CMD® Workshops seeking various things. Beginners first want to experience first-principles calculations, while there are also participants who want to apply. first-principles calculations to specific research topics. These diverse demands requires wide-ranging flexibility. For example, in most cases, a minimum requirement for conducting first-principles calculations is the ability to enter various commands as instructions on the computer terminal, or to conduct file operations at the UNIX® level. In the beginning, the instructors explained these operations as needed during the lectures. In recent workshops, however, a course on UNIX® has been held on the first day of the Beginner's Course. Furthermore, in addition to the lectures and hands-on training in the fundamentals of first-principles computing, each workshop features invited lecturers who introduce some case studies of advanced research to show how first-principles computing is applied in the research fields of materials and devices at universities, research laboratories and private companies.

After the end of each CMD® Workshop, an opinion survey is conducted for both participants and lecturers. This is done to know needs with regard to workshop content and system and to point out problems, so these comments can be reflected in future workshop planning and administration.

Expansion to Asian countries

Since around the 10th Workshop, the number of foreigners attending the workshop from countries in East Asia has increased. Most of these are graduate students studying abroad at Osaka University. There were nine foreign students among the participants at the 10th Workshop. Thanks to Prof. Kasai's effort, by the 19th workshop, this number had grown to 18. On the other hand, this increase in the foreign participants made it difficult to conduct the lectures and hands-on training in Japanese only, and not only the explanatory slides but the oral explanations came to be presented in both Japanese and English. This style of instruction has continued to date, but it has produced problems as well. It often happens that a participant's question causes the lecturer to engage in animated discussion of a certain subject and the explanation tends to be disproportionately in either Japanese or English, causing frustration with the lecture on the part of the participants.

Although this type of problem sometimes occurs, the acceptance of foreign students has produced major benefits. Interchange with people from the East Asian region through the CMD® Workshop became the inspiration in 2008 for the start of Asian CMD® Workshops in East Asia. In August 2008, the first Asian CMD® Workshop was held at Institut Teknologi Bandung (ITB) in Indonesia. In September of that same year, an Asian CMD® Workshop was held at De La Salle University in the Philippines. In the following year, 2009, Asian CMD® Workshops were held again in Indonesia and the Philippines and in Vietnam as well. In FY 2010 and FY 2011, the number of countries was expanded to four with the addition of Thailand.

In developing nations in East Asia and other regions, there has always been tremendous interest in and expectations for computational science, and there have been many highly motivated requests to hold CMD® Workshops where young people can be trained using PC-level computing resources.

CMD® Workshop in the Philippines. Photo: Prof. Wilson Diño.

CMD®20 Supercomputer Course

Tomoya Ono

Assistant Professor,
Research Center for Ultra-Precision Science & Technology, Osaka University

The Supercomputer Course in the CMD® Workshop is a relatively new course, which is the fourth in the 20th CMD® Workshop on March 2012.

Out of consideration for computing resources, the supercomputer course is limited to three to four participants. It is designed to enable participants to learn through one-on-one instruction in an environment with resources that closely approximate the one in which researchers actually conduct research. Applicants to attend the course have included graduate students, post-doctoral researchers and researchers at private companies — the people who will be leaders in the next generation of computational science. From among these applicants, the participants are selected based on their participation in the beginner's and advanced courses, their past coursework and so on.

The instructors are Ono (Osaka University) and Yoshiyuki Egami (Nagasaki University), in addition to Shoichiro Saito (Osaka University) as teaching assistant. In the Supercomputer Course, RSPACE code and STATE code are used alternately, and this time RSPACE was used. Usually the participants are asked in advance about what computing environment they would like, and the lecturers make the decision after consulting the participants. However, since the participants themselves read the academic papers prepared using RSPACE, they were able to come up with computing topics that were pertinent. Up to now, the supercomputer used for hands-on training was SX-9 at the Cybermedia Center, Osaka University, but this time Altix ICE at the Institute for Solid State Physics, the University of Tokyo was used.

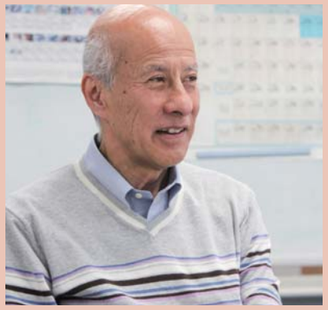
The first day of the hands-on training began with an introduction to the computer. After that, the participants began hands-on training using computer code. As many of the participants had never used computer code before, initially they pursued the work while consulting the combined manual and text. RSPACE code is parallelized with both process parallelization using MPI and thread parallelization using OpenMP. Altix ICE is designed for multi-node use, so the hands-on training was conducted so as to emphasize an awareness of process parallization using MPI. As RSPACE enables computing time to be reduced by increasing the number of cores used, undoubtedly the participants were able to get a real sense of the importance of massively parallel algorithms of the kind used in next-generation supercomputers.

Judging from the participant surveys conducted after the workshop, the students had difficulty understanding nodes, CPUs and cores and other elements of computer structure, and the role of process parallelization and thread parallelization in relation to these elements. We were made keenly aware that future workshops using massively parallel computers will need to have content explaining the structure of computers in addition to instruction in physics and chemistry.

From the second day on, the mood in the workshop was like that of an actual research lab. As in other courses, there were set break times, but the participants were completely immersed in their computing tasks. Some participants took breaks between jobs, while others worked straight through without taking any breaks. It seemed that the workshop ended just as the participants had begun to get used to the computing work.

We regret that there were some participants who were unable to achieve what they wanted to do in the workshop. However, in the participant surveys submitted after the Workshop, some participants were exuberant in expressing their desire to pursue joint research in the future. From the lecturers' perspective, this made it all worthwhile.

CMD® Workshop : Future Issues



Hisazumi Akai

Professor Emeritus, Osaka University / Director, Groningen Center for Education and Research, Supervisory Office for Overseas Centers for Education and Research, Osaka University

Looking back on the 20 workshops that have been held up to now, it seems to me that almost all of the lectures and hands-on sessions have been limited to the stage of quantum simulation. Quantum simulation is the process of elucidating the functions and physical properties of existing materials. In contrast, what we have set as a goal is computational materials design (CMD®) — quantum design in which materials and structures with newly desired functions and physical properties are designed theoretically.

From now on, I think we need to have a greater awareness of this "design" in hands-on practice and implement it at a higher level. Naturally, it is not possible for us to "design" something in hands-on sessions that cover a period of only five days. After all, this is something that is only rarely achieved even after many years of research. The CMD® Workshop should be a place where researchers learn design techniques and approaches and pick up hints on how to proceed, and then take these back to their own workplaces and laboratories to pursue research.

