# K Computer : The Computer That Leaps Through Time

The K Computer can perform $10^{16}$(=10,000,000,000,000,000) calculations per second (10 petaflops)*. This is an enormous number of calculations. If a human being performed these calculations by hand at a rate of one calculation every second, it would take 300 million years to complete. 300 million years ago, human beings had not yet evolved, and the Japanese archipelago did not exist. * K (kei) refers to the number $10^{16}$ in Taiwan, Korea and Japan.

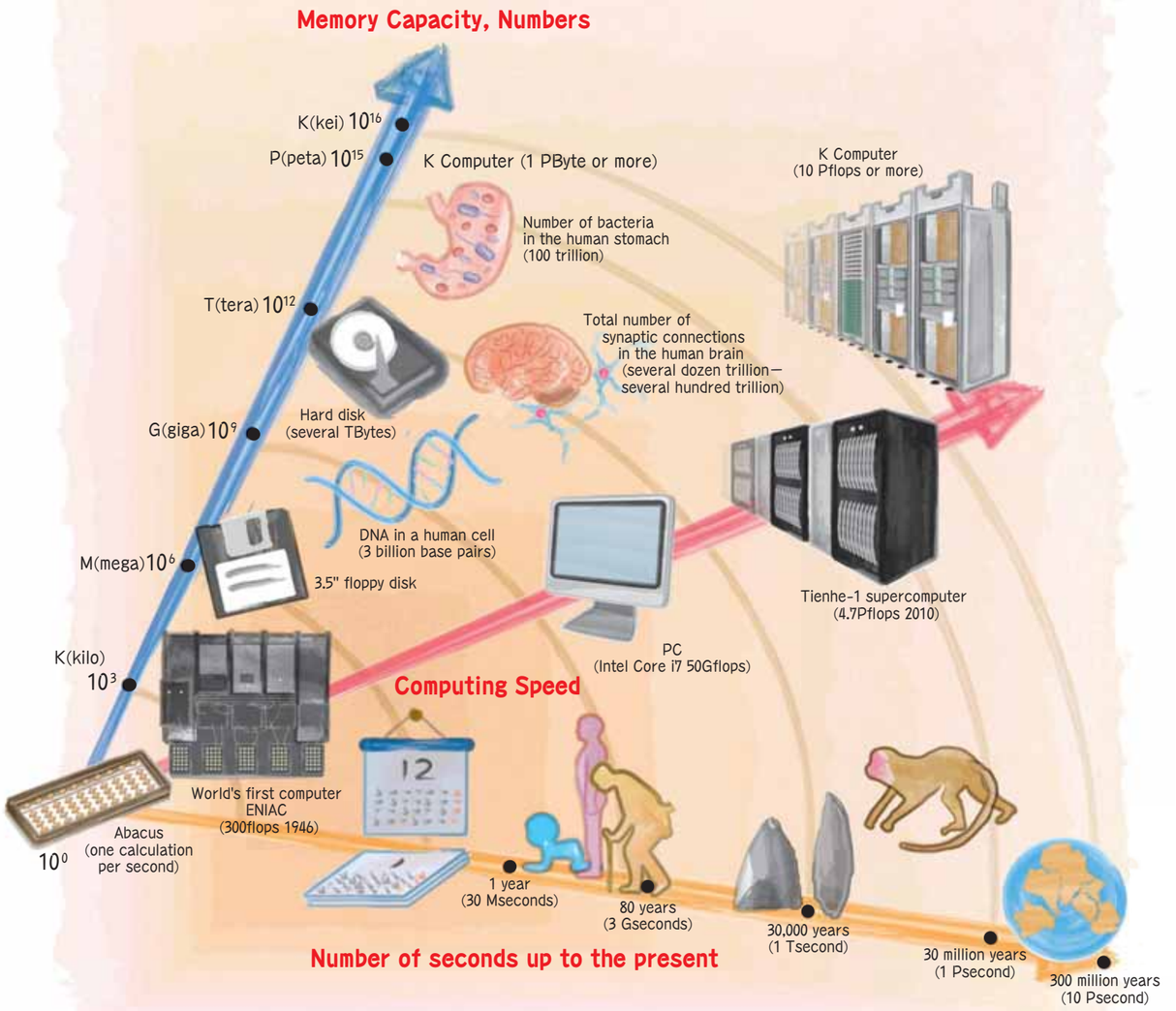


Illustration: Yuki Akimoto (Mabuchi Design Office)


**Torrent** : The Newsletter of the Computational Materials Science Initiative (CMSI) No.2, May 2011



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cmsi Computational Materials Science Initiative


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# torrent

# $10^{16}$ Weave New Materials



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

Young CMSI Researchers

# 1st CMSI Poster Award Recipients

"Torrent" is a forum for CMSI interchange. On January 5-7 2011, Workshop: "Computational Materials Science: Challenges and Prospects" was held. This workshop was organized jointly by ISSP, CMSI and the Next-Generation Functional Nanomaterials for Information Technology*. The three winners of the Poster Award at the workshop came together to discuss their individual research projects, their experiences using supercomputers, their interchange at CMSI, and the ties between young researchers.

* ISSP: the Institute for Solid State Physics, The University of Tokyo.
Next-Generation Functional Nanomaterials for Information Technology :
a group in Grand Challenges in Next-Generation Integrated Nanoscience Project.

■ Poster Award Recipients

**Takahiro Misawa**
Research Associate,
Department of Applied Physics,
School of Engineering, The University of Tokyo

**Hidemaro Suwa**
3rd year Ph.D candidate,
Department of Applied Physics,
School of Engineering, The University of Tokyo

**Hayato Shiba**
Research Assosiate,
Materials Design and Characterization
Laboratory, Institute for Solid State Physics,
The University of Tokyo

■ Moderator

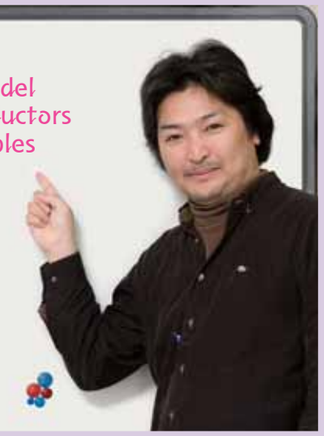
**Munekazu Ohno**
Associate Professor, Faculty of Engineering,
Hokkaido University

**You're all the type of people who love theory but also want visible output**

**Ohno :** Dr. Misawa was awarded the Grand Prize Poster award for his poster entitled "Analysis of an Effective Model for Iron-based Superconductor Using the Multivariable Variational Monte Carlo Method."Mr. Suwa was awarded the Outstanding Poster award for his poster entitled "Markov Chain Monte Carlo Method without Detailed Balance."Dr. Shiba was awarded the Judge's Special Prize for his poster entitled "Biomembrane Molecular Simulation That Explicitly Includes Solvent Molecules in an Effort to Achieve Massively Parallel Computing."
By coincidence, all three of you are specializing in condensed matter physics, but I imagine that you each had different motivations for going into that field. Could you begin by telling us a little about yourselves?
**Misawa :** Since my undergraduate days, I enjoyed thinking and computing on my own, so I thought I would go into theory. It was after I entered graduate school that I began to study condensed matter physics. I liked the fact that it's easier to compare calculations and experimental results than in the case of elemental particles and atomic nuclei. Even the research I've done up to now in the area of condensed matter physics has been close to experimentation.
**Suwa :** I think condensed matter physics is a field in which you can enjoy "things that can be known." Elementary particles are not really familiar to us, and in chemistry and biology you need to establish a lot of hypotheses and you don't really feel that you've understood things. But in condensed matter physics you can consider problems that seem close to you, working from axioms and principles with only a few hypotheses. In my undergraduate days, I had to conduct experiments in the course of researching for my graduation thesis, so when I entered graduate school I wanted to study theory. In the laboratory, we use primarily the Monte Carlo method, and since I became affiliated with the laboratory I've been hooked on how interesting that method is. The theme of the poster for

