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TORRENT

10^{16} Weave New Materials

Roundtable Discussion

Computational Materials Science Led by CMSI : Achievements in Advancing the Field and Next Steps

Interview with

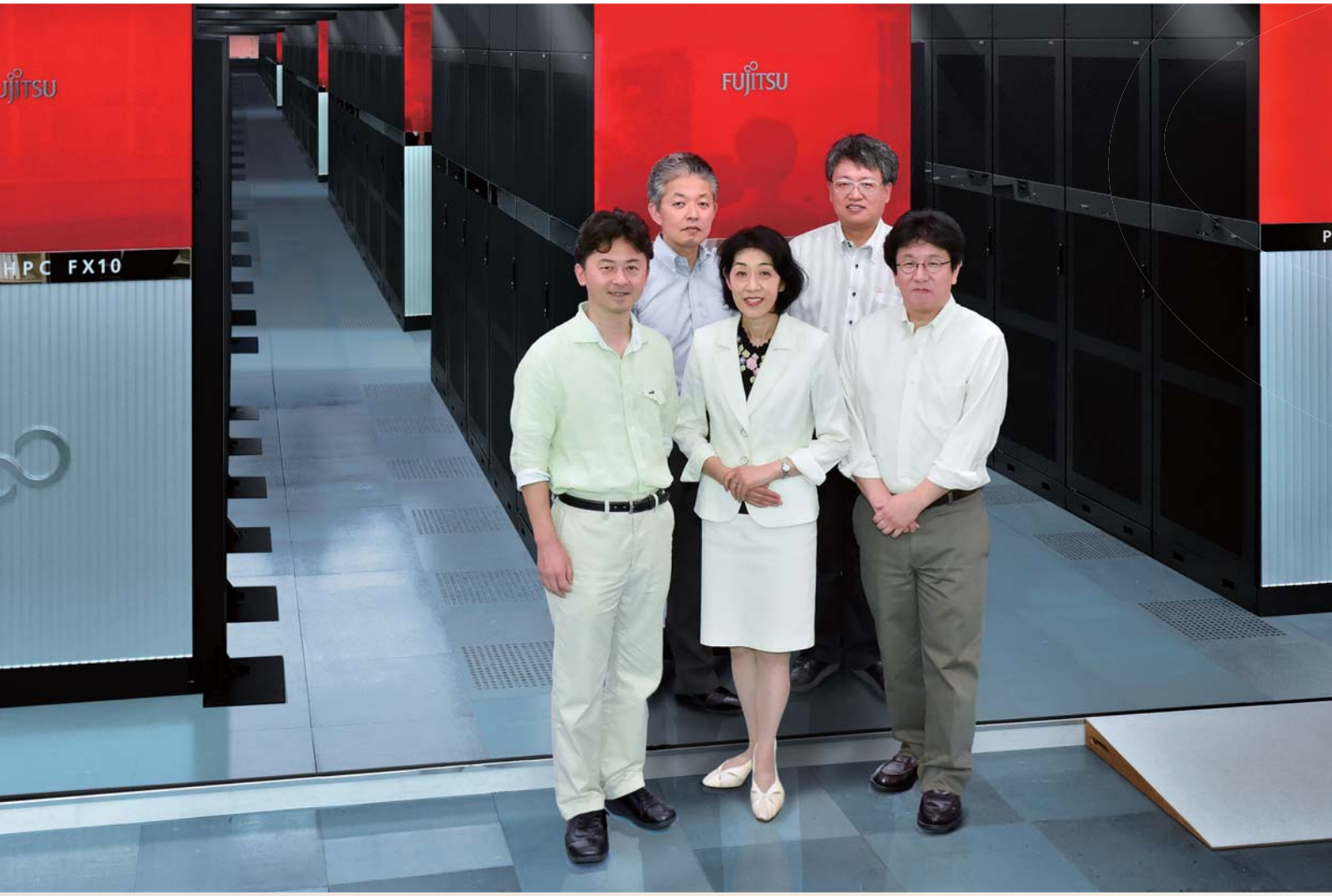
Tomohiro Takaki, Developer of Phase-Field Method

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

Roundtable Discussion

Computational Materials Science Led by CMSI:

Achievements in Advancing the Field and Next Steps



Participants
Chioko Kaneta
Expert, Fujitsu Laboratories Ltd.

Toshihiro Kawakatsu
Professor, Graduate School of Science, Tohoku University

Kengo Nakajima
Professor, Information Technology Center, The University of Tokyo

Nobuyuki Matubayasi
Professor, Graduate School of Engineering Science, Osaka University

Moderator
Synge Todo
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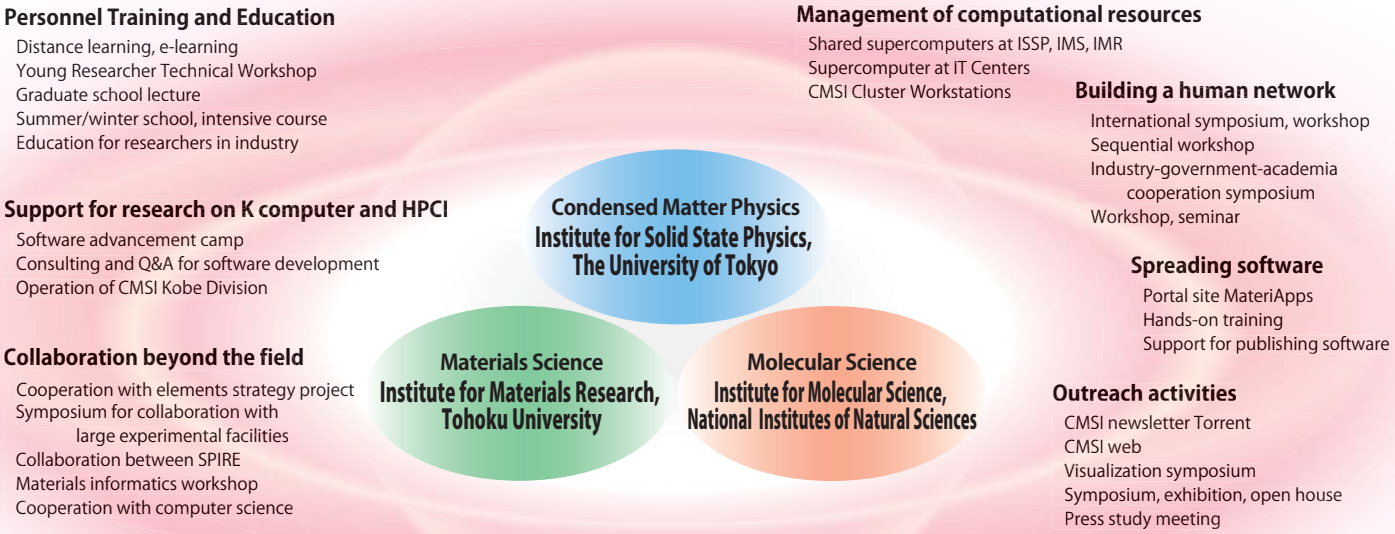
The computational materials science straddles the fields of condensed matter physics, molecular science, and materials science. CMSI has promoted various activities (Fig. in the next page) to advance the new horizons of computational materials science in the past three and a half years. We spoke to some of the people who have worked to advance the field from various positions, asking them to reflect on their activities and achievements up to now and to tell us about the next steps for the coming "Post-K" era.



Activities of CMSI for advancing the field of computational materials science: CMSI, centered on three operating institutions, the Institute for Solid State Physics (The University of Tokyo), the Institute for Molecular Science (National Institutes of Natural Sciences), and the Institute for Materials Research (Tohoku University), is promoting various activities together with 11 cooperative institutes, and also with researchers in universities, institutes and private companies.

"Shared awareness of issues" — the watchword for industry-government-academic collaboration

Todo(moderator): First, I'd like you to introduce yourselves and briefly describe what type of activities you've been involved in at CMSI.

Kaneta: My name is Chioko Kaneta, and I'm a researcher at Fujitsu Laboratories Ltd. I'm on the Industry-government-academia Cooperation Committee. We locate points of contact for industry, government and academia and hold workshops to promote collaboration. These are held several times a year, and I've been in charge of planning several of them.