Another issue that we need to consider from now on is how to create a mechanism to publicize our research achievements widely to ensure that they are used in society. The software used in the CMD® Workshop hands-on sessions is all freeware, so it can be used by anyone. There are many different approaches to the release and dissemination of scientific and engineering software, but in our community we use "CMD® Copymart®," a contract model for the distribution of digital contents. Unlike conventional rights management in which copying is prohibited, Copymart®, proposed by Zentaro Kitagawa, a professor emeritus at the Kyoto University, establishes a mechanism by which the agreement permits copying as long as permission has been obtained from the copyright holder in advance. Research on this type of copyright mechanism began even before the CMD® Workshop, and many discussions were held at the International Institute for Advanced Study. CMD® Copymart® was adopted in the lectures beginning with the 12th CMD® Workshop in an effort to popularize its use. We think CMD® Copymart® could be considered as one possible model to create such a mechanism because it is crucial to enable our research achievements to benefit society as widely as possible.

Interviewer: Masaaki Geshi (Project Associate Professor at Institute for NanoScience Design, Osaka University)

CMD® Workshop at the University of Riau, Indonesia

The three Asian CMD® Workshops in Indonesia were initially held at ITB, but in July 2011 the workshop was held at the University of Riau as a result of joint sponsorship with the Indonesian Chemical Society (Himpunan Kimia Indonesia / HKI). The workshop was held for four days, from July 19 to July 22. At this point, a brief overview of the workshop will be presented in addition to reports from two of the participants, Irma and Hani, who previously attended Osaka University as part of a Study Abroad program.

The most notable feature of the CMD® Workshop is that it includes not only lectures on the basic theory and detailed techniques of first-principles calculations and their application but also hands-on computer training using first-principles calculation code developed by the instructors. At these Asian CMD® Workshops, through the cooperation of ITB and the University of Riau, a computer server and 50 Linux® terminals were prepared.

Almost all of the 50 participants were people in the field of chemistry from HKI. Many of the participants were using Linux for the first time, and so a large amount of time was devoted to practicing UNIX® operations. The program for the CMD® Workshop is shown in Table 1. The hands-on computer training was conducted using six types of first-principles calculation code: HiLAPW, STATE-Senri, Osaka2k, RSPACE, MACHIKANEYAMA and NANIWA. Each lecture lasted approximately one hour, with approximately three hours allocated for practical training. Rather than theory, the emphasis was placed on actually experiencing various kinds of calculations.

From the host side, Prof. Hermawan of ITB provided an introductory lecture on first-principles calculation. There were many opportunities for interchange between participants and instructors, both during the lecture and during the lunch period and the fellowship gathering, so the positive aspects of the CMD® Workshops could be observed in the Asian CMD® Workshops as well. In particular, it is to be hoped that the fact that participants and instructors with such different cultural backgrounds were able to share the experience of the workshop over a four-day period will prove valuable in future mutual understanding and research interchange between Japan and Indonesia.

Table 1. Program of the CMD® Workshop held at the University of Riau, Indonesia.

	19-Jul	20-Jul	21-Jul	22-Jul
8:00				
9:00	Opening Introduction & Lecture Kasai	lecture Morikawa	lecture Ono	lecture Nakanishi
10:00	break	break	break	hands-on practice NANIWA Nakanishi
11:00	lecture Hermawan	hands-on practice STATE-Senri Morikawa	hands-on practice RSPACE Ono	break lecture Ogawa
12:00	lunch	lunch	lunch	Closing
13:00	UNIX® operation guide break	hands-on practice STATE-Senri Morikawa	hands-on practice RSPACE Ono	
14:00	lecture Oguchi	break lecture Shirai	break lecture Akai	
15:00	hands-on practice HiLAPW Oguchi	hands-on practice Osaka2k Shirai	hands-on practice MACHIKANEYAMA Akai	
16:00	break			
17:00	hands-on practice HiLAPW Oguchi	break hands-on practice Osaka2k Shirai	break hands-on practice MACHIKANEYAMA Akai	
18:00				

Prof. Hermawan at ITB, one of the lecturers in Asian CMD® Workshop held at the University of Riau.

Main building of the University of Riau, the venue of CMD® Workshop.

Prof. Akai giving the lecture.

A snapshot in the Workshop.

Report of the CMD® Workshop in Indonesia

Hanifadinna

Bandung Institute of Technology (ITB), Indonesia

Brief personal history on major study and research — I hold a bachelor degree in Engineering Physics from ITB, Indonesia. My undergraduate thesis was ab initio study for polypyrrole catalyst using Gaussian Software. After my undergraduate study I had an opportunity to stay for eleven months at Kasai's Laboratory, Osaka University. Now I am a master-course student in ITB and continuing research in computational materials science and engineering.

Experience in the previous workshop — When I was a research student in Osaka University I also have an opportunity to attend the CMD® workshop on March 2010 in Kyoto.

Purpose of attendance to present workshop — I hope within the CMD® workshop I can broaden my knowledge in the area of computational material design, especially for my present research and I also hope I can share to those who interest with this area.

How to use the skills and knowledge you got in the workshop — I will try to use it in my research, to get the calculation result if it is applicable.

What kind of calculations to perform with the "K" Computer — I want to perform an ab-initio molecular dynamic calculation for my further research.

Aspirations for future relation and cooperation to Japan — I hope there will be any program like CMD® which gives an impact for the education atmosphere in Indonesia and I hope some students could have an opportunity to learn in Japan because Japan is well known for advances in science, technology and industry while maintaining high belief in traditional cultures. With this condition, I believe the activity like CMD® becomes high motivation for many students and researchers in Indonesia in pursuing the advanced education.

Dream in research — I hope I can design a new advanced material in fuel cell technology and other applications with my knowledge in computational material design. I also hope that I can share my knowledge and experience with the students who are interested in fuel cell and quantum engineering. To train and find the potential individual who can help out my research project and maybe can develop it any further. After all, to make the continuity of research and to keep it going, it cannot be done by one person alone but nevertheless have to work as a team.

Ms. Hani (right), and Ms. Triati (left), a foreign student at Osaka University from ITB, who supported the CMD® Workshop in full scene.