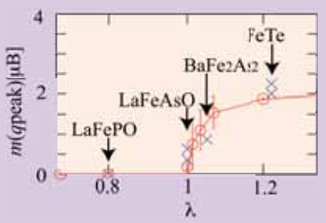
Grand Prize Poster award

## Magnetic properties of low-energy effective model for iron-based superconductors derived from first-principles downfolding method –Microscopic origin of diverse magnetic ordered moment–



**Takahiro Misawa**
Research Associate,
Department of Applied Physics,
School of Engineering,
The University of Tokyo

One of the central issues in recent solid-state physics is a strongly-correlated electron system where energy scales of interactions among electrons become comparable to those of band widths. In this system, it is known that the strong interactions among electrons induce many intriguing phenomena such as high-temperature superconducting phase.
It is one of the most important objectives of solid-state physics research to understand these intriguing phenomena from the "first-principles Hamiltonian" in solids, namely, the Hamiltonian that includes the periodic potential created by atoms and the Coulomb interaction among electrons. Because of huge degrees of freedom in the first-principles Hamiltonian, it is impossible to solve this Hamiltonian exactly even with the largest and fastest supercomputers that exist today. For this difficulty, up to now, many researchers have focused on the low-energy part of the system and derive low-energy effective model that reproduces intriguing phenomena observed in solids. Although this method has succeeded in explaining many intriguing phenomena in solids, in most cases the parameters of the effective model were determined "by hand," and its validity of these parameters is unclear and under hot debates. In recent years, we developed "first-principles downfolding method" as a bridge linking the first-principles Hamiltonian and the effective model. In this method, first, we calculate global band structures of solids based on the first-principles Hamiltonian. Then, in order to derive a low-energy effective model, we eliminate the degrees of freedom in the high-energy part, which is away from the Fermi energy, by using constrained random phase approximation. By using this method, without a priori hypothesis, we can determine the parameters of the effective model only from the structures of solids. By analyzing this effective model with high accuracy numerical calculation methods such as multivariable variational Monte Carlo method, we can clarify and predict the electronic properties of solids. In this study, we apply this method to recently discovered iron-based superconductors. We have shown that differences in interaction parameters induce the diverse magnetic properties of the iron-based superconductors (see figure). This is the first study to clarify the microscopic origins of these diverse magnetic properties from first-principles calculations.




Comparison between theoretical magnetic ordering moments m(qpeak) (red circles), and experimental values (blue Xs). The horizontal axis represents the scaling parameter $\lambda$ that uniformly scales the interaction parameters. Our theoretical results are in excellent agreement with experiment.

Outstanding Poster award

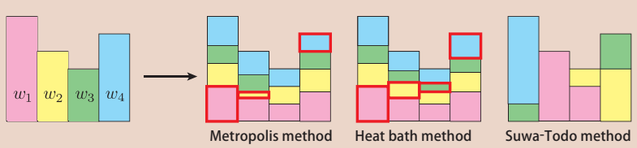
## Markov Chain Monte Carlo Method without Detailed Balance

Hidemaro Suwa
3rd year Ph.D candidate,
Department of Applied Physics,
School of Engineering,
The University of Tokyo

The emergences of phase transition and strongly correlated states, in which we are very interested, include an abundance of novel physics, and they are expected to have many applications in new material design and so on. The essence of these physical phenomena is that they are multi-particle (have multiple degrees of freedom), and it is not effective to conduct rough approximation that considers only average quantities among particles. Only through the skillful use of computers is it possible to analyze these problems that are difficult to solve using manual calculation by human beings.

However, these problems cannot be solved using a shotgun approach with computers on a large scale; the key is how cleverly and efficiently they can be used. This also applies to the Markov chain Monte Carlo method with which we are working. This method, in which multiple integrations are derived using a computer, has great general applicability, and it is becoming indispensable not only in physics but also in various other fields, such as, chemistry, biology, medicine, statistics and economics. Almost all of the Markov chain Monte Carlo methods up to now used a condition of "detailed balance," and for more than half a century the method continued to develop within the boundaries of this condition. However, the detailed balance was used because of the convenience for computation; it was not a fundamentally necessary condition. Accordingly, we broke with what had been up to now established and devised a new algorithm that can calculate correctly even without satisfying the detailed balance.

This algorithm uses a geometrical process called as "weight filling" that definitely minimizes the average rejection rate, which is the cause of reduced efficiency, making it even zero in most cases (see figure). This greatly improved calculation efficiency to anywhere from several times to more than a hundred times as much as that by conventional methods. Applying the algorithm to spin systems, which are quantum-mechanical problems, resulted in the discovery of a new phase transition for spins from a liquid state to a solid state. This method is applicable to almost all of the Markov chain Monte Carlo methods that are used in various fields, and it is expected to make wide-ranging contributions in the future.




Comparison of the "weight filling" process using the new method and existing methods. In this case, the rejection rate is reduced to zero by our method.



which I won the award was general modifications to the Monte Carlo method. I'd been thinking about that for a long time, and one day I suddenly got the idea.

**Shiba :** The other two are studying quantum systems, but I'm studying classical systems exclusively. I had a vague idea that I wanted to go into theoretical physics, but in the course of graduating from undergraduate school I was assigned to an experimental research laboratory. It was there that I encountered experiments of soft matter and linear non-equilibrium phenomena and other subjects. I thought the idea of "first just trying something" was interesting, and felt that there were aspects that were distinct from theorizing. At the laboratory I worked at in the master's program, we did full-on numerical calculation, so I began conducting simulations in which first I'd try something and then I'd try to figure out the results that were unexpected.

**Ohno :** So you all like theory and enjoy trying to understand things starting from axioms. But you also all want the output to be something that you can see. That's what you all have in common.

Do you collaborate with people conducting experiments, such as by having them use the output from calculation in their experiments?

**Misawa :** I solve the effective models for certain materials, so I hold close discussions with the people conducting experiments on the interpretation of the experimental facts and whether or not they are consistent with the theory.

**Ohno :** I myself conduct calculations in the field of materials science. In collaborations with the people conducting experiments, I often find there's a wide gap between what they expect from calculations and what is actually possible through calculation, and this gap can't be bridged. What is it like in condensed matter physics?

**Suwa :** It's the same. If there's something in the model presented by the theoreticians that can't be explained, the experimenters are actually pleased. The theoreticians try to resolve it, but the experimenters use it as a jumping-off-point.

**Ohno :** That's true. Both parties would probably be in agreement in the case of a simple system, but with a real-world system it's hard to put together a simulation that will produce experimental results.

Dr. Shiba, you work on classical molecular dynamics. Do you get the impression that using the new supercomputer will produce results that approach what is desired by the people doing experiments?