Nakajima: My name is Kengo Nakajima. I am a faculty member of the Information Technology Center, the University of Tokyo (ITC/U.Tokyo). I'm in charge of operating the supercomputer system at the Center. I'm also a member of CMSI Supercomputer Cooperation Committee, and many of CMSI researchers are using our supercomputer system (FUJITSU PRIMEHPC FX10). Moreover, I have given some lectures in seminars and summer school for young researchers organized by CMSI. My specialty is parallel numerical algorithms. We are also providing tutorials for parallel programming with hands-on sessions at ITC/U.Tokyo.

Kawakatsu: My name is Toshihiro Kawakatsu, and I'm a professor at Tohoku University. I belong to the Personnel Training and Education Committee. There is a center of education in the Faculty of Science at Tohoku University, and as the head of that center, I administer teaching programs in cooperation with the Computational Materials Research Initiative (CMRI) located within the Institute for Materials Research. During the last fiscal year and this fiscal year, we held a series of seminars on Multi-scale Materials Science. Each year we hold a workshop designed for company and university researchers on OCTA, a polymer materials design simulation software program. We invite the members of the OCTA development team to give lectures and hold practicums. The participants are either half-half from universities and companies, or two-to-one from companies.

Matubayasi: My name is Nobuyuki Matubayasi, and I'm a professor at Osaka University. My specialty is molecular science, and I'm studying the use of computational statistical mechanics for molecular aggregate systems. I'm focusing on the common functions in the various types of molecular aggregates. My goal is to develop a universal software program to analyze these functions and help to popularize the program as something that could help a lot of people.

Todo: Thank you. I'm the Chair of the Publicity Committee, and I'm involved in putting together Torrent and the CMSI website. Recently, I've been working to spread CMSI application software through developing MateriApps, a portal site for materials science simulation software. I'm also working on collaborations and exchanges with AICS (RIKEN Advanced Institute for Computational Science).

I'd like to begin with the topic of collaboration on the part of industry, government and academia. What do you think has changed as a result of CMSI activities? Also, in what ways do you think we've been successful, and in what ways do you think we're just going around in circles?

Kaneta: At the workshops I mentioned, sometimes the university people weren't interested in the presentations by people in industry. People in the sciences start with an interest in "why." People in industry first want to know "how." The points that they're interested in are different, so I really felt that there was a huge gap.

It's difficult to form a straight connec-

Chioko Kaneta

Industry-government-academia Cooperation Committee

"People in the sciences start with an interest in 'why.' People in industry first want to know 'how.' The question is how to connect these two."

tion between people in the sciences and people in industry, so first we should work to form a connection to engineering. Also, I think one of the final forms of the ideal collaboration between industry and academia might be training personnel and sending them to industry.

Todo: But even at CMSI, don't people in the materials field have very close relationships with the people in companies?

Kaneta: It's true that there are a lot of university laboratories that do contract research from private companies. But when you consider dissemination and penetration in the industries of the future, university laboratories can't cover it all, and besides it would be difficult for them to synchronize their efforts with industry trends. With only that, collaboration will wither away. So we should encourage undergraduate and graduate students who major in computational science to join companies and pile up achievements there, and that would stimulate the private companies. Then the benefits could flow back to the university. I think that unless we create a large movement like that, there will be no growth of the field as a whole.

Todo: Prof. Kawakatsu, you're involved in the development of OCTA. It was developed through collaboration between industry and academia, wasn't it?

Kawakatsu: Yes, OCTA was a project when I was at Nagoya University. People from more than 20 private companies gathered at a research institute at Nagoya University and developed the software. Only a few university people were involved. The software that was created was released publicly, free of charge, and it's now used by many people at both companies and universities, not only in Japan but in other countries as well.

Todo: What was the key to the success of OCTA?

Kawakatsu: I think it's the fact that they made all of the software free, and the fact that even now, after more than 10 years, the original members of the development team volunteer their time to improve the program. Its commercial version has been released as well by JSOL Corporation.

Kaneta: Yes, in the case of the most successful software that's been developed in other countries, it takes two or three decades before people come to use it, and people continue to improve it during that time, and there are user groups as well. Up to now, there haven't been any examples like that in Japan.

Todo: In that sense, OCTA is quite different from the other software that has been developed by academia.

Kawakatsu: A lot of companies use OCTA. But not many students use it. That's because students in the science departments prefer to create their own software.

Todo: Even if you've written the code, it's a lot of work to release something publicly and get everyone to use it.

Kawakatsu: You also have to write a manual.

Todo: At CMSI, we develop and improve a lot of software programs, and we want to make sure the best ones survive. What should CMSI do to accomplish this? Prof. Matubayasi, you're currently developing an application, and you're actually working with a company to try to expand its use. How does it feel to do that?

Matubayasi: I think they're happy with what we've done. We were talking about science a moment ago, and the good thing about science is that, even if there are various problems at each company, they are often seen as different faces of common problems. Science is there to provide approaches to those common problems. Even among companies in a different field of industry, it often happens that we're able to "translate" things into the same problems. If we do that, the program will come together as a single piece of software.

Todo: In terms of sending people to industry, I think computer companies conduct a lot of exchanges of that type, but what kind of efforts and arrangements are being made by universities? Prof. Nakajima, how do you view the fields of physics and chemistry, where supposedly there hasn't been much progress in personnel exchanges?

Nakajima: Generally speaking, research in computer science, especially in HPC (high-performance computing), should be practical. Therefore, it is rather easier for researchers in academia and in industry to share same type of awareness for future direction. This is the reason why information exchange and collaboration between academia and industry go well in the field of HPC. Moreover, many faculty members of Japanese universities in this area have experiences in industry. Recently, various types of choices for career-path's after graduation can be considered.
Many students of our university want to join Google. Topics and methods for research in HPC are not so different between academia and industry. Thus, information exchange and collaboration between academia an industry are conducted very smoothly.

Toshihiro Kawakatsu

Member of CMSI Personnel Training and Education Committee

"If remote lectures are distributed on demand, people can watch them anytime, so many people including company employees will be able to see them."

Training people who can create software, use software and tweak software

Todo: A shared awareness of issues on the part of industry and academia is something that needs to be cultivated in people starting from their graduate school days. At CMSI, we've tried to do this in the form of a series of workshops.

Kaneta: Universities do not exist solely for the benefit of industry. It is expected that academia basically aim for research that is at a high level. You don't need to answer all things what industry wants. I think it's only natural that each entity has its own approach.

Kawakatsu: If that's the case, then the Personnel Training and Education Committee only needs to cultivate students.

Kaneta: That's not what I mean. I just don't think that it would be good for everything to be facing in the same direction. For example, you don't gain the ability to create something simply because you understand the properties of a material. You have to go through an engineering process in which various materials are combined with one another to get products finally. And you also need competent people at the point between the basic and applied stages. So the question is how to train such people.

Matubayasi: It will be difficult unless those people in the middle are highly competent and hold a very high position. They have to be able to look at the basic research and conclude "We can use this, so let's put it over here" or "This is where we really need application personnel. There's something missing here, so we have to do something." And they need to be in a position to say "Do this." So it's not personnel training so much as cultivating true elites, right?

Kaneta: I think there are a lot of things that can be done at the engineer level as well, though that's not easy. Unless those things are done, I don't think there will be a true connection.

Nakajima: What kind of activity is expected to be done by academia for that ? Activities to promote the use of software on the part of the general public? Or building in things to make the software easy to use?

Kaneta: It depends on what value you see in those things. From a university professor's perspective, it's possible that activities to spread software would become just another chore to be done.

Todo: There's one more aspect. The population of people majoring in computational science has increased. Not all of them are capable of doing research, but we need to cultivate more and more people who go to industry and people who become those people in the middle. Various levels will be created — for example, some people will develop applications, and people who have the expertise to do something using those applications will go to industry and do some kind of work in company research & development and so on. At CMSI, the Division Researcher system has been established, and researchers work on various research projects to develop programs that are common to all fields. And they also work on activities to increase application use. The goal will be to cultivate people who can be in that middle position.

Kengo Nakajima
Member of CMSI Supercomputer Cooperation Committee

"Research and development in hardware and software of the next-generation supercomputer system have been conducted under intensive collaboration between academia and industry from the beginning."

Nakajima: How about the career-path's of these people ?

