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Torrent

What is CMSI?

Roundtable Discussion by Young CMSI Researchers

CMSI Calendar

Messages from CMSI Division Directors

CMSI Research Areas

Turning the Headwaters of Basic Science into a Torrent of Innovations in Functional Materials and Energy Conversion

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

Roundtable Discussion by Young CMSI Researchers

Furthering the Development of Computational Materials Science

Todo (moderator) : Today we have brought together four young researchers who are currently active in various fields of computational materials science. We'd like to ask them to speak frankly about the state of computer training, the state of software development and release in their respective fields, and about the issues that need to be resolved in these areas, as well as their expectations with regard to CMSI.
Could you begin by telling us a little about yourselves?

Udagawa : I graduated from the Graduate School of Science at the University of Tokyo with a major in physics. My specialty is model calculations for strongly-correlated electron systems. The fundamental area of inquiry in this field is the search for novel cooperative phenomena and order phenomena. In materials that have strong geometric frustrations, electrons sometimes act as if they have several hundred times the mass of free electrons, and I'm very interested in the mechanism that causes this phenomenon. In terms of hardware, I use the supercomputer at the Institute for Solid State Physics.

Ohba : I graduated from the School of Science at Nagoya University with a major in physics. I am currently employed at the Toyota Central R&D Labs, Inc. This is the research lab that conducts basic research for the Toyota Group. My work involves device simulations and first principle calculations for ferroelectric and hydrogen storage materials. Currently I'm working to develop simulation methods for lithium ion batteries. I'm also a third year student in the Ph.D program at Nagoya Institute of Technology.

Synge Todo
CMSI
Publicity Committee Chair
Lecturer, Department of Applied Physics, Graduate School of Engineering, The University of Tokyo

Sato : I'm currently studying in the Graduate School of Engineering Research at Hokkaido University with a major in materials science. My research topic is atomic diffusion in alloys. When heated, iron and aluminum atoms begin to move of their own accord and mingle with one another, and I'm attempting to calculate the way in which they will move and mingle with one another. I often use the Monte Carlo method. In terms of computers, I mainly use PC clusters, but I'd like to use a large computer as well.

Ishimura : After graduating from the Graduate School of Kyoto University with a major in synthetic biochemistry, I worked at the Institute for Molecular Science and the Toyota Central R&D Labs., Inc., and now I'm a assistant professor at Kobe University. My work involves quantum chemistry calculations. This involves calculating the electron state of molecules and developing algorithms and programs for accelerating and parallelizing simulations. I'm particularly interested in working with nanosize molecules, which has not been possible until now. At the Toyota R&D Labs, I developed and demonstrated a program to perform 2000-core quantum chemistry calculations.

Handmade Software / Self-Taught in Programming

Todo : What kind of software do you use?

Udagawa : In terms of simulation software, I generally write the software myself.

Sato : I also write my own software, but some people use commercial MD packages.

Tsuneyuki : At universities, having students write software is part of their education. But how about at companies? If commercial software is available, do you use it right away?

Ohba : Mainly we use programs that we've developed in-house. With regard to using commercial software, it depends on the price. If we do use it, we add things ourselves to expand the software.

Todo : At companies, do you provide full instruction in programming?

Ohba : We don't provide any instruction at all. Research teams use the standard software that's in use, or programs that more experienced members of the team have created. Everyone's self-taught. For that reason, each department sometimes uses different programs.

Todo : I get the feeling that recently a lot of the students haven't learned the languages that can be used for simulation when they first join the laboratory.

Shinji Tsuneyuki
CMSI
Representative Director
Professor, Institute for Solid State Physics / Graduate School of Science, The University of Tokyo

Ishimura : At Kyoto University there are classes in Fortran, so students can program in Fortran when they are assigned to the laboratory. At Kobe University, the department uses C, and students entering the laboratory have to study Fortran. In the class of parallelization and optimization, source code is provided in both C and Fortran, and students write their own programs.

Udagawa : In the field of condensed matter physics, too, there's a mix of both C and Fortran. In my lab, my boss and I use different languages.

Sato : Fortran is used for computer practice in the department. In the lab it's all over the place: the professor uses Fortran, the research associate uses C, and I use C, too. Students learn programming through one-on-one instruction from a teacher.

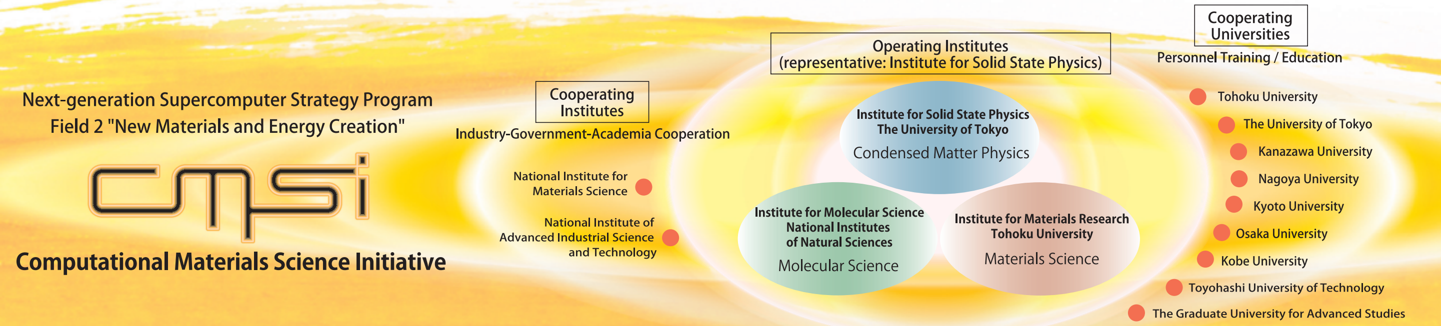
Todo : So I guess when you enter graduate school, the language you use is determined by who teaches you.