Report of the CMD® Workshop in Indonesia

Irma Syafitri

Bandung Institute of Technology (ITB), Indonesia

Brief personal history on major study and research — In 4th year at ITB, my project was "Immobilization of leucine on polypyrrole for biosensor applications: A density functional theory study." After that, I joined Akai's group in Department of Physics, Osaka University. I had two research topics "Metal-to-insulator transition in yttrium trihydride" and "Knight shift of hydrogen in NiTi," by using KKR method. My current project at ITB is "Immobilization of leucine on polypyrrole for biosensor applications by water solvent: A density functional theory study."

Experience in the previous workshop — In 2009, I became one of the committee in Asia CMD® workshop at ITB. In that time, I helped the things which needed in the CMD® workshop, such as place of activities, consumption, or certificate. In 2009, I became one of the participants in CMD® Workshop at International Institute for Advanced Study, Kyoto. In the workshop, I was learned some kind of the CMD® tools, such as ABCAP, ES-opt, HiLAPW, MACHIKANEYAMA, NANIWA, Osaka2k, STATE-Senri, and TSPACE. In this workshop, we can learn the CMD® tools from the developers directly. By these tools we can calculate the properties of the material such as the electronic structures of metals, semiconductors and compounds, etc.

Purpose of attendance to the present workshop — My purpose in the current CMD® workshop is to learn more how to use CMD® tools that I did not learn in the previous workshop and make good relation with Japan university lecturers.

How to use the skills and knowledges you got in the workshop — After attended this workshop I will use this knowledge and skills in research, workplace and living environment.

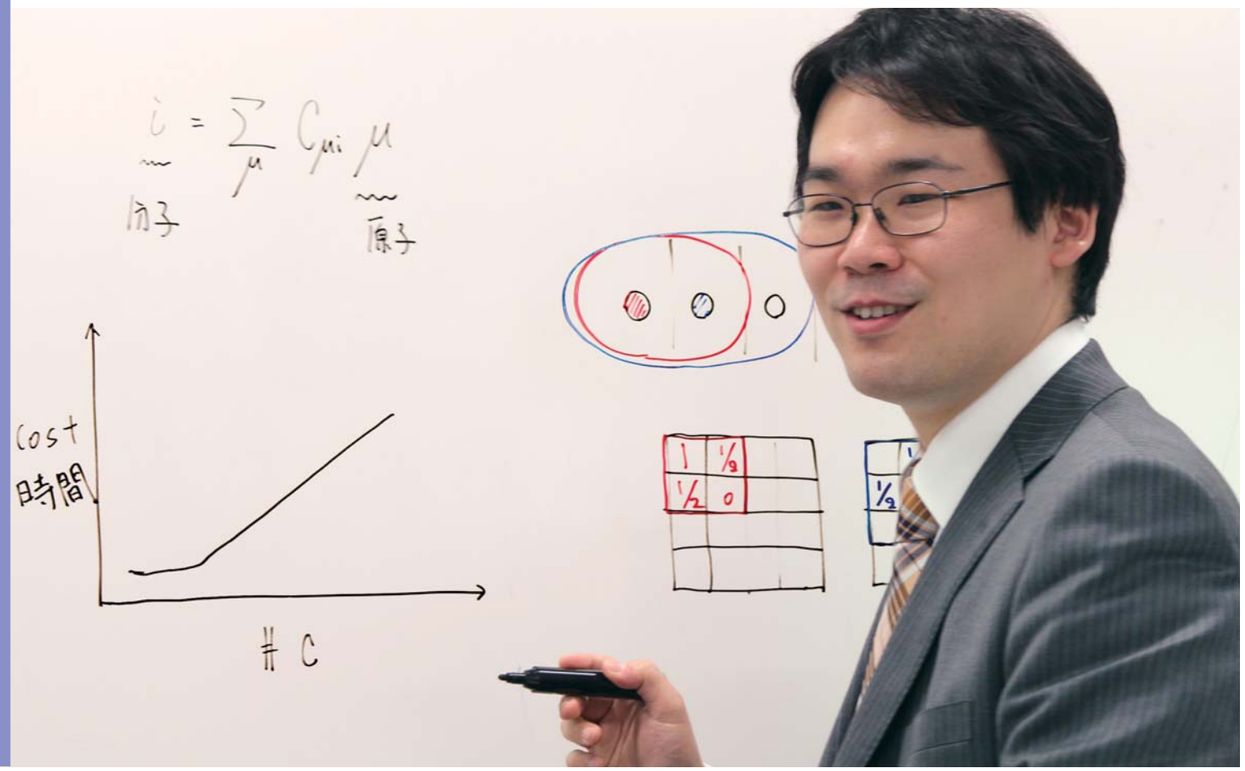
Ms. Irma.

What kind of calculations to perform with the "K" Computer — By this "K" Computer we can calculate the properties of the material in the big size input file, such as electronic structures of metals, semiconductors and compounds, etc. I hope it can help our project and research for Japan and Asian nations.

Aspirations for future relation and cooperation to Japan — By this CMD® workshop, I can make good relation with Japan University lecturers, so that in the future I can make cooperation in research field.

Dreams in research — I hope I can find new theory in computational material design. At least, I can show the phase diagram of metal-to-insulator transitions of YHx. This is a challenge for me in order to solve this problem, so in the future it can be useful to find new technologies and new theories.

Interview with Masato Kobayashi, developer of DC



Interviewee:
Masato Kobayashi
Assistant Professor,
Waseda Institute for Advanced Study,
Waseda University

Interviewer:
Yu Yachi
Ph.D. Candidate, Division of General Culture,
Graduate School of Humanities and Sociology,
The University of Tokyo

"Divide each difficulty into as many parts as is feasible and necessary to resolve it," said the philosopher Rene Descartes. Since ancient times, the idea of "divide and conquer" has been widely used in the realm of politics, etc. But in recent years it has also been applied to methods of calculation for large-scale systems — in particular, as a method of speeding up electronic structure calculations. Masato Kobayashi, who has studied the divide-and-conquer method, is working to incorporate electron correlations in order to further increase the accuracy of this method. He has succeeded in developing DC, new application software based on his original idea.

Computers and quantum chemical calculations

"Everyone is fascinated when they do a laboratory experiment and see the blue color of copper ions appear. But why is the color blue? That's something very difficult to figure out. These kinds of fundamental questions can be understood through quantum chemistry. That's why I was attracted to it." So says Dr. Masato Kobayashi in explaining why he chose the path of quantum chemistry.

The behavior of electrons and atomic nuclei determines the structure and properties of all matter. Quantum chemistry provides theoretical explanations for this behavior. Electronic structure — electron density, energy state, spin state and so on — can be calculated by solving the Schrödinger equation. In practice, it is not possible to exactly solve equations for many-body systems made up of numerous electrons and atomic nuclei. For this reason, approximation is used for calculation.