Matubayasi: If we create organizations that are like semipublic corporations and get private companies to contribute to them as well, and if we can get people to recognize that there is real value in joining those entities, I think that will become a good career path.

Kaneta: But even if companies are looking for people in the simulation field to work on materials development, they're not looking for application developers; they're looking for experienced users. It would be a plus if they could write short amounts of code to analyze the simulation results and so on, but there are almost no companies that write applications on their own. If there's a good application, they bring it in. What they need is talented people who can use various applications and hardware to solve problems in materials development and device development.

Do you think universities are successfully training experienced users?

Kawakatsu: Maybe not.

Nakajima: I've also studied how to train computer science personnel at the university. We divide the people to be trained into three categories: 1st category is the people who can use computers and application programs, 2nd is the people who can develop applications, and the 3rd category is a kind of ultimate personnel who can cover both of science and numerical algorithms. I think different course materials should be provided for each category of people. The 1st category will become the group of users of application programs.

Kawakatsu: Is it all right if application users don't understand the theory behind the application?

Nakajima: No, they need to do that. We're formulating a teaching program to ensure that the people who can use programs also study the minimum necessary theory and algorithms while they're at the university.

Kaneta: However, the programs right now are getting enormous. So rather than not allowing them to use the program until they've read every inch of it, it's good enough if they're able to study the things that they become curious about in the course of using the program.

Matubayasi: "This program produces these great results, so it must be backed by tremendous theory, so I'm going to study it." I think that's the sequence that will ultimately be most efficient.

Todo: So what do you think should be taught to train people who can use programs?

Nakajima: Basically, it doesn't matter whether it's commercial code or a program that the professor teaching the class has made by himself or herself, the students should be taught to use it and be able to compute the various results accurately. It's also important to cultivate the sense that will enable them to evaluate the results — in other words, an engineering sense.

Moreover, they should also study the minimum necessary things related to computer science, so that while they're at the university they acquire enough knowledge to have a discussion with the people who develop applications. I think that will enable them to be quite successful as users.

Computer education in anticipation of the Post-K Supercomputer

Todo: I'd like to turn now to the issue of the Post-K Supercomputer, the successor to the K computer. We need to educate people about a computer that will have 10 million cores. But the programs and applications that can be used on such a platform have not yet been developed. At CMSI, we're distributing a series of remote lectures by computer specialists like Prof. Nakajima and application developers. These have been very successful, and a lot of students have taken the course. But I'm worried about whether we can do this on a higher level in the future, up to the exascale level.

Matubayasi: Some of my students participated in those remote lectures, but many felt that it was quite difficult. I think it's unlikely to achieve its objectives with only one lecture a week. I think it will be difficult to make it effective unless you make participants gather and stay somewhere for a while and teach them intensively.

Todo: Through practicums?

Matubayasi: Through training.

Kawakatsu: I wonder if that will get students to attend.

Matubayasi: This may sound extreme, but you have to make them go to class whether they understand or not. They don't know which industry they'll be working in. So you need to get them to learn even just all of the essential terms and have them take home all of the references. The thinking should be that they may not understand the content now, but eventually the day will come when they'll look at those references.

Kaneta: It's true that it's important for them to remember when they hit a wall that "oh, that's right, I remember getting a reference for that."

Matubayasi: Another point is that when the Post-K Supercomputer becomes a reality, I think training people who can be involved in the programming for that computer will be a separate issue. They'll have to actually fine-tune the thing, so it won't be a matter of lecture learning.

Todo: AICS holds an HPC Summer School every year. Is that for graduate students?

Nakajima: We have a lot of graduate students, but there are some post-doctoral researchers as well. The content is very basic. First we aim at a level that enables them to be able to understand and to program to some degree using the Message Passing Interface (MPI) protocol. The summer school is held for five days, but we don't just try to teach everything about parallel programming in a haphazard manner. We establish a target application and teach the techniques needed to parallelize that application. In our experience up to now, that's more effective as a short-term teaching program. Currently we're covering issues relating to three-dimensional steady-state heat transfer using the finite element method. However, some people don't know anything about the finite element method, so the first day's lectures cover the finite element method itself and its programming. Next we cover the MPI needed for the parallel finite element method. Then we talk about actual parallelization. Finally, we also cover OpenMP and give the students an entry-level knowledge of hybrid parallel programming. That concludes the five-day course.

We cover a lot of content, but this year we were able to secure about two hours of practice time each day. I think if the students spend that amount of time, they'll understand not only in theory but to some degree they'll have had the experience of programming for themselves, and that will stay with them. We haven't received any feedback yet, so I don't know how it was received by the students in the program. But they all worked very hard, all the way through to the end, so I think this year's approach was comparatively successful. If you spend a solid week intensively doing something, you retain a lot.

Todo: I feel that that type of education is pretty general, so rather than CMSI doing it, having it done by AICS or by the Information Technology Center and then having other institutions offer other types of education might be better. Prof. Nakajima, from your perspective, how much content and how much time should the ideal computer education have in order to create the ideal program for training computer scientists?

Nakajima: The most important thing is to train intermediate people, which are the 3rd category of people mentioned a moment ago, and make them people who can become a bridge between various fields. But in some ways it's difficult to do that in education. A lot of different programs are being tried. For example, some universities are having students major in physics and also assigning another academic advisor from the computer science field. One possibility is a dual degree program of Ph.D in science and M.S in computer science with 3-4 years. To begin with, we can put in place those kind of programs on the university side.

When it comes to intermediate personnel who can be useful in the real world, it would be difficult unless they first get some degree of practical work experience. In that sense, collaboration between industry and academia will be important.

Todo: By practical work experience, do you mean actually doing development and research at a company?

Nakajima: Yes, that kind of thing. I think training people who can meet a variety of needs isn't something that can be done at the university alone.

Kaneta: If you go into a company environment, you learn how applications are being used, and you see that there's a different attitude toward the awareness of issues. When a problem arises, the most important thing is time. You have a limited amount of time and limited resources, and you have to think how you can use those skillfully to resolve the problem — if not 100%, then 80%. For that reason, you have to make a lot of judgment calls. Not just that "this program is good, so I'll use it" but that there may be other options, or that a certain application is not as precise, but it's fast, so it might be better to use that one, and so on.

In that sense, we should train students not to learn just one application but so they're able to use at least two or three to some degree, and to train them so they're able to consider which one to use when a problem arises. That's what will really help them in an actual workplace setting.

Nobuyuki Matubayasi

Member of CMSI Strategic Subject (Research Group 3) Committee

"I think that increased use of applications at companies will show the connection between computational science and society, and that will be helpful in training personnel who can contribute to both science and engineering."

Change of consciousness needed for CMSI and academia

Todo: A moment ago we talked about how people who are doing simulations in the sciences can't get hired by companies. Is there anything that CMSI can do to provide support?

Kaneta: Actually, people with a science background have a good grasp of the fundamentals, so they should do well wherever they go. But a lot of people don't understand that.

Nakajima: So isn't creating opportunities where they can learn that the most important thing?

Kawakatsu: People who come out of sciences should try to do their best at their company.

Nakajima: That's true as well.

Kaneta: More directly, I think it would also be possible to produce results in simulations of hot topics in the materials field and present them with a big splash, not at academic society meetings that corporate people will never attend, but at places where people from corporations will go, in order to promote those individuals in a strategic manner.

Matubayasi: So we should not only hold presentations that show "these are the things we're doing at CMSI, so you should come" but also go to places where corporate people gather and hold lecture meetings and presentations.

Kawakatsu: It's true that physics students usually try to go to physics association meetings, but they're afraid of academic society meetings and workshops where there are a lot of corporate types, so they tend not to go to those.

Todo: So professors need to be educated as well. The dream of industry-academia collaboration will wither away unless we change the consciousness and make a steady effort. And we also need to teach students how to tie a necktie and the proper way to present a name card.

Kaneta: Unless we expand the base, ultimately we won't be able to secure research budgets, either. So if we're thinking about the future, it's something we should definitely do.

Todo: In terms of strategic programs, up to now we've pursued twin tracks simultaneously: the study of research issues and advancement of the field. But the study of issues in preparation for the Post-K Supercomputer is scheduled to begin in the latter half of this year. On the other hand, it's not yet clear in what form projects for activities to advance the field will continue.