**Shiba :** With classical model simulations, it's easy to expand the scale of calculations to match the capacity of the computer being used, so it may be possible to get to the point desired by the experimenters to some degree. However, it's not possible to conduct many calculations on an unlimited basis, so it's a problem that depends on what you select. It's not that it's impossible technically, but I get the impression that we need to consider more carefully exactly what calculations should be done.

**Ohno :** Is there anything that you on the calculation side would like from the experimentation side?

**Shiba :** Up to now, the collaboration has been possible only when the experiments have been done for those things for which calculations could be carried out. Now, however, there's a strong sense that calculations are trying to keep up with experimentation, or that calculations are performed in order to further develop what's being done in experimentation. I think that these two may slowly be coming closer to one another due to the increased scale of computing. So collaboration is important.

**Misawa :** In quantum systems, optical lattices have recently become popular, and collaborations are underway between theoreticians who are working to solve the Hubbard model and people who are conducting experiments with optical lattices. It's even becoming possible to vary control parameters at one's disposal in experiments as in computational studies.

### What are the expectations for the K Computer, and what will we be able to do with it?

**Ohno :** I'd like to ask you about your involvement with supercomputers. Have you ever thought, "I'll bet I could do such-and-such if I had the K Computer?"

**Suwa :** In classical systems, if it were possible to use it for mesoscopic system simulations, it might be possible to study transport phenomena and so on more carefully.

**Shiba :** When it comes to soft matter, there's a gap between macroscopic description of hydrodynamics and the microscopic description of phenomena, and it's difficult to bridge this gap. I think efforts to bridge the gap are needed, but on the other hand I'd like to find a single method that would enable us to punch right through it.

**Suwa :** In quantum systems, there are few calculations that are well parallelized, and there is a fundamental difficulty with parallelizing the calculations that can be used with the broad-based models that I want to use. To master the K Computer, methods themselves will need to be developed.

**Misawa :** If the K Computer uses several tens of thousands of dedicated cores, it would be easy to search for many things systematically.

**Ohno :** Normally we are conducting researches within the machine power we have. So, if a new large-capacity machine is suddenly given to us, it's true that it would be a bit difficult to answer when someone asked us "OK, now what's your research topic?" To use the K Computer, we'll need to improve our knowledge of computer science apart from our direct research topics.

It's getting so that you can't produce results without some knowledge of computers, even if you know a lot about condensed matter physics. On the other hand, just because you know a lot about computers doesn't mean you can produce results in condensed matter physics. How do you think that balance should be maintained?

**Suwa :** Rather than mastering the details of parallelization technique, I'd like to work on basic computing methods.

**Shiba :** For the past several months, I've been doing nothing but parallelization, and I've used supercomputers here and there. And I've realized that it's important to actually buckle down and get hands-on experience rather than focusing only on theory.

**Ohno :** What percentage of your time do you spend developing code and algorithms and conducting parallelization processing? And what about with regard to the research for which you won the award?

**Misawa :** I use partly resources created by other people, so the amount that I create myself from scratch comes to about 20%. It was actually the computing time that took longer. Computation time is proportional to $N^3$, where N is system size, so if the system size doubles, the computation time will increase eight-fold.

**Shiba :** I began conducting parallel computing in earnest in September of last year, and I was practically a hermit for three months. So for this project it was 100%. (Laugh)

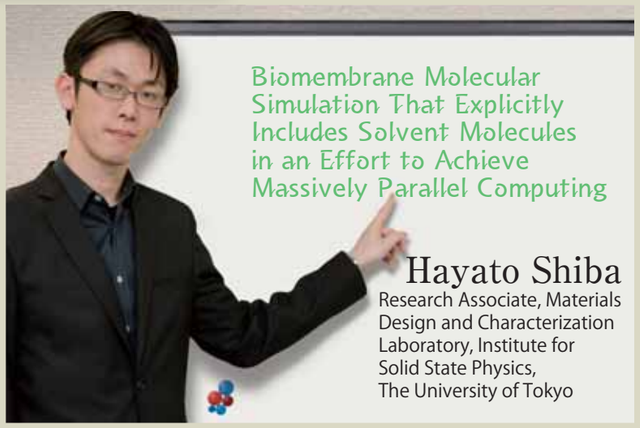
**Suwa :** My normal approach up to now has

"I'd like to come up with a variety of venues to connect young researchers with one another. Torrent is one example."

■ Moderator

Munekazu Ohno
Associate Professor,
Faculty of Engineering,
Hokkaido University

Judge's Special Prize



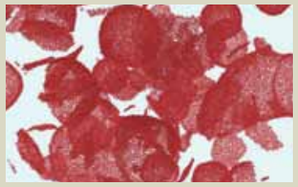
## Biomembrane Molecular Simulation That Explicitly Includes Solvent Molecules in an Effort to Achieve Massively Parallel Computing

**Hayato Shiba**
Research Associate, Materials Design and Characterization Laboratory, Institute for Solid State Physics, The University of Tokyo

An endless variety of cell membranes, red blood cells and other membrane structures formed by molecular assemblies can be found in the body. These membrane structures are molecular assemblies that have lipid molecules and surfactants that accompany hydrophilic and hydrophobic groups as their main structural components. They have many intriguing aspects, ranging from the properties of the individual molecules to their macro structural formation, uneven distribution of various components within the cell membrane and so on, and they constitute a boundary area that is being approached from not only biology but chemistry and physics as well. These materials are one example of the soft matter accompanying nonequilibrium phenomena that are controlled by large spatial and temporal scales. They are currently the subjects of wide-ranging exploration, from carefully controlled scientific experiments to practical industrial applications.

From a physics perspective, the effect on membrane structure, form transition and time-dependent dynamics of the properties that are derived from the membrane elasticity of the two-dimensional membrane, in-plane flow, crystallization and so on have been debated since the 1980s. The "coarse-grained molecular dynamics method" is a method that has been used since the 1990s as a convenient way of studying large spatio-temporal scale dynamics. As it is difficult to include all of the all-atom molecules in the simulation, this method uses a single particle to represent the degree of freedom of multiple atoms to the extent that this is able to reproduce the macroscopic structure and dynamics.

Particularly in calculations in the field of chemistry, methods of solving the movement of membrane molecules as part of the same system as solvent molecules have become quite popular in order to study the effect of environmental solvents surrounding the membrane (osmotic pressure). However, there are many matters that need to be explained from a physics perspective as well. We decided to include the solvent into a meshless membrane model with a large degree of coarse-graining as part of the same system. The meshless membrane model is a highly idealized coarse-grained molecule model based on membrane elasticity theory, in which the shape of the monolayer membrane is formed spontaneously. It enables membrane cleavage, vesicle self-assembly and fusion and so on to be reproduced. Our aim is to use this model to gain a complete picture of nonequilibrium phenomena, such as the structural transitions of the membrane in which solvents are involved.



In the midst of nearly a million solvent particles (not shown), the particles (red) that have been made coarse-grained based on a meshless membrane model form a quasi two-dimensional membrane structure. Creating a rational visualization method for solvent degree of freedom is also an important research topic.

been to take something I know nothing about and tackle it starting with an analysis of methods, in order to try to understand it all at once. So my main focus is on program and algorithm development.

### Physicists need to be flexible: crude in the micro scale but refined in the macro scale

**Ohno :** The advantage of CMSI is being able to work with people from different fields. What is your impression of the other fields? Does the philosophy that you have when you conduct calculations differ depending on the field?