Nevertheless, even when a computer with high-level computational ability like the K Computer is used, it takes an enormous amount of time to execute calculations with highly accurate approximation, those capable of adequately recreating the properties of matter. If the number of atoms is N, computing time increases proportionally to N^{5-7}. Suppose a computer takes one second to perform calculations for a single atom. That computer would need from 30 seconds to two minutes to perform calculations for two atoms. If there are 100 atoms, the computer would need anywhere from 300 years to three million years.

Hardware advancements alone will not be sufficient to decrease this enormous computing time. The real key will be to develop software that uses a completely new theory for approximation calculations and can take advantage of the latest hardware. That key is now in place, in the form of the divide-and-conquer method and the DC application software based on this method.

"Divide difficulty into parts"

The "divide-and-conquer" method takes the approach of dividing a problem that cannot be calculated as is into smaller partial systems and then solving those small problems. In quantum chemistry, the divide-and-conquer method divides large molecules up, performs calculations for each part, and then adds up the results.

Although the concept is simple, in practice a variety of measures are needed. First, the target molecule must be divided up into several non-overlapping subsystems. This means that the impact of the surrounding domains will not be included in the calculations, resulting in low accuracy. For this reason, the subsystems with the peripheral atoms added as buffer domains are calculated separately (Fig. 1). Then, the results of all subsystems are accumulated with excluding contributions from the buffer domains. The process is repeated until the electron density derived in this manner converges to a certain value at every point in the space. With the divide-and-conquer method, calculations are performed with the entire system divided up into subsystems of a uniform size, so the calculation time is directly proportional to N. Using the previous example, calculations for 100 atoms could be performed in 100 seconds. Moreover, as the calculations for each subsystem are performed independently, they can be done efficiently using parallel computing with modern supercomputers like the K Computer that are made up of numerous processing nodes. One of the features of the divide-and-conquer method is that even if the subsystems are made smaller, for example divided up into individual atoms, the accuracy is not greatly reduced. Dr. Kobayashi focused on this attribute and wanted to create a program that would be easy for anyone to use.

Encounter with Energy Density Analysis

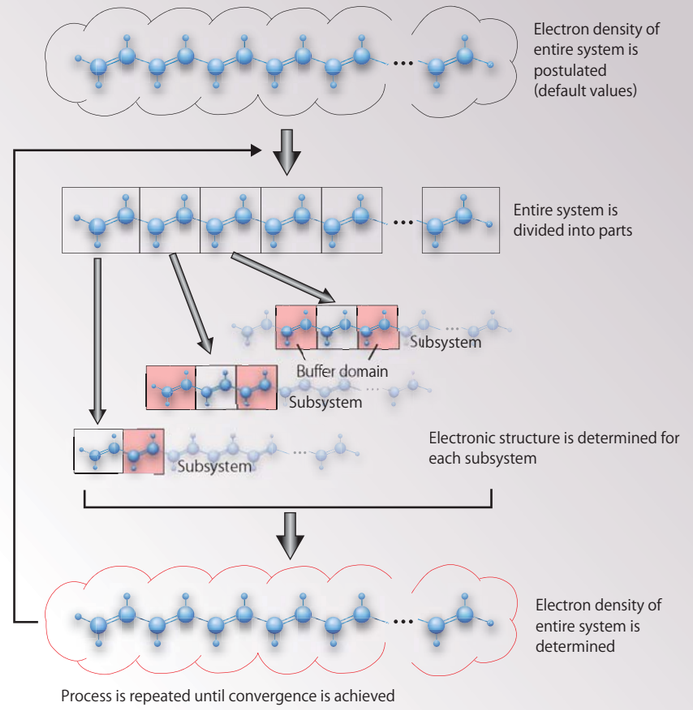
To achieve higher calculation accuracy, the effect of electron correlation must be incorporated. With the conventional divide-and-conquer method, the interaction between electrons is averaged. The difference between this averaged interaction and the exact interaction is referred to as "correlation energy."

However, there was a major problem with applying the divide-and-conquer method to calculations that incorporate electron correlation. The values derived with the conventional divide-and-conquer method were those for the correlation energy for each subsystem including the buffer domains, and simply adding these up will result in duplicate calculation. It was essential that this problem be resolved.

One day, Dr. Kobayashi heard a presentation on Energy Density Analysis (EDA) at a laboratory seminar. That gave him the idea to incorporate EDA into the divide-and-conquer method.

Energy Density Analysis is an analysis technique in which the energy of the entire molecule is allocated to individual atoms. Dr. Kobayashi thought that EDA might make it possible to derive the correlation energy for individual domains without including the buffer domains. Adding these together

Fig. 1 Basic process of divide-and-conquer calculation



In divide-and-conquer method, the computations are performed for subsystems with the surrounding atoms (buffer domains) added to individually divided non-overlapping domains. This method makes it possible to maintain high accuracy.

Masato Kobayashi

Dr. Kobayashi creates computational theory for quantum chemistry, and he also does all of the programming himself. He is particularly hardcore in the latter sense, ever since coming in contact with BASIC in his elementary school days. He is a strong supporter of releasing software for free, saying that he is happy just to know that the software is being used by many people. In his spare time, he enjoys playing the tuba. Dr. Kobayashi's diverse talents and his outlook of finding enjoyment in the pure pursuit of knowledge are sure to result in a bright future.

would enable even the correlation energy to be determined in a calculation time that was proportional to *N*. This became the EDA divide-and-conquer method developed by Dr. Kobayashi.

"In physics, it might be taboo to apply an analysis method like EDA to calculation theory," says Dr. Kobayashi. "For that reason, I was very uneasy as to whether it would actually work. But I tried several different methods, and the method that uses EDA gave the most accurate results, and the calculation time was also short."