Nakajima: More large-scale computers and research into algorithms will both be important issues for the achievement of the Post-K Supercomputer. Cooperation between individual fields extending across industry, government and academia will be essential. I hope that is promoted at CMSI as well.

Kaneta: A lot of application programs have been developed, but I'm really worried what will become of them once the project ends. As a mechanism for preserving the good ones, I think if we build a platform that would allow programs with different hierarchies to be linked and used in combination with one another, it would make it easier for them to be used in industry as well.

Todo: The big question is who's going to do that.

Kawakatsu: It would only be necessary to build a common platform and format and make it possible for people to link to them and use them.

Todo: There's also the question of what to do with simulation results. Because the output is incompatible with various platforms.

Kawakatsu: The common format will help with that as well.

Kaneta: The national budget is such that, even if you can get money to build a new application, there's not enough to nurture it from that point on. You need to make your request very loudly.

Matubayasi: It might be more effective if industry makes the request instead of a university professor, saying things like "This is an industry need" or "Industry will suffer if we don't cultivate this."

Nakajima: The JST (Japan Agency for Science and Technology) has an industrial applications framework that can apparently be used for ongoing support of things that have been researched and developed.

Matubayasi: I think that should be the role of university-affiliated research institutions.

Todo: At CMSI, there's currently a perception that the Institute for Solid State Physics and Institute for Molecular Science are for joint use within academia only, and it's difficult for corporate people to get in. A change of consciousness is needed.

Matubayasi: I agree. We have the space, so we should also have people from various companies come in to enable daily exchanges. If we put the university research centers on the first, third and fifth floors and used the second and fourth floors as space that we could lease to various companies, it would be ideal.

Todo: I think the role of affiliated research institutions is going to change greatly in some ways in the next five-year plan. I think they should not handle only administration and leasing of machines; they should play a role in providing various kinds of support. A change of consciousness will be needed to achieve that. You could say that, in preparation for the Post-K Exascale Supercomputer, a change of consciousness is needed not only at CMSI but throughout academia in Japan.

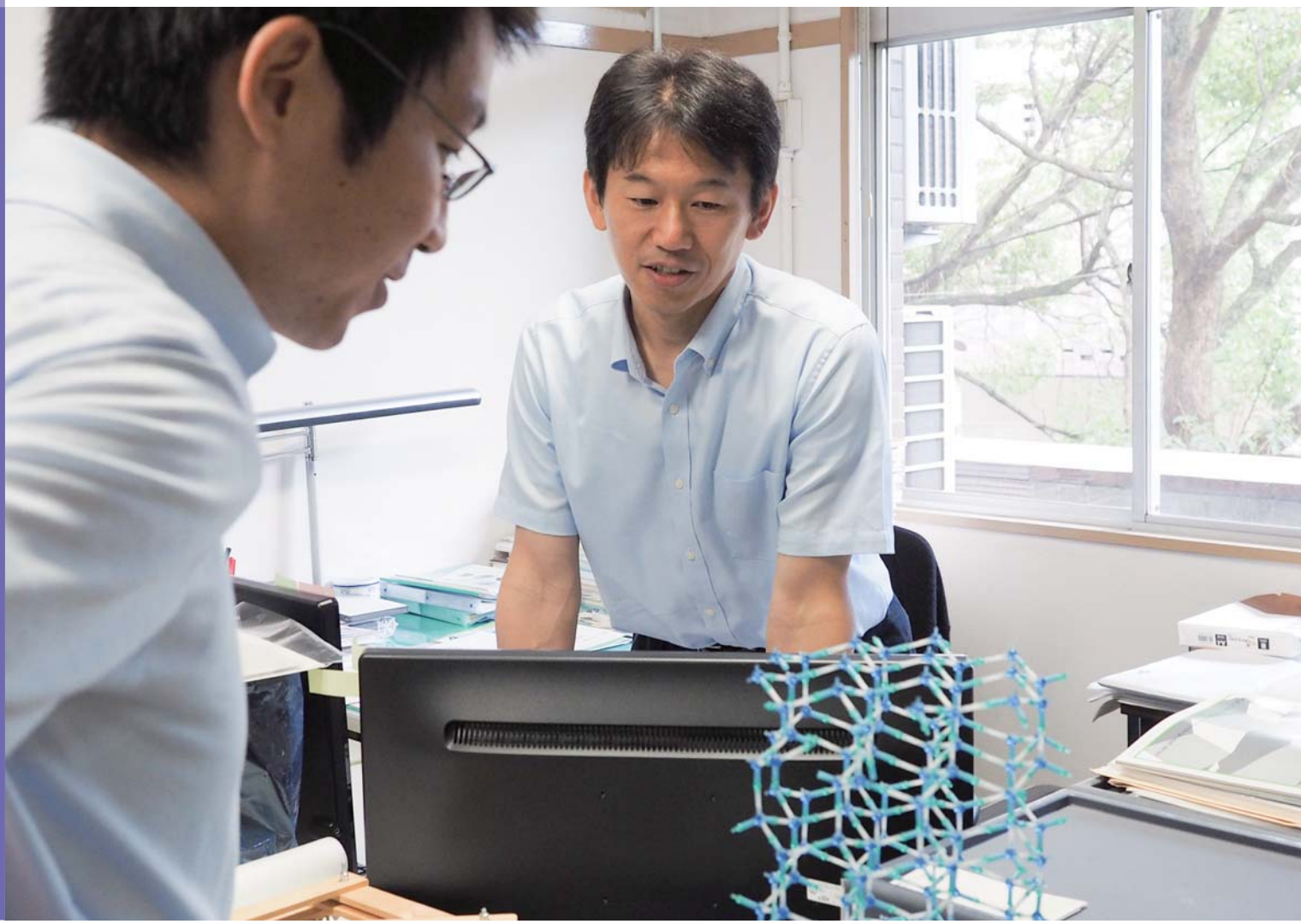
Synge Todo

Chair of CMSI Publicity Committee

"The population of students majoring in computational science is increasing, so there is a need to train people at various levels, including those bound for industry and those at the interface between industry and academia."

(Recorded September 5,2014 at Hongo Campus, The University of Tokyo)
Photography cooperation: Information Technology Center, The University of Tokyo
Text : Sakiko Fukushima
Photos : Shuich Yuri

Interview with Tomohiro Takaki, Developer of Phase-Field Method



Interviewee:
Tomohiro Takaki
Associate Professor,
Graduate School of Science and Technology,
Kyoto Institute of Technology

Interviewer:
Shingo Yonezawa
Assistant Professor,
Graduate School of Science,
Kyoto University

Blurring the boundaries can sometimes produce better results. For example, if you go to Kyoto's famous Gion Festival, you can see European and Middle Eastern objects among the decorations on the festival floats. You realize that not adhering strictly to the boundaries between Japanese and Western elements has helped to perfect Kyoto's dazzling traditional culture. Even in the world of computational science that is strictly ruled by ones and zeros, there are methods in which computations are performed successfully by blurring the boundaries. In this issue, we focus on one such method, the Phase-Field (PF) method, and its developer Tomohiro Takaki, Associate Professor at Kyoto Institute of Technology.

A Computational Technique that Blurs Boundaries

Our world is a world of many interfaces. When you put ice into a glass of water, the boundary between ice and water becomes an interface. If you magnify the interior of the metal around you, you can detect the presence of crystal grain boundaries and composition boundaries, and these interfaces hold the key to the nature of that material. Moreover, interfaces can change position and grow. In the former case, the interface will move if the ice melts or the water freezes. In the latter case, the interfaces in the metal material will be transformed by temperature and external pressure. Such interface behavior is extremely important to both science and engineering.

So how can interfacial changes be correctly simulated? A simple answer is to calculate the moment-by-moment changes in the location of the interface (Fig. 1(a)). However, the shape of interfaces frequently becomes complex. For example, it is well known that snow crystals have an extraordinarily complex structure. This is surely because the interface between ice and water vapor in clouds developed in a complex fashion. The more complex an interface is, the more difficult it is to perform calculations when the method of tracking the interface is employed. Particularly in the case of extremely detailed shapes, it becomes impossible to correctly calculate the energy originating from the curvature of the interface, and this can deal a fatal blow to the effort to accurately simulate the interface.