**Shiba :** When researchers studying the soft matter in physical systems look at molecular dynamics, they construct bold models. But I get the impression that molecular science researchers construct rigorous models and bring them to a supercomputer.

**Ohno :** I see. So the term "first principle" is used differently in molecular science and materials science. Apparently chemical science researchers use rigorous calculations that take into account exact electron correlation, and I understand that they refer to that as "first principles."

**Suwa :** In a sense, physicists are sometimes on the casual side. (Laugh)

**Ohno :** In physics, you often don't try to be any more rigorous than is necessary. As a result, it's possible that we may be broad in the micro realm and exacting in the macro realm.

Do you have a desire for expanded interchange with other fields? In materials and condensed matter physics, we sometimes study similar materials, but the two fields also have different academic societies, so you couldn't say there's much interchange. But it's interesting once you start working together, as you get a lot of different perspectives. Wouldn't you agree?

**Suwa :** The Monte Carlo method that I'm working on is employed in a broad range of fields, and there's a great need for it. I think listening to the views of a lot of different people would give you new ideas about the method. The Monte Carlo method originated in the field of physics in the 1950s, and it spread from there. Since the 1990s, it's been used in statistics and other fields as well. But it took 40 years for that to happen. I think that having as much interchange as possible with other fields and having a shared awareness of issues would have a positive effect in enabling methods to spread more quickly. I'm personally making an effort to check out the methods used in a variety of fields.

**Ohno :** Mr. Suwa's work has a great ripple effect, so it'll be interesting if it attracts the attention of people in other fields.

**Suwa :** What's difficult about interchange between different fields is the fact that the terminology is different. I think that's the reason that interchange hasn't made much progress.

**Shiba :** In physics, the models are sometimes changed completely, but in chemistry the models of each atom are put into a library and used over and over. Molecular dynamics in physics is conducted from a stance of flexibility. I think constructing a framework for molecular dynamics that could accommodate massively parallel processing would be useful for both sides.

**Suwa :** Physicists are interested in mechanisms, while chemists are interested in the materials themselves. When modeling as well, physicists create abstractions that omit the details, while chemists use the properties of atoms and molecules as is.

**Misawa :** Don't you find that many quantum chemistry researchers are concerned with quantitative attributes? In physics, many people adopt the stance of trying to think of the minimum model that will enable you to understand the essence, so their approach is qualitative. The research for which I won the award is close to quantum chemistry, and its goal is to create an actual model based on the first principles and solve it completely. But even in that effort, I have a strong awareness that I need to identify the essence that is concealed within that model. In that sense, I guess it's a physics model. I'm greedy. (Laugh)

### Enabling interchange with different fields, information sharing and links between young researchers at CMSI

**Ohno :** What do you hope to get from the interchange provided by CMSI, regardless of whether or not you use supercomputers?

**Misawa :** I'd love to get large-scale computing expertise from other fields. Although it would be difficult to turn it into an academic paper, I'd like to be able to exchange information. At the first CMSI research seminar, I got to give a presentation to people I would not normally meet, and that was stimulating.

**Ohno :** It's been six months since CMSI was founded, and there is starting to be a demand for greater knowledge about the techniques of computer use. What do you think would prove useful in this regard?

**Suwa :** Open programs, for example.

**Ohno :** If we created a map, not for individual research topics but for a method-based one, for example one based around the Monte Carlo method as a way of showing that CMSI includes these kinds of research topics, I think that would attract people based on the method. It's interesting to exchange information with people who use different methods, so I think it would be good if there were a map that could serve as a catalyst.

**Suwa :** I'd like to see small-scale meetings where the discussion could really get down to the nitty-gritty.

**Shiba :** I agree. I wonder if it would be possible to have vendors to participate in that kind of meeting as well.

**Ohno :** That's an interesting idea.

**Shiba :** It would be great if we could share expertise for use when consulting vendors and topics for consultation. Normally things end with no one being able to see what was discussed or the results of the discussion.

**Ohno :** In the case of experiments, in some cases the techniques and so on are included in the written paper, and sometimes they're the essence that's needed to view the phenomenon. However, information like such-and-such a computer has a certain peculiarity is not made public. On the contrary, it's kept hidden.

**Suwa :** It would be great if there were a forum where everyone could freely upload that kind of information and people could consult it if they encountered a problem. I think having a Q & A section on the CMSI website would be helpful.

**Ohno :** It would be good if the circle of young researchers could be expanded as well.

**Suwa :** I'd also like to see method development get more recognition. The development of methods doesn't get much acknowledgement as compared to overseas.

**Ohno :** I get the impression that it's difficult to get funding for method development. But without methods, there would be no progress.

Lastly, I'd like you to tell us your expectations for CMSI and any candid advice you may have.

**Misawa :** It's not clear to me what shape the organization is taking.

**Shiba :** I don't have a clear overall picture of what gets decided, and in what manner.

**Ohno :** Originally, the most important mission of CMSI was to discuss and decide who should use the next-generation supercomputer and for what purpose. Subsequently, a variety of objectives were added, but I'd like the focus to be on how to select embryonic research in a way that will make everybody happy.

**Suwa :** In that case, by all means let me use the next-generation supercomputer.

**Ohno :** In April 2011, use of the K Computer will begin at last in Kobe. In the near future, we'll have to nail down what will be needed after that. Each generation of a supercomputer lasts five years, so I'd like you to not be shy about speaking up as soon as possible regarding the next generation.

**All :** Understood. We'll do that.

**Ohno :** I have high hopes for your work at CMSI.

(Recorded on February 24, 2011 at the Department of Science, The University of Tokyo)

Text : Etsuko Furukori
Photos : Shuichi Yuri

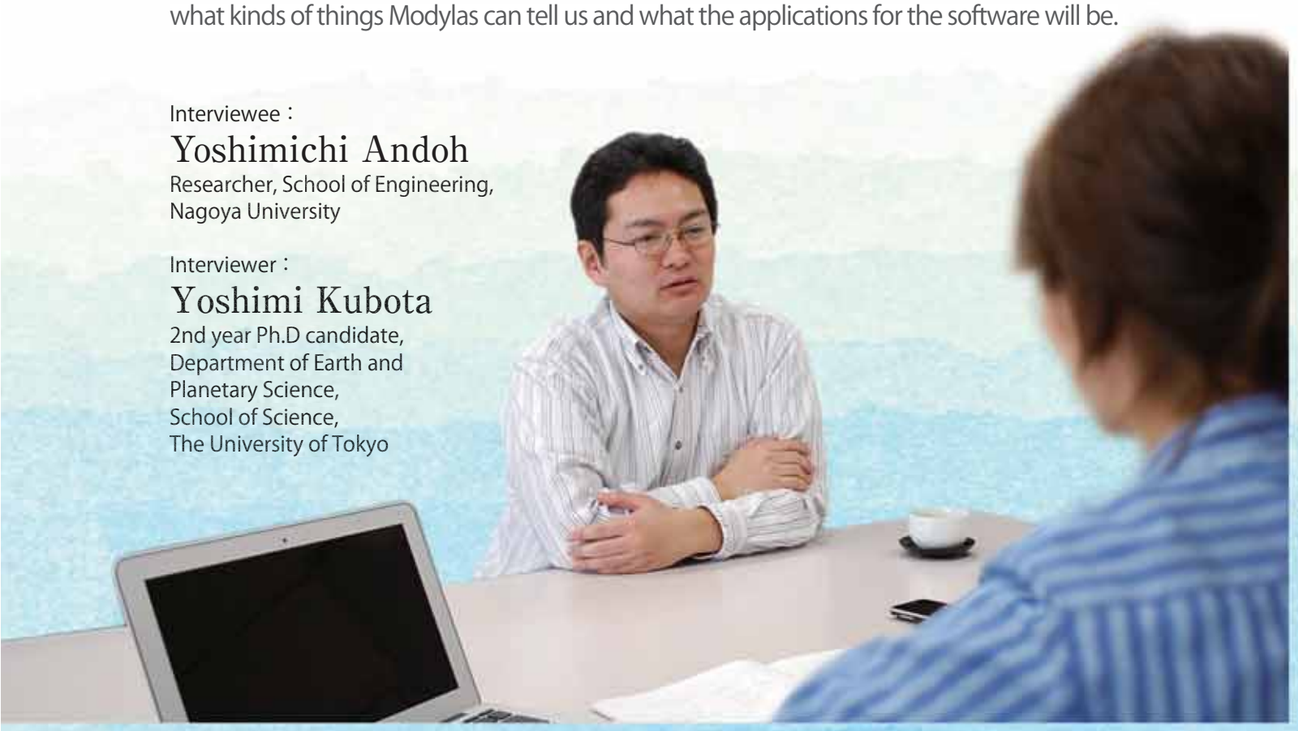
From the Front Lines of Application Development