Calculating larger systems with higher accuracy

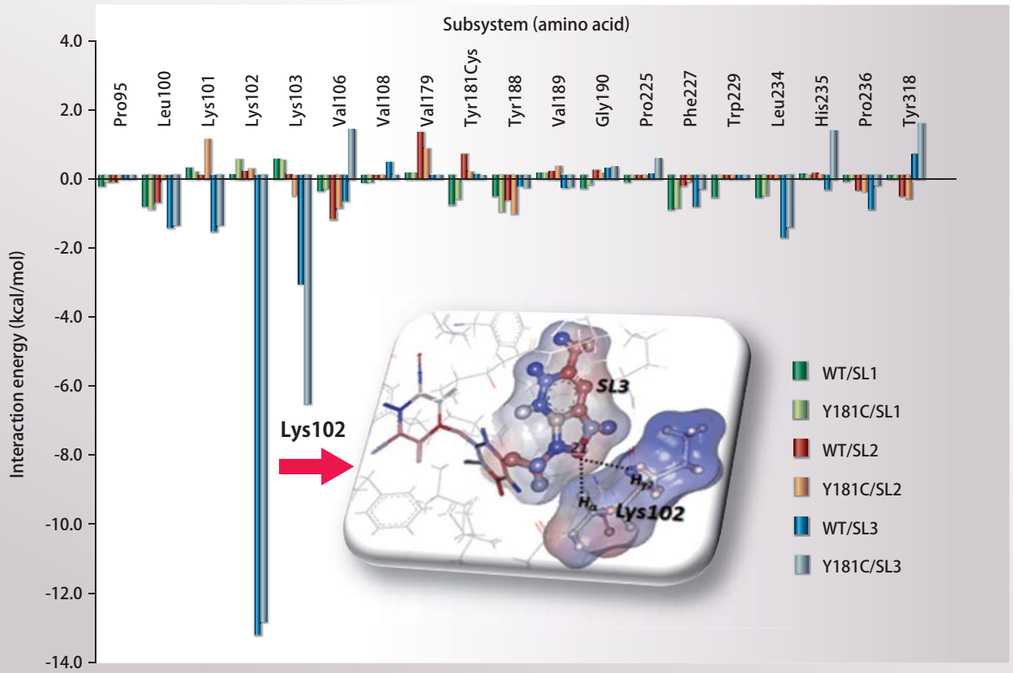
Combining Energy Density Analysis with the divide-and-conquer method made it possible to quickly perform highly accurate calculations that include electron correlation. This method is well-suited to the investigation of substances in which electrons are not localized and move from place to place. With the K Computer, it is even possible to perform ultra-high accuracy calculations for nanosize materials. For example, the power generation efficiency of organic solar cells is greatly affected by the electrical properties of charge transport materials like pentacene. Using the divide-and-conquer method to calculate the charge mobility is making it possible to design solar cell materials that have greater efficiency.

Moreover, Energy Density Analysis makes it possible to calculate the correlation energy for each domain, enabling direct analysis to determine, for example, locations where interaction is strong, or locations that are unstable and where the bond is about to break. For example, it is possible to conduct a detailed investigation of the bond between the HIV (AIDS virus) and the reverse transcriptase inhibitor that is designed to inhibit the virus (Fig.2). In the future, this type of information will not only make it possible to safely pursue the development of more effective drugs and enable the costs to be greatly reduced, it may even make it possible to predict side effects.

At present, DC, the EDA divide-and-conquer application software, is available to the general public as freeware. It is incorporated into GAMESS, the world's most commonly used freeware for quantum chemical calculations, as an option. Dr. Kobayashi had customized GAMESS so he and his colleagues could use his own method within the program. In order to make his software available to as many people as possible, he contacted Iowa State University, which manages GAMESS, and got the program formally adopted.

More recently, Dr. Kobayashi has just started adapting the program for the K Computer. The K Computer is made up of 640,000 cores. "It's completely unlike any supercomputer up to now, so the software requires special tuning," he says. "I still have several hurdles to overcome. It' s a challenge for the future." I was struck by the obvious joy in his voice.

Fig. 2 Interaction between AIDS virus and medicine determined using the EDA divide-and-conquer method



Use of the EDA divide-and-conquer method makes it possible to handle large systems that combine biomolecules and drugs. The figure shows the interaction energy between the AIDS HIV-1 reverse transcriptase and the MK-4965 inhibitor. As the figure shows, the MK-4965 subligand 3 (SL3) has a particularly strong interaction with lysine 102 (Lys102) and lysine 103 (Lys103). This kind of detailed information on interactions is expected to lead to new drug development.

Application SPEC Sheet [DC]	
Code Name	DC
Method / Algorithm	HF, MP2, CC and density-functional-theory calculation using the divide-and-conquer (DC) method
Overview / Features of Code	Fast quantum chemical calculation methods are currently attracting attention worldwide, and a variety of approaches have been devised. The divide-and-conquer (DC) method is characterized by its ability to be applied to delocalized electron states as well, and by its ability to execute highly accurate MP2 and CC calculations.
Materials for Simulation	Nano materials and biomolecules
Development Leader	Hiromi Nakai
Developers / Developing Institutions	Nakai Research Group, School of Advanced Science and Engineering, Waseda University Waseda Institute for Advanced Study
Development Period	Development since 2005
Development Language / Number of Lines of Source Code	Fortran / Approximately 800,000 lines (including GAMESS main program)
Operating Environment	K Computer
Parallelization Method	DDI (implemented by MPI+ARMCI) / OpenMP hybrid
Status of Parallelization	Currently 94.80% parallelization efficiency on 72 nodes with respect to 36 nodes
Software Release	Source code has been opened to the public
Related / Competing Applications	FMO-MP2, OpenMX, Conquest, etc.
Other Functions	Input data format is designed to be generally compatible with FMO-MP2; input data can be created using a GUI that is compatible with FMO-MP2

Yu Yachi

Based on her love of natural science, Ms. Yachi entered the Natural Sciences I program at the University of Tokyo. Yet she was unable to leave behind her desire to pursue philosophy and literature, and she went on to study in the Faculty of Letters. Her research topic is "What is reality, and what is fiction?" She uses a wide-ranging approach from perspectives that include analytic philosophy, mythology and cognitive neuroscience. In her quest to link academia with society and the natural sciences with the humanities, Ms. Yachi is currently attending the Science Interpreter Training Program. She is also active as a writer.

2nd CMSI Poster Award

The 2nd CMSI Workshop was held on January 30 and 31, 2012 at the Institute for Materials Research at Tohoku University. In this Workshop, the activities of CMSI during the past year have been reported and evaluated. The sessions featured 23 oral presentations, categorized into the four CMSI research fields of "Fundamental science of novel quantum states and new materials," "Next-generation advanced device science," "Energy conversion," and "Molecular function and matter transformation."