With such a conventional approach, the same mathematical formula can not be used to express both sides of the interface, so the range in which the mathematical formula can be used (= the interface) has to always be defined. To put it another way, various mathematical formulas and variables changes at the interface in a discontinuous manner, and this is a problem. If this is the case, we can approach the problem from a different perspective and try blurring the interface a bit (Fig. 1 (b)). When we do that, the discontinuities are resolved and the mathematical formulas are connected to one another smoothly throughout the entire region that includes the interface. However, it in turn becomes impossible to properly determine the interface with this approach, so an additional variable ϕ is introduced. This variable is defined for the entire region and changes precipitously but smoothly in the neighborhood of the interface. For example, ϕ is determined so that $\phi = 1$ in ice and $\phi = 0$ in water, and at the interface ϕ changes smoothly from 1 to 0. Moreover, the "real" interface is set at the position where ϕ is equal to 0.5. As this variable ϕ is like a "field" that defines the phase on both sides of the interface, it is known as the Phase-Field (PF). Subsequently, by simultaneously computing equations that express the relationship between ϕ and various other quantities and equations that denote the time changes for these quantities, it is possible to calculate the changes in the interface. Moreover, the curvature energy in the interface is incorporated naturally into this model. In other words, one can accurately simulate interfaces with complex shapes, which are difficult to calculate with the conventional method. The method that introduces this PF to handle systems that include interfaces is known as the Phase-Field method (PF method).

It was Ryo Kobayashi of Hiroshima University who demonstrated the utility of the PF method. Kobayashi is a very famous applied mathematician who, among other achievements, has received the Ig Nobel Prize twice for research into path determination by slime mold. He used the PF method to simulate the growth of dendrites in metal, successfully recreating their distinctive fractal-like structure. There is an anecdotal account that the research paper for this study was not released for a long time after the first demonstration, and Kobayashi finally published a paper on it several years later at the request of overseas researchers. Even so, it has become an extremely influential paper that has been cited more than 600 times.

Takaki's Encounter with the Phase-Field Method

Even before he encountered the PF method, Takaki had been pursuing research into experiments and simulations involving machine components. His primary simulation technique was the finite element method, in which the object is

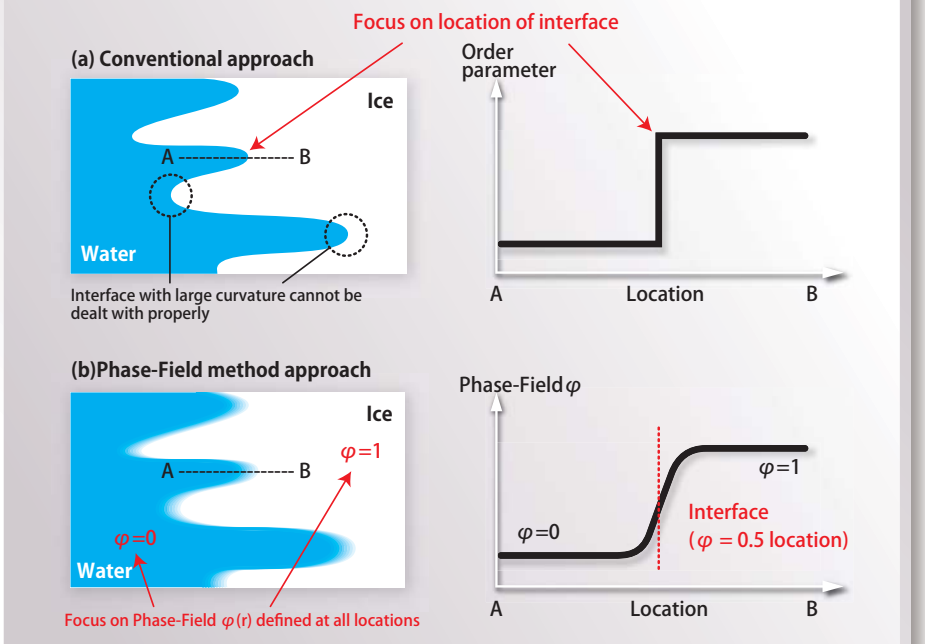
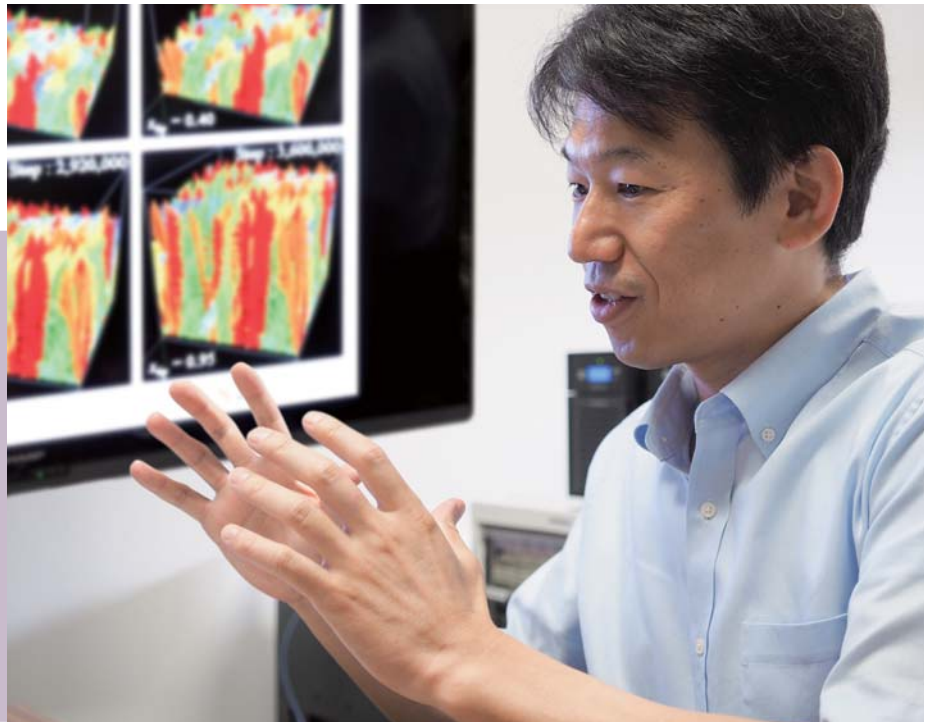


Fig. 1 Difference between (a) conventional approach and (b) Phase-Field method approach for a system that includes interfaces



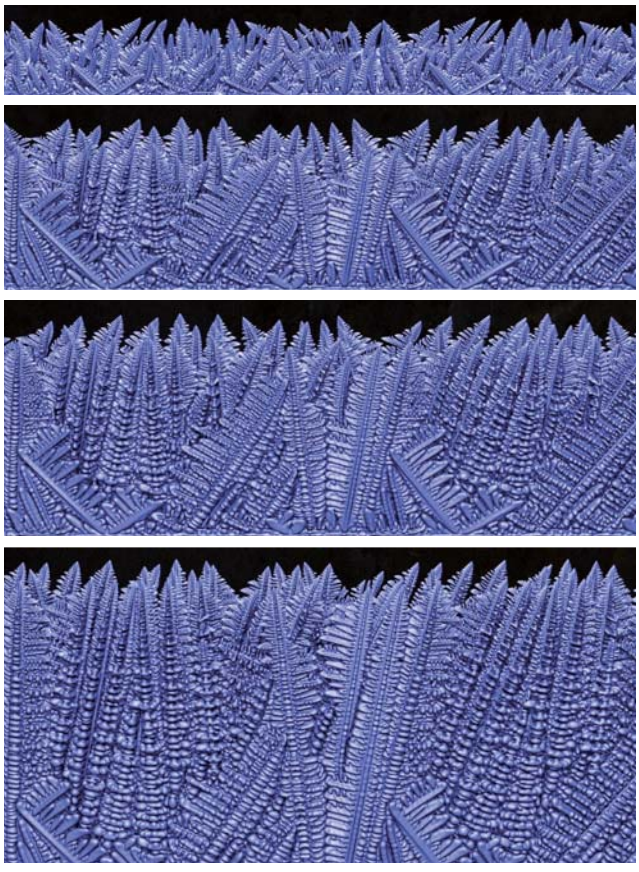
Tomohiro Takaki

Associate Professor at Kyoto Institute of Technology. Currently conducting research in an effort to expand the use of the Phase-Field method in many other fields in addition to the machine field. Has received many awards for his work on the Phase-Field method, including the Gordon Bell Prize (Scalability / Time to Solution Prize) in 2011, the APACM Award for Young Investigators in Computational Mechanics, and the Certificate of Merit for Best Presentation, JSME Medal for Outstanding Paper and the Computational Mechanics Achievement Award of the Japan Society of Mechanical Engineers.

divided into tiny domains to perform computations. Beginning around 2000, however, finite element method software for general use gradually became available, and companies came to actively use this method as well. Under these circumstances, Takaki began to wonder whether it was appropriate to conduct research at a university that could be performed even by private sector companies. At around the same time, the PF method was included in a topic presented to him by his former instructor, Yoshihiro Tomita. The focus of Takaki's research at that time was the mechanical properties of macroscopic materials, and these are strongly controlled by ever finer microscopic crystalline structures. For example, to make a Japanese sword, the swordsmith heats and hammers steel to create a steel body that is far tougher than the original material, and the changes in the crystalline structure play a major role in this process. Takaki was attracted to the PF method, which can be used even for the formation of crystalline structures, and he sensed that it had great future potential, so he made it his research target.