# Modylas Developer : Yoshimichi Andoh

Modylas, a program that can calculate the trajectories of 10 million atoms simultaneously, will soon be a reality. We talked to developer Yoshimichi Andoh, a researcher at the Susumu Okazaki Laboratory at Nagoya University who is playing a central role in the development project, to ask what kinds of things Modylas can tell us and what the applications for the software will be.

Interviewee :
Yoshimichi Andoh
Researcher, School of Engineering,
Nagoya University

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



## What kind of program is Modylas?

I liked the name Modylas, so I began by asking where it came from. "Modylas" stands for MOlecular DYnamics simulation software for LArge System.

In molecular dynamics (MD) calculations, the initial coordinates of all of the atoms making up the groups of molecules (systems), as well as a variety of force-field parameters describing the interactions between atoms, are entered, and then, the Newtonian equations of motion for the all atoms are numerically solved in order to analyze the structure and changes (dynamics) of the system. Since calculating the interactions between atoms requires an enormous number of calculations, the scale of the systems that can be handled has increased with progress in computers. However, existing supercomputers can only handle systems that are several hundred thousand to several million atoms in size (Fig. 1).

Yoshimichi Andoh is a specialist in molecular dynamics. He is both well-versed in computer science and a skilled computer programmer. But even for him, it was not easy to develop software for an advanced supercomputer.

"The K Computer is a complex computer made up of more than 80,000 computing nodes. The key to bringing out the maximum capabilities of the K Computer is the construction of algorithms that reduce the number of communications, enabling the computer to calculate efficiently. Developing Modylas often required the most advanced technologies that only a specialist in computer science would understand. Up to now, for crucial sections I had pursued research jointly with a software development engineer (from Fujitsu). But in order to conduct joint research smoothly, it was necessary to have a good understanding of computers. And computer science is a field in which new technical terms are being produced all the time. So we sometimes had trouble communicating."

The biggest problem was how to efficiently incorporate the Coulomb force (electrostatic force), one of the forces that acts between atoms, into the MD calculations. The Coulomb force operates to a far enough distance that it can even be felt by human beings. As the Coulomb force is thought to control phenomena in the micro world at the atomic level as well, naturally it must be accurately included in simulations.

"On supercomputers up to now, the Particle-Mesh Ewald (PME) method has been used to calculate the Coulomb force. This is an approximation calculation method that employs the fast Fourier transformation (FFT). Although it was sufficiently precise, there was a problem in that, as the number of calculation nodes increases, the traffic of communications between nodes resulting from the FFT becomes enormous, and this decreases calculation efficiency. In the case of the K Computer, which will consist of more than 80,000 nodes, a more efficient method of calculating the Coulomb force will have to be used in place of the PME method. Accordingly, we developed a new program for calculating the Coulomb force, based on the Fast Multipole Method (FMM). With the FMM, the force from nearby particles is calculated precisely, while the contribution from more distant particles is treated as a group. This results in an algorithm that is capable of high-speed simulation while still preserving a high level of precision (Fig. 2). Nevertheless, as the program is far more complex in structure than the PME method, it has almost never been used in actual MD software. We're the first to implement it in MD software on the assumption that it will run on a supercomputer made up of several tens of thousands of nodes." The implementation of FMM is now the biggest selling point of Modylas.

## What can Modylas tell us?

So what kind of simulations will be possible using Modylas? Modylas can conduct molecular dynamics calculations for systems made up of 10 million atoms, which would take 500 years on existing supercomputers. The origins of the structural stability of biological macromolecular aggregates in the body such as viruses is a topic that is of great interest to scientists. Moreover, highly efficient MD calculation software will be useful for a wide variety of nanoscale research areas, such as predicting protein structures and elucidating the origin of the structure change in cell membranes caused by some diseases.

Dr. Andoh says that another of the pluses of this research is being able to see clear images in simulations. On the day of the interview, he showed me an actual image of a virus particle in water, and I was able to see immediately that it had a very interesting structure. The shell of the virus, made of a protein called a capsid, takes a certain form in which the same parts of the protein clump together.

"By performing calculations on the K computer, it will be possible to track the behavior of all of the approximately 10 million atoms, ranging from the atoms that make up the surrounding water molecules to the atoms that make up the virus. Up to now, we have not clearly understood in scientific terms why viruses become stable when they form this structure. I want to solve this riddle at the atomic level through simulations on the supercomputer."

## What are the applications for Modylas?

A great deal of attention has focused on applications for Modylas in the area of drug discovery. It is difficult to determine through experimentation how viruses infect cells, or the molecular mechanism of the response between viruses and immune systems. Researchers hope that all-atom MD simulations will become a new method that can be used instead.

"By quantifying the interaction between a virus and a receptor as free energy, we will be able to clarify, at the molecular level, the reason that a virus attaches itself to a specific receptor in the human body. And if we make it so a different molecule with a similar structure attaches itself to the connector on the virus before the virus attaches itself to the receptor, we'll be able to block the virus from intruding into the interior of the cell. Understanding the structure of a virus will also lead to the development of drugs that can block that virus."

"In addition, this is also expected to be able to contribute to the development of drug

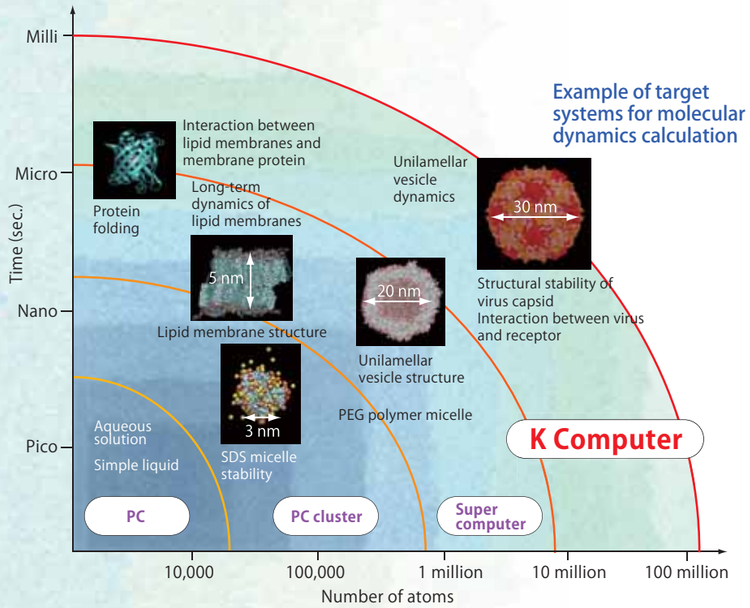



Fig. 1 Size and time scale of the systems that are the subject of molecular dynamics (MD) calculations
The scale of calculations has expanded along with progress in computers and algorithms. The first attempt at MD calculations, in 1957, was performed for a system consisting of only 100 atoms.