The poster session featured 53 posters. The poster presentation was held on the evening of the first day, with one minute allotted for the presentation of each poster, followed by a discussion that lasted for two hours. From among these presentations, poster awards were presented to young researchers and graduate students 35 years of age or under whose posters were an outstanding preview of upcoming research. The three awards in the 2nd CMSI Poster Awards were given to Masato Kobayashi (School of Advanced Science and Engineering, Waseda University (at that time)), who is also featured in the "From the Front Lines of Application Development" section, for his poster entitled "Development of Divide-and-conquer (DC) Quantum Chemistry Calculation Programs;" Yasunobu Ando (Graduate School of Science, The University of Tokyo (at that time)) for his poster entitled "Study of Electrical Double Layer Capacitance of a Solid-liquid Interface Using First Principle Molecular Dynamics;" and Hiroshi Watanabe (Institute for Solid State Physics, The University of Tokyo) for his poster entitled "Effect of System Noises in Massively Parallel Classical Molecular Dynamics." The awards were presented at the reception held on the first day, and the three recipients received warm applause.

1 Graduate Interview

From First-principles Calculations to the World of Game Programming

This section will present profiles of some of the young researchers who have studied computational materials science and are now active in various industries. The first interview features Teppei Ono, who has begun a career as a game programmer. CMSI Division Researcher Yusuke Konishi went to visit Ono and ask about his graduate school research, the reason that he chose that career, what the work is like and so on.

Yusuke Konishi

Nanosystem Research Institute, National Institute of Advanced Industrial Science and Technology (AIST)
CMSI Industry-Government-Academia Cooperation Division Researcher

Teppei Ono

Advanced Technology Division, Square Enix Co., Ltd.

Mr. Ono majored in physics at the Graduate School of Science, The University of Tokyo and studied applications for GPU programming in first-principles calculations. After graduating with his Master's Degree, he joined Square Enix.

What is the attraction of game programming?

Konishi: Could you start by explaining what kind of work you do?

Ono: The Advanced Technology Division where I work functions as a technical support team for the company. I work on developing game engines. Game production involves various tasks: graphics, animation, AI, physics calculations and so on. When we develop a new game, it's becoming difficult to do everything from scratch, so we use existing systems and libraries. The function of the game engine is to create this common infrastructure and systems and put a development environment in place. I'm in charge of tool programming.

Konishi: Exactly where is that in the entire game production process from planning to completion?

Ono: The development of the game engine itself is separate from the game production process. The game engine is ultimately only a means of producing the game. Using the game engine makes each step in the game production process go more efficiently and ensures high quality (Figure on the next page).

Konishi: Can this common infrastructure be used for making software that will run on any platform — say, game machines, PCs, smart phones and so on?

Ono: The ideal is to be able to use the game engine so things made on the PC will run on any machine. It's important to design the game engine so a different code can be substituted for the sections that won't run well under a different environment.

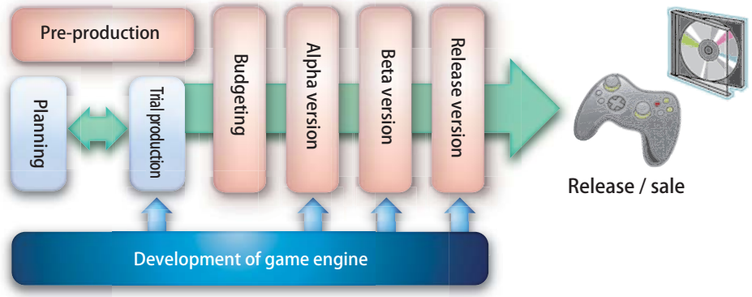
Konishi: What aspect of programming do you like best?

Ono: I really enjoy the fact that mastering the skills makes you more adept at writing programs.

Konishi: Isn't the real thrill also the fact that a new product may become a bit hit and sell several million copies?

Ono: I've only worked here for two years, so I haven't had that experience. But of course I'd love to release a game that completely revolutionizes things.

Game engine and sample game production process



What was your motivation for changing from physics to game programming?

Konishi: What was your original motivation for choosing this type of work? It's rare for someone who studied physics to go into this line of work.

Ono: At the end of my first year of college, I started studying programming so I could create game software as a hobby. I began with a two-dimensional game, and when I had gained some skill, I began working on creating three-dimensional games. In the course of doing this, I experienced the enjoyment when I completed a game, and I also became very attracted by the difficulty and depth of game programming.

But then I ran into problems that I couldn't solve no matter how hard I tried. And the programs became enormous and impossible to manage. It was frustrating.

Konishi: When was this?

Ono: Around the end of my third year of college. I thought I had given up, but for some reason I couldn't stop looking at the source code. So I decided to give it another try. I started to study programming again from the ground up. And I found I was able to write far more advanced programs than before. That was a major turning point for me, and I decided to make game programming my career.

Konishi: Of all of the game companies you could have chosen, why did you choose Square Enix?

Ono: I simply liked one of the games they marketed. Also, they make their technology a selling point. I was interested in them because they used advanced technology for game programming.

Are you using what you learned in graduate school?

Konishi: What kind of research did you do in your graduate school days?

Ono: Around the time that CUDA (a programming environment for GPUs) had just come out, I was working on increasing the speed of the diffusion Monte Carlo, a kind of first-principles calculation, by using GPUs. The Monte Carlo method is well-suited to parallel computing, and I was able to achieve a greater than ten-fold increase in speed. So in that respect I was able to produce achievements. But even though I was able to perform calculations for molecules up to a certain size, there were problems with program stability and so on, so I wasn't able to apply it to larger systems.

Another research topic was single precision operations on GPUs. The GPUs nowadays are capable of double precision operations, but at the time they hadn't been developed, and I was exploring how far it was possible to calculate with only single precision.

Konishi: With single precision it seems like the rounding error would be a big problem. Was it?

Ono: Yes, I came to the conclusion that using only single precision would be difficult when high accuracy was needed. And I was happy that I was able to confirm that, leaving aside the question of GPUs, even if low-cost fast calculation units were available, they also would not be much help if we could only perform single precision operations.

Konishi: Are you using your graduate school research in your job now?

Ono: I'm using the knowledge I gained about GPUs in my job. I may not actually use numerical simulations themselves in games, but in the course of producing more realistic games in the future, I think it's possible that I'll use numerical simulations for advance data preparation.

Advice for students

Konishi: Lastly, as someone who has studied computational materials science, do you have any advice for students?

Ono: The programming I started doing in my student days was kind of my own style, and I wish I had studied design more seriously. After I joined the company, I began full-fledged study of design patterns. But if I'd mastered that while I was still a student, I might had produced better results in my research as well.

Since other people may use or expand on the code I'm creating in my job now, I'm being careful to create programs that are flexible and versatile. This is something that's needed in scientific numerical computing as well, especially for large-scale programs.

Konishi: The kind that we'll be working with if we start using the K Computer.