Immediately after he began studying the PF method, Takaki was able to understand the strengths of the method. Firstly, one of the major characteristics of the PF method is its great compatibility with various other methods. For example, when combined with thermal diffusion equations, it can describe phenomena like coagulation that produce latent heat. When combined with fluid equations, it can describe the movement of interfaces with a presence of convection currents. As he had expected, Takaki also confirmed that the PF method has extremely high compatibility with the machine field. At academic societies that he belonged to in the machine field, initially there were only a few people who gave presentations on the PF method, but almost immediately the method was accepted and its use became more widespread. Takaki speaks humbly about that time. "In some ways, I was just in time to ride the wave." But rather it can be said that he played a central role in creating that wave.

Even after he moved to Kyoto Institute of Technology in 2007, Takaki pursued research centering on the PF method. Many researchers study the PF method as a means of applying it in their own field of research. In contrast, Takaki says that he wants to do anything and everything that can be done with a central focus on the PF method itself. In the sense of using the PF method as a point of departure for research, Takaki may be the only PF method specialist in Japan. At present, he is engaged in research in a wide range of fields — not only the growth of crystalline structures and changes in those structures, but also growth models for nerve cells, simulations of crack progression within materials, optimization of the struc-



Simulation of dendrite-growth simulation using the PF method, awarded for Gordon Bell Prize in 2011. Figures are provided by a courtesy of Aoki Lab at Tokyo Institute of Technology.

tural configuration for supporting force and so on.

Even Greater Power with Supercomputers

One problem with the PF method is that of computation time. In order to describe complex interfacial structures, a fine mesh is needed for calculation, and this increases the quantity of calculations that must be performed. In particular, three-dimensional computations are needed for the simulations to be useful in the real world. But the number of meshes needed for three-dimensional calculations is several orders of magnitude greater than two-dimensional calculations, something that is beyond the capabilities of ordinary computers.

This is where supercomputers can demonstrate their true power. The great affinity between supercomputers and the PF method was demonstrated in various ways in 2011, when Takaki and coworkers received the Gordon Bell Prize, sometimes called the Nobel Prize of the supercomputing world. The prize was awarded for the work of a group including Takaki in the three-dimensional simulation of the dendrite growth of an alloy with an extremely fine mesh (several thousand × several thousand × several thousand), performed using the Tsubame 2.0 supercomputer at Tokyo Institute of Technology. Because the PF method requires a comparatively large number of computations for each mesh, it is a method that makes it easy for supercomputers to prove their worth. Many modifications were made to the memory access method and so on, resulting in the achievement of an extremely high execution performance of 2 petaflops. Takaki says that the receipt of the Gordon Bell Prize brought the PF method to the attention of many people outside the field. Future generations will undoubtedly see the award as one of the turning points for the PF method.

Another method in which supercomputers are expected to demonstrate their effectiveness is multi-scale computing. First, a macro scale test specimen is partitioned using the finite element method, and the deformation, internal stress and other attributes are calculated for each section. Normally that would be the end of it, but thanks to Takaki, it is now possible to use the PF method to calculate the changes in crystalline structure produced inside each element. As the mechanical properties of each element are changed as a result of these structural changes, the finite element method and PF method are performed again with these changes reflected. This process makes it possible to simulate macro-scale deformation while incorporating real-world phenomena on the micro level (for example, increased hardness of heavily-deformed sections). Such multi-scale computations take a very long time, so up to now only small domains could be handled. But if a supercomputer is used, multi-scale computation of real-world size materials will become possible.

The Future of the Phase-Field Method

How will the PF method develop from this point on? Takaki thinks that, as a first step, it will be important to conduct coagulation simulations that more accurately reflect the effect of convection currents. When a substance coagulates, convection currents must be produced on the liquid side, and therefore there should be many phenomena that cannot be reproduced unless these are accurately taken into consideration. He also thinks that it will be necessary to build a methodology that links the PF method with first-principles calculations and other atomic scale computations. If these efforts bear fruit, it will become possible to simulate various processes in material manufacture, and this will produce innovations in material research. Secondly, Takaki thinks that steady efforts to compare theory and experiments in greater detail will also be important.

Takaki is also working to expand the use of the PF method through a wide variety of activities. He has created a website (http://www.pfm.kit.ac.jp/) to collect issues relating to the PF method, and he has also published books aimed at beginners, held workshops and so on. On the other hand, the completion of a stand-alone application is still a work in progress. By itself, the PF method holds little interest; it becomes capable of performing meaningful simulations when it is combined with other equations. Because of this characteristic, it is likely to be difficult to develop a general PF method application that can be used for anything and everything. Takaki's first step will be to release it as a tool that can be incorporated into other programs, like a library, in order to enable as many people as possible to use the PF method.

In the meantime, the further innovations produced by Takaki and the PF method are coming soon to an interface near you.

◆Interviewer's Postscript

Shingo Yonezawa

This interview was conducted on a hot summer day in August. But it was one surprise after another, with Prof. Takaki showing me several very interesting simulation results. I was particularly impressed with the multi-scale simulation. I was surprised at what can be accomplished with the Phase-Field method. To tell the truth, the basic equation used in the Phase-Field method takes almost the same form as the equation describing the superconducting state, which is my own research area. So I felt a real sense of affinity as I conducted this interview.

5th Visiting Our Graduates

Graduate :
Shoichiro Saito

Technology Section 4, Functional Design Technology Center, Corporate Research and Development Division, Corporate Technology Sector, Nitto Denko Corporation

Majored in computational physics in the Graduate School of Engineering at Osaka University and received his doctorate for research into first-principles calculations of the interfaces between semiconductors and insulators. Subsequently joined Nitto Denko Corporation.

In Search of Simulations that Can Be Applied to Product Development

In this fifth installment of "Visiting Our Graduates," we visited Shoichiro Saito at Nitto Denko Corporation. We asked him about topics ranging from the research he conducted in his university days to the adhesive simulations he is performing with the use of the K Computer.

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

Research and Development Involving Use of the K Computer

Konishi : Let me begin by asking you about the research and development you're working on at Nitto Denko.

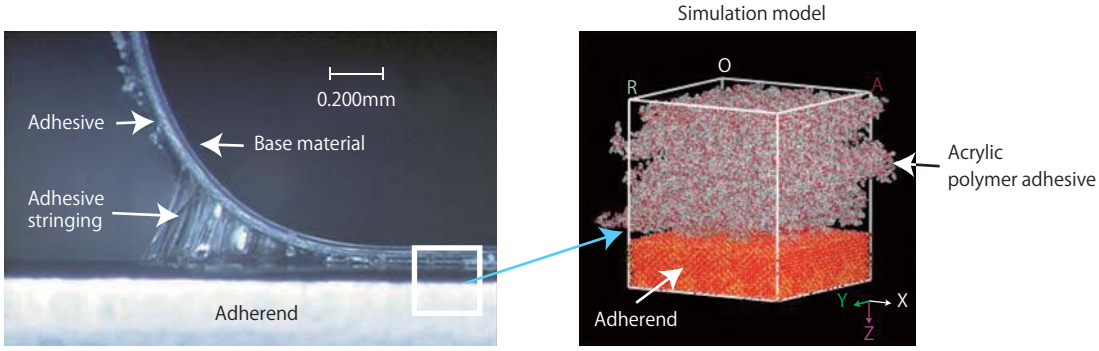
Saito : Nitto Denko is a well-known manufacturer of adhesive tapes, polymer membranes, medical products, information materials and so on. My job can be roughly divided into two activities. One is to resolve problems that are directly related to product development. When we're developing various products, we need to resolve technical issues that impede the development process as quickly as possible using numerical simulation technologies. My other main task is to develop molecular simulation technologies that are expected to be needed in future products development efforts. In my department, we handle everything from micro molecular simulations to macro continuum simulations.