## Andoh Yoshimichi

When Dr. Andoh first entered college, he was interested in aerospace engineering. But in his fourth year of the undergraduate course, he became fascinated by the varied phenomena created by countless molecules, and he decided to study molecular science. He majored in open environmental science and got his Ph.D for molecular dynamics research into the gas-liquid interface in an alcohol aqueous solution. Subsequently, he conducted research at the Institute for Molecular Science within the National Institutes of Natural Sciences. Since 2008, he has focused on the development of Modylas at the University of Nagoya, under the direction of Professor Susumu Okazaki. Another of his goals is to complete the "Rokko Zenzan Trekking" event held in Kobe, home of the K Computer.

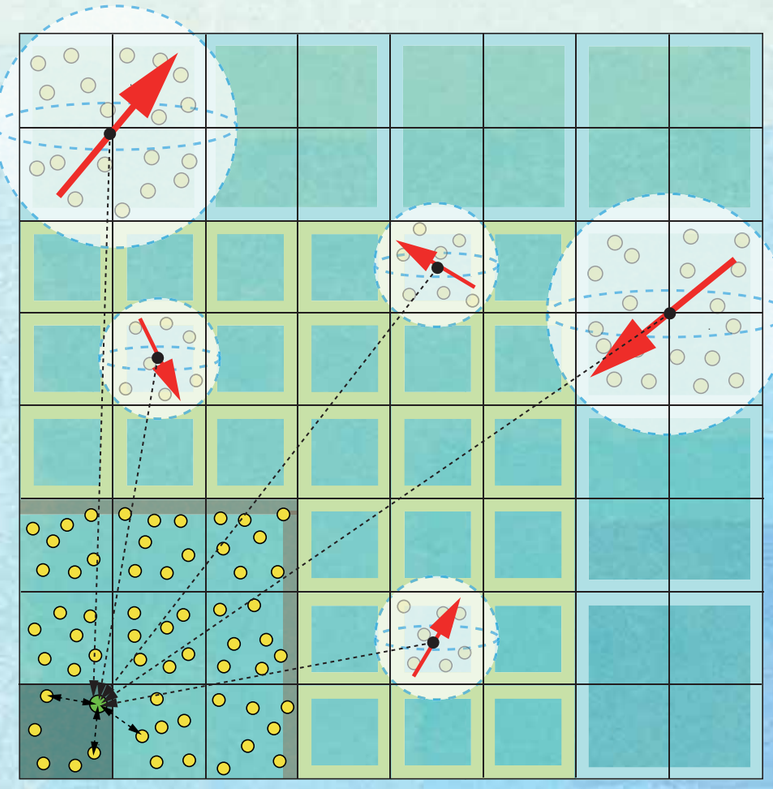


Fig. 2　Calculation of the Coulomb interaction using the FMM
Interactions with nearby particles are calculated rigorously. Contributions from more distant particles are clumped together and expressed as multipoles. For particles that are even farther away, a hierarchy is introduced, clumping together particles in an even wider area. This enables calculations to be conducted at high speed without sacrificing calculation precision.

delivery systems (DDS) that use the vesicles, which are matter transport carriers within cells. Vesicles are bag-like structures with the aqueous phase enclosed in a lipid bilayer membrane. The drug is injected into the interior of the vesicle, or into the lipid bilayer membrane, to deliver it efficiently to the affected area in the body. In this DDS development research, we still don't have a clear understanding of basic matters such as the interaction between the lipid membranes making up the vesicle and the encapsulated drug, or the interaction between the vesicle and the cell membrane that is the target of membrane fusion. So new knowledge obtained through MD simulation is needed."
Currently the calculation efficiency is poor for non-dense systems such as foam formation and the formation of stars in outer space, so these systems appear to be not really suitable for calculation by Modylas. Modylas is particularly good at calculating systems that are filled with materials and have a generally uniform density, as in the case of simulations of viruses in which the water and the target protein are entered and calculations are performed. As long as there is a good idea, Dr. Andoh hopes Modylas will be used for a variety of targets regardless of whether or not they are biomolecules.

### "I want to lead the world with unique software developed in Japan"

There are not many researchers like Dr. Andoh, who combines a basic knowledge of physics and chemistry with programming skills.
"Currently the researchers in the molecular dynamics field who do both MD code programming and research are a minority. Ideally I'd like them to become a majority."
There is also a great significance in passing on essential knowledge in Japanese software development to the next generation.
"Currently the molecular dynamics community in Japan does not have software that can be used by anyone and is capable of highly efficient calculations that put it on par with the rest of the world. In contrast, the U. S. and Europe began pursuing software development around 20 years ago through joint research projects that brought together specialists in various fields such as computer science and physics. So in terms of organizational capabilities, Japan is quite a bit behind. Naturally it's possible to import software from the United States and use that. But we would only be using the software, and my fear is that through successive generations we would gradually lose an understanding of the basic principles that form the essence of the software. This could be said about any field. But in order to prevent this kind of hollowing-out of knowledge, it's crucial that we start from scratch to create unique state-of-the-art software in Japan."
From this point on, researchers in molecular dynamics and various other fields with specialist knowledge will come together to begin the final tuning of Modylas on the K Computer. Bringing together specialists from different fields will undoubtedly result in a definite increase in the calculation speed of each of the software parts. In this process, Dr. Andoh will continue to serve as the "captain" of the Modylas project and work to optimize overall performance.
"Up to now, we've resolved the difference in terminology among different fields through close communication. In the future as well, we plan to work together to bring the project to a successful conclusion."
The goal is to create a program that reaches the top level on the world stage.

## Yoshimi Kubota

Ms. Kubota's specialty is the fields of paleoclimatology and paleoceanography, whose goal is to reconstruct past global climates. Her research topic in the Ph.D course is climate change in East Asia during the past 40,000 years. She is also interested in the relationship between the growth and decay of civilization and climate change.
As a member (and representative for FY 2011) of the group "0 to 1" (from 0 to 1) made up of volunteers at the Graduate School of Science at The University of Tokyo, she takes part in events to communicate the enjoyment of science and activities to discuss science-related problems. She is also active as a science writer.

### 【Dr. Andoh as seen from an interviewer's perspective】

At 5:00 p. m. on March 11, the day of the Great East Japan Earthquake, Dr. Andoh sent us the following email: "In this type of emergency, it would be especially difficult for Ms. Kubota to travel to Nagoya. So I think it would be a good idea if we postponed tomorrow's interview." As a result, the interview that had been scheduled for the 12th was postponed.
This solicitude reflects Dr. Andoh's character. The care he takes in his research activities needs no introduction, but the solicitude he shows toward joint researchers and the way he takes care of his juniors are also hallmarks of his character. In simulations for the K Computer, he not only takes the lead in pursuing software development but also plays a crucial role in establishing communication among specialists. Dr. Andoh himself is conscious of his role as the "captain" of the Modylas project team.