Ono: Yes. And in terms of the programming environment, I think more and more development will be done by multiple programmers from now on, so we'll have to use version control software.

Konishi: CMSI will also have to work hard to develop the framework for teaching the expertise needed for large-scale software development.

(April 25, 2012 at the Square Enix head office)

Profiles of Division Researchers

This section will introduce the Division Researchers who joined CMSI in April 2012.

Kazuya Ishimura

Molecular Science Division Researcher
Institute for Molecular Science, National Institutes of Natural Sciences

I majored in quantum chemistry at the Graduate School of Engineering at Kyoto University and received my Doctorate (of Science) from the Graduate University for Advanced Studies. Currently I'm conducting research into methods and techniques for performing large-scale quantum chemical calculations at Institute for Molecular Science.

Motivation for applying for the position
I wanted to use what I'd learned about large-scale parallel computing to develop basic programs for use on the K Computer.

Mission / Role
To develop programs for performing high-speed, highly parallel quantum chemistry calculations and make them public so they can contribute to other areas of research as well. I'd also like to provide development-related expertise in order to create an environment that will facilitate participation by many researchers.

Ambition
I want to use the K Computer to create guidelines for the design of catalysts, secondary cells and other materials.

Tsuyoshi Okubo

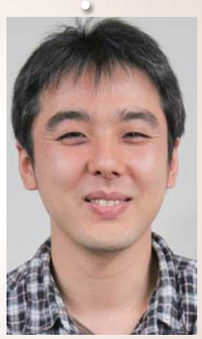
Condensed Matter Physics Division Researcher
Institute for Solid State Physics, The University of Tokyo

I majored in physics at the Graduate School of Sciences at Kyushu University. After receiving my Doctorate (of Science), I studied ordering and dynamics of frustrated magnets at the Graduate School of Science at Osaka University.

Motivation for applying for the position
I believe that progress in large-scale parallel computing using the K Computer opens up a new world of condensed matter physics research that is qualitatively very different than what has been done before, and I wanted to contribute to that project.

Mission / Role
To develop innovative algorithms and techniques for computational condensed matter physics using large-scale parallel computing, and to use them to conduct condensed matter physics research.

Ambition
I want to enjoy tackling new challenges and developing algorithms, and use them to pursue intriguing physics research.



Hiroaki Nishizawa

Molecular Science Division Researcher
Institute for Molecular Science, National Institutes of Natural Sciences / Faculty of Science and Engineering, Waseda University

I majored in quantum chemistry at Waseda University where I received my Doctorate (of Science). I worked on theoretical development of nonadiabatic theory.

Motivation for applying for the position
I developed programs not only as part of my research but as a hobby as well, so I thought I would be able to put that skill to use.

Mission / Role
To create advanced parallel computing programs using quantum molecular dynamics and the DC method, a linear scaling quantum chemistry calculation method, and conduct experimental research into chemical reactions.

Ambition
To develop software that is easy for people conducting experiments to use, and is not only functional but highly usable.

Tomoko Mizuguchi

Molecular Science Division Researcher
Institute for Chemical Research, Kyoto University

I majored in physics at the Graduate School of Sciences at Kyushu University where I received my Doctorate. Later I studied glass transition using molecular dynamics at Lille 1 University in France.

Motivation for applying for the position
I wanted to expand on the systematic separation method for time scales and interaction in glass systems, in order to learn more about multi-component heterogeneous systems with more complex interactions among molecules.

Mission / Role
To achieve advances in methods of fusing large-scale MD simulations and solution theory, in order to learn more about issues involved in intermolecular interaction in nanoscale heterogeneous systems.

Ambition
I want to combine molecular science research and software operation advancement in order to help establish methods for analysis and control of molecular ensemble functions at the atomic and molecular level.

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.

Tatsuya Sakashita

Condensed Matter Physics Division Researcher
Institute for Solid State Physics, The University of Tokyo / CMSI Kobe Branch

I majored in pure mathematics at Hiroshima University and the Graduate School of Science at Osaka University. Later I studied quantum information theory at the Graduate School of Information Systems of the University of Electro-Communications where I received my Doctorate (of Engineering).

Motivation for applying for the position
The implementation of large-scale computing in quantum information theory, which I was doing in my doctoral studies, required a deep understanding of eigenvalue computation. I wanted to apply this experience to parallelization on a next-generation supercomputer.

Mission / Role
To work on efficient implementation related to linear calculations including eigenvalue computation, in order to efficiently implement ALPS, QDS and other statistical mechanics simulation programs.

Ambition
My goal is to achieve ideal implementation in every sense — from the standpoint of linear calculation, computer architecture, condensed matter physics theory and so on.

CMSI Calendar

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

●1st K Computer Condensed Matter Physics Seminar
Date : April 18, 2012
Venue : Advanced Institute for Computational Science (AICS)

●CMSI Industry-Government-Academia Cooperation Symposium "Current State of OCTA Use in Industry"
Date : May 8, 2012
Venue : Akihabara Conference Center

●1st CMSI Informational Exchange Workshop on K Computer Use
Date : May 10, 2012
Venue : Advanced Institute for Computational Science (AICS)

●2nd K Computer Condensed Matter Physics Seminar
Date : May 23, 2012
Venue : Advanced Institute for Computational Science (AICS)

●Field 2 x Field 5 Interdisciplinary Exchange Workshop
Date : May 30, 2012
Venue : Institute for Solid State Physics, The University of Tokyo

●3rd K Computer Condensed Matter Physics Seminar
Date : June 13, 2012
Venue : Advanced Institute for Computational Science (AICS)

●K Computer Symposium 2012 and 2nd HPCI 5 Field Joint Workshop
Date : June 14 - 15, 2012
Venue : Kobe University Integrated Research Center Convention Hall

●3rd Computational Materials Science Symposium
Date : June 18 - 19, 2012
Venue : Institute for Materials Research, Tohoku University (Building 2 Lecture Hall)

●MASP2012 Workshops and Symposiums
Workshops June 25 - July 1, 2012
July 3 - 11, 2012
Symposiums July 2, 2012
July 12 - 13, 2012
Venue : Institute for Solid State Physics, The University of Tokyo

●4th Joint Research Seminar, HPCI Strategic Program
Date : July 10, 2012
Venue : Advanced Institute for Computational Science (AICS)

●6th CMSI Young Researcher Technical Workshop
Date : July 17 - 19, 2012
Venue : Yamaha Resort (Shizuoka Prefecture)

●4th K Computer Condensed Matter Physics Seminar
Date : July 26, 2012
VVenue : Advanced Institute for Computational Science (AICS)