Konishi : So you're in charge of micro calculations such as electronic structure calculations?

Saito : Yes, I use electronic structure calculations as well. I'm also trying to use molecular dynamics methods to perform simulations for diffusion and other types of systems where movement is crucial.

Konishi : I understand you're also using the K Computer. What type of research are you conducting?

Saito : I used the K Computer to perform simulations for an adhesive made up of several million atoms. As adhesives are composed of polymers made up of an enormous number of atoms, it's necessary to use a high-performance supercomputer in order to perform simulations for all atoms on a spatial scale that is close to reality. If you perform the simulation as a model of a system that is closer to reality than is possible with conventional methods, you can hope to get knowledge that will be helpful in developing real-world materials. It was from that perspective that we began a research project on the topic using the K Computer. In this project, I'm primarily in charge of modeling the molecular structure of the adhesive. As the simulation software, I'm using a highly parallelized molecular dynamics program for large-scale molecular systems.



Experiment in which an adhesive is separated from an adherend / Simulation model in which a polymer adhesive is attached firmly to an adherend

Konishi : What kind of results have you gotten?

Saito : I conducted a simulation of the separation of the adhesive from the adherend, and I learned that the behavior of the force produced at the time of separation was qualitatively similar to the behavior observed in experiments.

Konishi : Have you had trouble with anything when performing simulations?

Saito : To begin with, when I actually tried executing the program on the K Computer, an error occurred and the program stopped. The environment that we use on the computers at Nitto Denko is different from that of the K Computer, so transferring the program to the K Computer as is doesn't work. I spent quite a bit of time to port the program to the K Computer architecture.

I was in charge of everything from modeling the molecular structure of the adhesive through model stabilization. The molecular model of the adhesive included not only the degree of freedom to adapt to the number of atoms but also the degree of freedom for the interactions between molecules and so on. So I had a hard time finalizing metastable structures.

Things Learned in Student Days: The Basic Rules for Communicating Correct Information

Konishi : You earned your degree at the Graduate School of Engineering at Osaka University. What kind of research did you do there?

Saito : Beginning in my fourth year of undergraduate school, I conducted research into first-principles calculations, working under Assistant Professor Tomoya Ono (the present post: Associate Professor in University of Tsukuba). From a laboratory studying electronic devices in the same department, Dr. Ono received a request for an analysis of the interfacial properties of a germanium using first-principles calculations. At the time, there was interest in germanium as a possible substitute for silicon. I was a fourth year undergraduate student at the time, and I was put in charge of the analysis. I worked on it until I graduated with my graduate school degree. In graduate school, my primary research was not limited to the interfacial properties of germanium materials; I also studied semiconductor-insulator interfaces.

Konishi : What things that you learned during your student days are you applying in your current job?

Saito : When you consider properties using electronic structure theory, you're able to deepen your understanding of many of the phenomena you observe in experiments, and I think my knowledge is helpful in that regard. I'm able to use what I learned in my student days, so I think I'm taking advantage of the things in my arsenal.

Konishi : What kind of things did you learn through your graduate school activities?

Saito : I learned a lot about logical sentence construction from Dr. Ono. Starting with the basics, I was taught how to communicate correct information and not pretend like I know more than I do, not only in academic papers but in emails and daily conversation as well. That's something we need in order to be a full-fledged member of society as well, and I make an effort to do that even now.

Konishi : What was your motivation for wanting to join a company?

Saito : When I got my doctorate, I agonized about whether to remain at the university or go to a company. Even if I had been able to remain at the university, I think there's a possibility that I might simply shift from a learning role to a teaching role. I thought there were a lot of things that I still needed to learn, and so I thought an environment like a company where I had superiors and senior associates would be better. That was the major reason. So I looked for a company that was hiring personnel to conduct molecular simulations, and I wound up joining Nitto Denko.

Toward Mesoscale Simulations

Konishi : I understand that you're in your second year at the company. Tell me about your work goals.

Saito : The company climate at Nitto Denko is "providing support to people who want to tackle challenges." I plan to take on new challenges in areas other than the framework of molecular simulations.

Konishi : Will you be doing computational simulations?

Saito : I think that simulations will come to play a major role in product development in Japan in the future. Supposedly exascale computers will become a reality in the near future. If we become able to use such computers, I think it will become possible to perform mesoscale simulations starting from micro models. I'd like to design products that reflect the results of those simulations. I'd also like to develop simulation technologies that can be applied to product development, so customers are able to see the value of simulations.

Institute for Solid State Physics The University of Tokyo

Hiroshi Noguchi
Associate Professor, Materials Design and Characterization Laboratory / Center of Computational Materials Science, Institute for Solid State Physics, The University of Tokyo

The Condesed Matter Physics Division pursues research into large-scale computing in the field of condensed matter physics. To that end, it makes its supercomputer available for shared use. The Division also supports software development and dissemination in order to increase computer use on the part of both theoretical and experimental researchers. We asked Associate Professor Hiroshi Noguchi to talk about the Division's activities.

Providing existing software as well to meet needs

The Condensed Matter Physics Division of CMSI is located within the Center of Computational Materials Science (CCMS) in the Institute for Solid State Physics (ISSP) at The University of Tokyo. ISSP moved from Tokyo's Roppongi district to Kashiwa City in Chiba Prefecture in 2000. At that time, the campus itself was brand new, and there was not much in the area. Following the beginning of service by the Tsukuba Express railway line in 2005, however, the population grew steadily, and now the shopping center in front of the station is a place of vibrant activity, filled with parents and their young children.

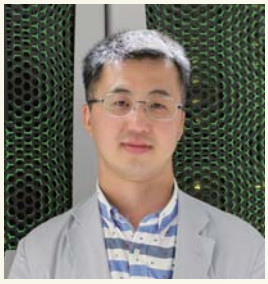
ISSP has made its supercomputer available for shared use nationwide since 1995. The Institute considers its primary mission to be providing computers suitable for performing condensed matter physics simulations, and it has configured its computer specifications to achieve that goal, upgrading the systems around once every five years. The first supercomputer at ISSP, FUJITSU VPP500/40, was introduced in 1995, and currently the fourth generation systems, NEC SX9 (System A) and SGI Altix ICE 8400EX (System B), that have been installed July 2010, are in operations. Since 2000, two types of computers have been in service: System A, which is primarily used for vector computations, and System B, which is used for massively parallel scalar computations. In addition, in April 2013 a 4.5 generation FUJITSU PRIMEHPC FX10 (System C) began operating for the purpose of cooperation with the K computer. Systems A and B are scheduled to be upgraded the next fiscal year, and preparations for introduction are underway.

Up until recently, almost all of the users of the ISSP supercomputers have performed calculations using simulation code that they have written themselves. Recently, however, users who perform first-principles calculations in particular have increasingly used existing third-party software. The Institute has begun providing compiled execution binaries for VASP (a plane wave first-principles simulation software), OpenMX (a localized basis first-principles simulation software) and ALPS (libraries for strongly-correlated quantum lattice models). (Note: users must purchase their own user license in order to use VASP.)

Research for creation of an advanced parallel computing environment

Shared use of the ISSP supercomputers is open to any applicant, provided that the objective is research in the field of condensed matter physics by researchers in research institution in Japan. In addition to two regular application periods each year (June and December), "anytime" applications are also accepted — Class D for urgent large-scale simulation, and Class A for trial use. CPU time and other computing resources are allocated based on an evaluation by review committee members, in particular regarding whether or not the large-scale calculations can only be executed on the ISSP supercomputer systems and so on. Currently 88 researchers volunteer their time to serve on the review process. In addition to general shared use, 20% of the computing resources are provided to CMSI.