Photos : Hisashi Okumura (Institute for Molecular Science)

Application SPEC Sheet [Modylas]

| | |
|---|---|
| Code name | Modylas |
| Method / algorithm | Molecular dynamics method |
| Overview / features of code | Made up of a close-range particle calculation section and a long-range FMM calculation section. The basic cells are completely domain segmented and overall communications are eliminated to the greatest extent possible, in order to create a molecular dynamics calculation program capable of more than 10,000 parallelization processes. |
| Target materials | Biomolecular assemblies in the aqueous phase (viruses, lipid bilayer membranes and micelles) |
| Development leader | Susumu Okazaki (Nagoya University) |
| Developers / developing institutions | Yoshinori Andoh, Kazushi Fujimoto, Atushi Yamada (Nagoya University), Noriyuki Yoshii (Himeji Dokkyo University), Kazutomo Kawaguchi (Kanazawa University), Kensuke Iwahashi, Fumiyasu Mizutani (Institute for Molecular Science), Fujitsu (as of FY2010) |
| Development period | Conceptual design began in FY 2006; completion at the end of FY 2011 |
| Development language / number of lines of source code | Fortran / approximately 20,000 lines |
| Hardware environment | Can run on Tsukuba T2K (Linux), Fujitsu FX1 (Solaris), K Computer (Linux), other standard supercomputers |
| Parallelization method | Hybrid parallelization (MPI and OpenMP) |
| Parallelization status | Maximum degree of parallelization 8192 cores; process parallelization rate approximately 100% (for particle calculation section); 60% (FMM section) |
| Software release | Provision in binary format to joint researchers |
| Related / competing software | Related: REM, ermod / Competing: NAMD (U. S.) |
| Other functions | Cooperation with NANO-IGNITION and GIANT (both developed at Institute for Molecular Science) |

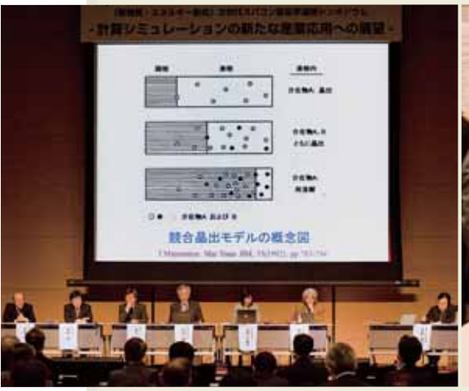
# CMSI Calendar

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

**●February 7, 2011**

CMSI Industry-Government-Academia Cooperation Symposium : "Prospects for New Industrial Applications for Computer Simulations"
Venue : Akihabara Convention Hall

The Industry-Government-Academia Cooperation Symposium, which was planned by the Industry-Government-Academia Cooperation Subcommittee and sponsored by CMSI, attracted 150 participants from the areas of industry, government and academia. The objective of the symposium was to study current industry use of computer simulations from the different perspectives of industry, government and academia, and to discuss future approaches.
The director of the Office for the Promotion of Computing Science at the Ministry of Education, Culture, Sports, Science and Technology summarized the government's guidelines as follows: "In the large-scale supercomputer project centering on the K Computer, industry, government and academia must work together to increase the nation's industrial competitiveness." To that end, the issue of large-scale software development was raised in the keynote address: "In order for Japan to lead the world in the use of supercomputers by industry, software that can make maximum use of large-scale parallelized supercomputers must be efficiently developed."
The speakers who followed proposed specific efforts such as "building a strategic framework for the development, maintenance and management of large-scale calculation software and its use in industry" and "establishment of targets through close cooperation with experimenters." The matters that were discussed in the panel discussion that began in the evening included "program organization and provision from a user's perspective" and "movement of personnel between industry, government and academia and creation of venues to promote interchange." A spirited exchange of views between speakers and attendees was also held in the question and answer session that concluded the symposium.
Note : Detailed information on presentations by two of the invited speakers is provided on Pages 13 and 14.




**●CMSI Researcher Workshops**
Date : Scheduled for July 7-8 and November 2011 and March 2012
Venue CMSI Kobe Branch
Program : Discussion of application advancement

**●TCCI Symposium**
Date : August 11-12, 2011
Venue : CMSI Kobe Branch

**●Center of Computational Materials Science Symposium**
Date : September 12-13, 2011
Venue : Institute for Solid State Physics, The University of Tokyo

**●Get-together for computational molecular science experimenters**
Date : Scheduled for November 2011
Venue : Kyoto

**●CMSI / Institute for Materials Research Joint Seminar**
Date : Scheduled for December 2011
Venue : Institute for Materials Research, Tohoku University

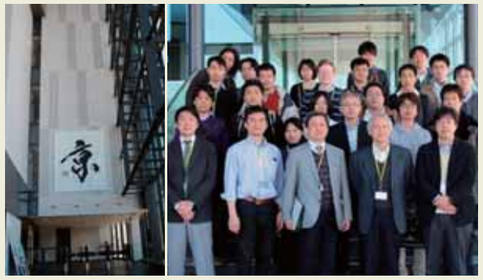
**●CMSI Industry-Government-Academia Cooperation Symposium**
Date : Scheduled for February 2012
Venue : Not yet decided

**●CMD® Workshops (Organized by CMSI and Osaka University)**
With Tutorial Course
- 19th September 5-9, 2011
  Venue : Cybermedia Center, Osaka University
- 20th March 6-10, 2012
  Venue : International Institute for Advanced Studies (Kyoto)
- Asian CMD® Workshop in Indonesia
  (supported by Institut Teknologi Bandung)
  Date : July 19-22, 2011
  Venue : Pekanbaru (planned)
- Asian CMD® Workshop in the Philippines
  (supported by De La Salle University)
  Date : Early October 2011 (to be finalized)
- Asian CMD® Workshop in Vietnam
  ((supported by Saigon University)
  Date : Mid-December 2011 (planned)
- Asian CMD® Workshop in Thailand
  Date : Mid-February 2012 (planned)

# K Computer News

## Opening of CMSI Kobe Branch

On April 4, the CMSI Kobe Branch opened at the Advanced Institute for Computational Science (AICS), home of the "K Computer," the next-generation supercomputer. The Center immediately became a gathering place for CMSI researchers aiming to become world leaders in research through the use of the K Computer. The brand-new facility and environment are now the venue for spirited debates that transcend specialist fields. A get-together was also held on April 6 at the Kobe Kachoen (bird and flower park), located next to AICS. The response clearly shows a desire to deepen exchanges with different fields, and to have such exchanges lead to the creation of innovation.
The Center is planning to hold a seminar on application advancement and other events. For details, see the CMSI webpage (http://cms-initiative.jp). We invite you to visit the CMSI Kobe Branch.