●1st Research Field "New Quantum / New Material Phase Basic Science" Summer School
Date : August 20 - 25, 2012
Venue : Zao Takamiya Village Hotel Jurin (Yamagata Prefecture)

●CMD®21
Date : September 3 - 7, 2012
Venue : Building G, Graduate School of Engineering Science, Osaka University

●Massively Parallel Technology Workshop
Date : Not yet decided
Venue : Not yet decided

●Advanced Institute for Computational Science (AICS) Open House
Date : October 20, 2012
Venue : Advanced Institute for Computational Science (AICS)

●Computational Condensed Matter Physics Symposium (in cooperation with SPring-8 and J-PARC)
Date : October 22 - 23, 2012
Venue : Institute for Solid State Physics, The University of Tokyo

●3rd Research Workshop of the Theoretical and Computational Chemistry Initiative (TCCI)
Date : October 2012 (exact date not yet decided)
Venue : Not yet decided

●SC12 (plans for a booth exhibit)
Date : November 10 - 16, 2012
Venue : Salt Lake City, Utah, USA.

●3rd CMSI Workshop
Date : December 3 - 5, 2012
Venue : Institute for Molecular Science

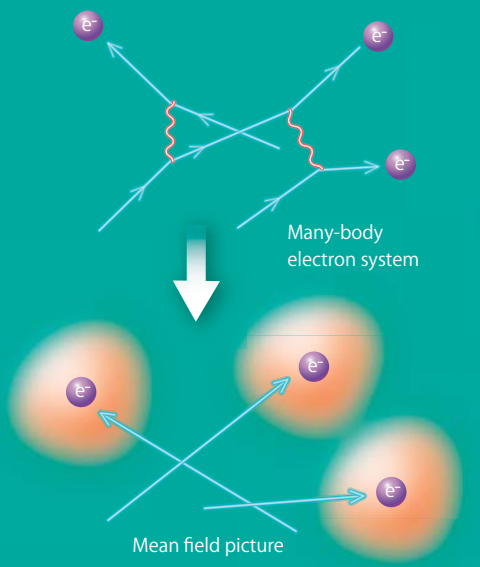
●TCCI Winter School (molecular simulation)
Date : December 11 - 14, 2012
Venue : Institute for Molecular Science

Effects of electron correlation

The key concept behind the application DC featured in this issue is "electron correlation." What properties of matter does electron correlation bring about?

Mean field approximation: the point of departure for materials science

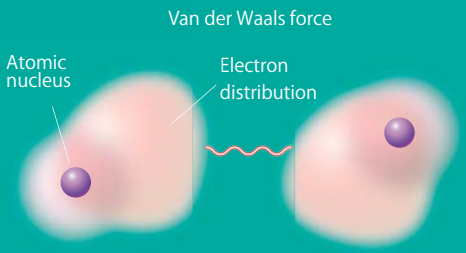
Inside objects, numerous electrons are in motion, repelling one another as they move. It is not possible to predict the motion of these numerous electrons even using the most advanced computers available. Since the birth of quantum mechanics, however, scientists have used a theory called mean field approximation as their starting point for explaining the properties of matter.



In the mean field theory, "multiple electrons interacting with one another" are replaced by "a single electron under the influence of the averaged electric field from other electrons."

Electron correlation: fluctuation from the mean field

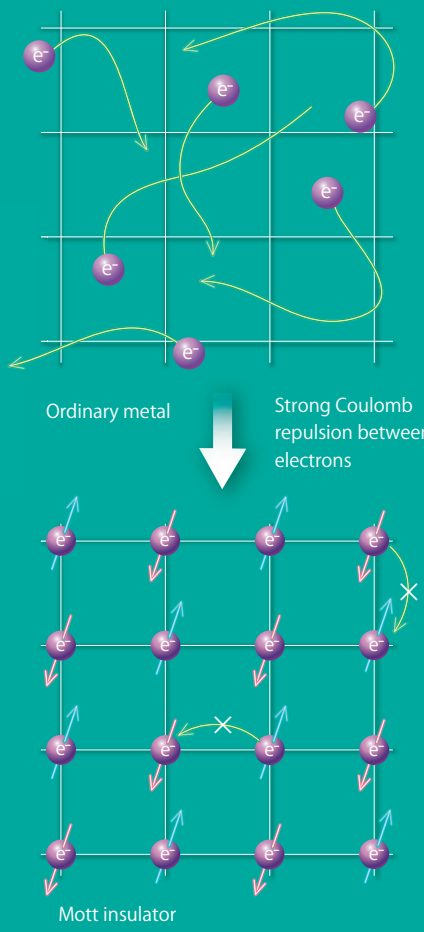
It should be noted that there are many phenomena in nature that cannot be expressed using the mean field theory. One of these is the van der Waals force between neutral atoms or molecules to form dry ice and other molecular crystals and liquids. This force is produced by the deviation and fluctuation from the mean electron distribution. This type of deviation and fluctuation from the mean field is known as "electron correlation."



The electron distribution of neutral atomic molecules fluctuates electrically within an extremely short time window. This fluctuation distorts the distribution of electrons in other atomic molecules.

Electron correlation turns electrons into magnets

Individual electrons function as tiny magnets. The fact that iron and nickel exhibit the properties of magnets overall is also a manifestation of electron correlation. In addition to magnetism, due to a strong electron correlation effect, some transition metal oxides and the like function as insulators that do not allow electricity to flow. These are known as Mott insulators.



In a Mott insulator, the quantum-mechanical nature of electrons to spread in the form of a wave is suppressed by electron correlation, and as a result electrons does not carry electric currents.

Cooperation : Youhei Yamaji (The University of Tokyo)

Electron correlation in next-generation technology

Progress in technology has made it possible to confine electrons to a space the length of several hundred atoms, known as a "quantum dot," and even add or withdraw individual electrons from the dot. It has also been discovered that, in situations in which the electric current hardly flows at high temperatures, the current will begin to flow if the temperature is reduced, due to correlation between the electrons in the dot and the electrons in a circuit. This clearly demonstrates that electron correlation will be crucial to our understanding of next-generation electronic circuits.

Torrent No.5 July 2012

Cover:
Tropical fruits that entertain us by all their own shapes and tastes are reminiscent of unlimited possibilities.
Like a wealth of researches in CMSI.

Torrent : The Newsletter of the Computational Materials Science Initiative (CMSI) No.5, July 2012

CMSI is a research network promoting Field 2 "New Materials and Energy Creation" within HPCI Strategy Program (SPIRE) of the MEXT, Japan.

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