The supercomputers are operated by the Supercomputer Center of the Materials Design Division in the Materials Design and



Hiroyuki Yata

After graduating from the Faculty of Science in The University of Tokyo, joined the Institute for Solid State Physics in 1995, the year in which the supercomputer went into operation. Currently working to develop systems that are easy for users to use and operators to operate.

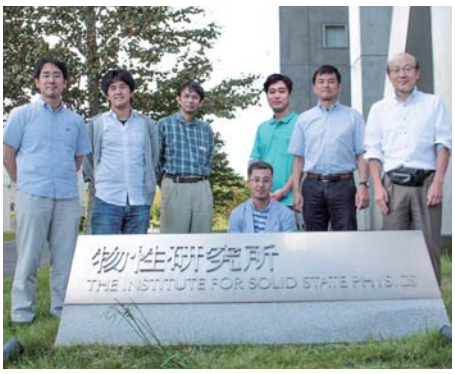
Characterization Laboratory in ISSP. The core personnel are Professor Naoki Kawashima, Associate Professor Osamu Sugino and myself; two research associates, Hiroshi Watanabe and Shusuke Kasamatsu; and three technical staff, Hiroyuki Yata, Takaki Fukuda and Shigeyuki Araki. We pursue work activities with the cooperation of the other professors within the Institute and at other institutions. We couldn't do it without the hard work of the research associates and technical associates in particular, so we're deeply indebted to them.

The Materials Design Division also works to develop, release and spread software, and we are making plans to create an environment that will make it easier for shared computer users to perform advanced parallel computing. To this end, starting in April 2015 we will have two new project researchers to provide development support.

As a CMSI core division

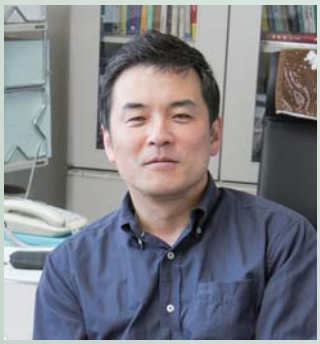
CCMS was established in April 2011 to support CMSI activities. In addition to Center Director Shinji Tsuneyuki and Professor Naoki Kawashima, CCMS has three professors, three associate professors, five research associates, 12 project researchers, two project academic support specialists and five clerical support staff members. This makes it seem like a very large institution, but many of the members serve in concurrent posts or work in Kobe or other distant locations, so not many of the staff members are resident in Kashiwa.

In contrast to the Materials Design Division, which primarily makes its supercomputer available for shared use, CCMS focuses primarily on software dissemination and development support. As an activity on the part of CMSI as a whole, CCMS built the MateriApps portal site in 2013 to introduce software. CCMS also plans workshops and symposiums, and in October it holds the ALPS tutorial. Through these activities, our goal is to build an environment that makes it easy for not only theoretical but also experimental researchers to perform numerical calculations.



Materials Design Division members operating the supercomputers

From left to right : Watanabe, Kasamatsu (Research Associate), Araki, Yata, Fukuda (Technical Staff), Kawashima (Professor), Sugino (Associate Professor)



Message from the Director of the Condesed Matter Physics Division

Naoki Kawashima

During my graduate school days in the late 1980s, computers became readily available for use even by students, and one after another algorithms were created ingeniously exploiting characteristics of physical systems in question . It was a time at which, in most cases, we only needed to consider how fast we could calculate using a single processor, and we simply accepted that algorithms themselves had universal value. The times have changed, and now we have entered the era of large-scale parallel computing. But the question of what is the fastest materials calculation algorithm for the distributed memory parallel computing model is still a universal one that is not affected by the specifics of the hardware. It is my hope that we can build an environment that allows computational materials science researchers the freedom to boldly seek answers to this universal question.

CMSI Calendar

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

●On-line Lecture: CMRI seminar on Multiscale Materials Science - computational approach -
Date : November 7, 2014
Venue: To be delivered from Tohoku University to 13 CMSI sites

●CMRI Symposium/ International Workshop on Multiscale Computational Materials Science
Date : November 10-11, 2014
Venue: Institute for Materials Research, Tohoku University

●International Symposium on Extended Molecular Dynamics and Enhanced Sampling: Nosé Dynamics 30 Years (NOSE30)
Date : November 10-11, 2014
Venue: Hiyoshi Campus, Keio University

●The 4th Symposium of Center of Computational Materials Science of ISSP / Joint Research for ISSP Supercomputer
Date : November 12-14, 2014
Venue: ISSP, The University of Tokyo

●9th CMSI Symposium on Industry-Government-Academia Cooperation "Carbon Composite Material and Molecular Simulation"
Date : November 20, 2014
Venue: Akihabara Dai Building

●4th International Workshop on Massively Parallel Programming Now - Toward post-K Computers
Date : November 23-24, 2014
Venue: Hongo campus, The University of Tokyo

●International Symposium on Computics – Quantum Simulation & Design (ISC – QSD) 2014
Date : December 1-3, 2014
Venue: Koshiba Hall (Tokyo)

●3D Projection Conference on Molecular Science (3DCMS2014)
Date : December 5-6, 2014
Venue: Iizuka Campus, Information Technology Department, Kyushu Institute of Technology

●5th CMSI Symposium
Date : December 8-10, 2014
Venue: Tohoku University

●TCCI Winter College: Quantum Chemistry
Date : December 15-16, 2014
Venue: Okazaki Conference Center at NINS

●10th CMSI Symposium on Industry-Government-Academia Cooperation "Computational Materials Science in Structural Metal (Iron and Steel)"
Date : November 19, 2014
Venue: 5F of Akihabara Dai Building

Profiles of Division Researchers

This section will introduce the Division Researchers who joined CMSI in April 2014

David Sulzer

Molecular Science Division Researcher

Graduate School of Information Science, Nagoya University

Graduated in physical-chemistry at the University of Strasbourg (France), and received a doctorate in theoretical chemistry in the same university. Engaged in research to enhance solar panel using theoretical methods at the Graduate School of Information Science, Nagoya University.

Ambition

Provide a better understanding of the process occurring in DSSC and propose new molecules that could enhance the overall efficiency and cost of currently available solar panels.

Motivation for applying for the position

To decipher the properties of matter and propose new technologies, I would like to develop and apply quantum chemistry methods.
I think that using them to help finding alternative and more ecological ways to produce energy is an important and motivating purpose.

Mission/Role

To develop a new approach to model and understand the electron transfer process in Dye Sensitizers Solar Cells (DSSC) at the edge between molecular and solid state simulations.

Yasutaka Nishihara

Molecular Science Division Researcher

Institute of Molecular and Cellular Biosciences, The University of Tokyo

Majored in theoretical chemistry at the Graduate School of Science at Kyoto University and received a Doctorate (of Science).
Currently conducting research into the relationship between protein structures and functions at the Institute of Molecular and Cellular Biosciences of The University of Tokyo.

Ambition

To identify the movements of proteins on molecular level, in order to understand the mechanisms for protein functions and help to establish techniques for controlling these functions.

Motivation for applying for the position

Research on protein structural changes are shifting to ever-broader spatial scales and ever-longer time scales. For this reason, large-scale parallel computing is needed, and I would like to acquire and apply those techniques.

Mission/Role

To improve cascade-type massive parallel molecular simulation method, in order to develop method for efficiently inducing structural changes in protein and membrane systems.

Moshiour Rahaman

Condensed Matter Physics Division Researcher

Department of Materials Engineering,
The University of Tokyo

Majored in Materials Science at KTH Royal Institute of Technology, Stockholm and received his Ph.D.

Ambition

Understanding the physical properties of materials using the state-of-the-art first-principles method.

Motivation for applying for the position

Conducting research at the nanoscale level in materials science.

Mission/Role

To develop the non-equilibrium Green's function (NEFG) techniques combined with real-space density functional theory (RSDFT) for investigating the electron transport of nano-materials.

Torrent
No.10 October 2014

Cover：What do you think this figure shows? It likes a forest, doesn't it? This is the result computed solidification of a metal by supercomputer. Supercomputer enables us to walk in the metallic forest and to see it from far away. Such large scale computation is key to make clear various mulstiscale phenomena. (CG: Tomohiro Takaki, Kyoto Institute of Technology)

Torrent : The Newsletter of the Computational Materials Science Initiative (CMSI) No.10, October 2014

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