Bringing Together Industry, Government and Academia-Invited Talk
at CMSI Industry-Government-Academia Cooperation Symposium

# The Computational Science Anticipated by Researchers Working to Create New Materials and Energy

Kazuhito Hashimoto
Professor, Research Center for Advanced Science and Technology /
Graduate School of Engineering, The University of Tokyo

In basic research in Japan, particularly in the areas of theory and calculation, many talented individuals appear to think that their role is basic research alone — that they are not suited for applied research, that applied research is not as interesting as basic research and so on. But these are misconceptions. Applied research, too, requires a tremendous amount of creativity.
I myself come from a basic chemistry background. But around 1990, I realized that titanium oxide could be used for decomposition of bacteria and contamination. This is a mere application. Fortunately, however, in the course of my research I discovered a new phenomenon of science in which a surface becomes extremely hydrophilic when it is exposed to light. Subsequently I developed this as a practical technology, and its applications have continued to expand to encompass fields ranging from construction to agriculture and civil engineering.
The deployment of research into different fields is actually not that difficult. People who have highly original ideas in the area of basic research appear to be able to produce highly original ideas in applied research as well. In applied research that maintains a focus on the practical applications of the research, it is essential to create a forum for mutual exchange of information with researchers in different fields and the marketplace. In that sense, I think it is important for the three CMSI centers and the Kobe supercomputer center to invite company personnel to maintain a presence at the facility on an ongoing basis.

As experimenters, we conduct material design that uses band calculations in an effort to discover highly efficient organic solar cells and visible light photocatalytic materials. In many cases, however, the results of our calculations and the things that we are actually able to synthesize at our current level of calculation are completely different. So what we do is to continue to produce one material after another until we get lucky and produce one that works. The thing we hope for from computational science specialists is to provide basic support for our intuition. The analysis of mechanisms is also important, but what we really want is a working theory of the direction in which we should proceed in order to increase the likelihood of producing a useful material.
In the field of applied research for functional members and nanomaterials, the list of things that we hope for from academia is growing steadily longer. If we take one of the missions of research to be contributing to society through our research, it is only by pursuing applied research in cooperation with experimental scientists and companies that we will be able to preserve our "scholarly endeavors" as well. I believe that this is the kind of world that we are entering.

Photo : Shuichi Yuri

Bringing Together Industry, Government and Academia-Invited Talk
at CMSI Industry-Government-Academia Cooperation Symposium

# HPC Challenges for the Next Decade and Beyond—From Discovery to Applications at the Nano-Bio-Med Frontier

Michael L. Klein
Professor, Institute for Computational Molecular Science,
Temple University, Philadelphia PA 19122 USA

As George Whitesides said recently in Nature Magazine—scientists should try to solve problems that are important and recognizable to society. Practical problems can be more challenging than those typical academics tackle; e.g., catalysis and polymers started in industry before becoming exotic fields within theoretical physics and synthetic chemistry.

Things in biology are not so simple. For example, consider a hybrid system of a DNA and a carbon nanotube. This is interesting because a device like this can pick up characteristics of functionalized DNAs, which are more and more important in biological environments. This is the intersection between biology, physics, and nanotechnology. Each time a DNA strand binds to a carbon nanotube it will take on a different structure. In order to discover the ideal packing we need to repeat the simulation hundreds of times and it required an IBM 'Blue Gene' using 2048 processors for one month. It's not just heroic calculations we need that use hundreds of thousands of processors. We also need capacity computing to gain time to solution.

The K computer will be a significant step on the pathway to empowering computation as a tool to complement experiment. But the real breakthrough during the last 30 years was about algorithms; the Feynman path-integral representation of quantum mechanics, the Nosé thermostat to simulate the canonical ensemble, and the Car-Parrinello method, which gave us the ability to simulate silicon both as a semiconductor and as a liquid metallic system. The latter, was a really significant breakthrough. It took a decade before the method was used widely, but since then it has become routine. So, algorithms have played a key role, and in the latter case we had to wait for big machines to catch up.

In biology, interesting things are micron size. They are assemblies of nanoscale machines. And these machines in the cell wall are membrane proteins that either transport ions or particles in and out of the cell. By understanding how these machines work, we can use the design principles from nature to do things that nature didn't do. This is a frontier area of material science. But the length scales are not appropriate to density functional theory. Heroic calculations on current supercomputers would allow us to handle about ten thousand lipids. But we are still a long way short of an interesting size. That has led to the idea of using different methods for different scales; the bridging of length scales. Unfortunately, the trouble is where we want to join a quantum method to a classical atomistic method. There are as many methodologies for doing this as there are groups doing calculations, and it's an intrinsically tough problem to deal with. In summary, we need more than just the big hardware. We need algorithms. We do need heroic calculations that could only possibly be done on a K computer type machine. But we also need capacity computing. The latter is especially important to solve real world problems.

Photo : Shuichi Yuri



CMSI Computational Materials Science Initiative

Development of Human Resources

# CMD®18 Workshop : A First-Hand Report

Hiromi Shima
Department of Physics, Graduate School of Science,
Tokyo University of Science (at the time)

The 18th Computational Materials Design (CMD®) Workshop supported by CMSI was held March 8-12 at the International Institute for Advanced Studies. More than 700 persons from universities and companies have participated in a series of workshops, which center on the design of materials using an actual supercomputer. Hiromi Shima reports on her experiences when she attended the most recent workshop.

I'm engaged in materials research into ferroelectric thin films and piezoelectric substances. So I'm what is commonly referred to as an experimenter. My reason for participating in the most recent workshop was that I wanted to get a foot in the door to begin to learn how to perform simulations. It often happens in the search for materials that we need to combine two or more types of materials to achieve the physical properties we're looking for. Recently it occurred to me that my research would go much more efficiently if I could predict to a certain degree through simulations what combinations would be best. I realized that I needed to study to learn how to do this, and I sat at my desk any number of times trying to study, but for some reason I was unable to maintain the effort.

Although I had applied to attend the workshop, I'm such a beginner that I was afraid the lectures and hands-on training would be over my head. It was even my first time to use the UNIX system in the hands-on training, so the only thing I could do was to type at the keyboard furiously as instructed. But in the course of finishing the series of calculations for each of the codes, I gradually came to understand what I was doing. I think this was due to the training style, in which lecturers explained everything clearly, starting with the basics, and then tutors followed up on what the lecturers had told us. We learned three computation codes in the five-day workshop. Thinking back on it now that I've completed the workshop, I realize that the order in which they were covered was extremely well thought-out.

I couldn't say that I now have a thorough understanding of the CMD® method or I'm at the level where I could actually perform simulations for my own material systems. But with regard to calculation I think I've progressed from being a complete lay person to the beginner level. The most important result of this experience, and the one that will have an impact on the future as well, is that I got a definite response from being interested in something and working hard at it.

Photo : Masaaki Geshi (Osaka University)

## Tutorial Courses

Attendees can select the course they want to attend.

**Computational Nanomaterials Design Beginner's Course**
- Lectures on the latest CMD® case studies and special lectures
- Lectures on fundamentals of ab-initio calculations
- Introductory hands-on training in ab-initio calculations (covering 3 simulation codes)

**Computational Nanomaterials Design Advanced Course**
- Lectures on the latest CMD® case studies and special lectures
- CMD® Intensive hands-on training (concentrating on 2 simulation codes chosen by the participant from among the 5 codes offered)

**Computational Nanomaterials Design Expert Course**
- Lectures on the latest CMD® case studies and special lectures
- CMD® practicum

**Computational Nanomaterials Design Supercomputer Course**
- Lectures on the latest CMD® case studies and special lectures
- CMD® practicum (RSPACE)

Capacity: 25 trainees
Participation fee for trainees: No charge (but trainees are responsible for their own travel costs and meals)