Tsuneyuki : Did you get any instruction in computational theory?

Ohba : No. I learned it through private workshops and so on. When I first joined the company, I was in the same laboratory as the

What is CMSI?

The Computational Materials Science Initiative (CMSI) is a research network established on September 27, 2010 as Field 2 "New Materials and Energy Creation" of the Next-Generation Supercomputer Strategy Program (FY 2010 - 2015).
The Initiative is centered on three operating institutions — the Institute for Solid State Physics (The University of Tokyo), the Institute for Molecular Science (National Institutes of Natural Sciences) and the Institute for Materials Research (Tohoku University) — and includes 11 cooperating institutes and universities. It is an open community that invites all universities, research institutes, companies and other entities with an interest in computational materials science to become members.
The objective of CMSI is to expand and deepen the headwaters of basic science and turn it into a "torrent" of innovations in functional materials and energy conversion. The three research fields — condensed matter physics, molecular science and materials science — are fully integrated with one another, with the aim of achieving a new type of science that can overcome the barriers between disciplines. Another major objective is to train the young researchers who will lead the computational materials science in the future.



fluids team, and there were people studying diagonalization theory. So I just picked it up.

Todo: I had thought it would be taught a little more systematically. I guess I was wrong. (Laugh)

Tsuneyuki: How did you study parallelization?

Ishimura: I'm self-taught. We have started a class this year, but it's at the beginner level, not the supercomputer level. In other words, that's for master's students to be able to write a program for PC clusters.

Todo: In my case, I learned parallelization by attending workshops at the Supercomputer

Masafumi Udagawa
Research Associate,
Department of Applied Physics,
Graduate School of Engineering,
The University of Tokyo

Center of the Institute for Solid State Physics. At the time, the only parallel computers were supercomputers. Have you ever attended that kind of workshop?

All: I know such workshops exist, but I've never attended one.

Todo: So that means all of you are completely self-taught?

All: Yes. (Laugh)

Sato: Learning by yourself is convenient since you can begin studying immediately when it becomes necessary.

Ohba: I studied by myself by asking people around me and people who really knew what they were doing. I also did research on the Web and modified the programs by myself as needed.

Todo: When I'm having graduate students do parallel computing, I wonder if it would be better to tell them to do research on the Web and then begin programming. It would be convenient if there were a collection of resources online.

Ishimura: There are still only young people in the lab, but we're planning to create a system in which the senior students teach the junior students.

Tsuneyuki: Are there any moves to create a university-wide curriculum?

Ishimura: I think instruction is beginning little by little and it will gradually take shape. Our department specializes in computational science, but the faculty members majored in a variety of areas like math, physics, chemistry and biology. The common thread is that they all use computers. From the standpoint of a physics or chemistry major, parallelization is ultimately just a means to an end. It's not the end itself.

Todo: They feel that if they go too deeply into it, they won't be able to get back to their original area of specialization?

Ishimura: Yes, you could say that about me, too. (Laugh)

Can Software Development Enhance Your Reputation?

Tsuneyuki: Work such as parallelization is hard to turn into an academic paper. How can you make it enhance your reputation? I think that's something that absolutely must be done in order to ensure progress in computational science. Do you have any ideas as to how to accomplish this?

Ishimura: Personally, I think it must have enhanced my reputation, since I got hired as a research associate.

Todo: In other words, academic posts need to be increased.

Ishimura: The professors need to do their part. (Laugh)

Tsuneyuki: People who have strong computer skills are needed in condensed matter physics, too, so I'd love to hire then. But I know that at the faculty meeting the minute I say an applicant's previous achievements were in software parallelization, the result will be that he or she won't get hired.

Ishimura: I think we also have to do our best to release programs that boost our name recognition.

Todo: Do you all release the programs that you develop to the public?

Ishimura: At the Institute for Molecular Science, I expanded a program called GAMESS, and a portion of that program was released. I played a leading role in the development effort, but subsequently we worked together to debug it and do various other types of work on it.

Tsuneyuki: What was the reaction?

Ohba: In the case of Gaussian, the paper will be cited with the name of developers.

Ishimura: That wasn't so in the case of GAMESS. You only got your name included in the list of developers at the end of the program. It's not like I got hired just because I developed the program.

Todo: I'm working on the project for a program called ALPS. There we write a paper with about 20 authors like elementary particle physics. And by the license people who want

Nobuko Ohba
Researcher,
Materials Design Lab.
Materials Fundamentals Research Div.,
Toyota Central R&D Labs., Inc.

Kazuya Ishimura
Assistant Professor,
Department of Computational
Science Graduate School of System Informatics,
Kobe University

to use the program to write papers are obliged to cite our paper.

Ishimura: If we can show through this Initiative that there's a way to increase your name recognition by releasing software, I think the number of young people who decide to try it will increase.

Sato: In companies, does program development enhance your reputation?

Ohba: If the purpose of your work is creating software, then I think you'll get credit for it. But I think it would be difficult if that weren't the case. Executives would ask, "So you created software. What now? Are you going to sell it?"

Todo: I think one of the advantages of open source software is that you can release it, even in imperfect form, and then many people will lend their knowledge and help improve it. Mr. Sato, do you release software?

Sato: No. I create software for my own use, and it's enough if I understand it. So I don't write programs carefully with the intention of ensuring that they can be used by as many people as possible. Also, our community isn't that large, so I don't think there are that many users.

Todo: People from other countries are pretty up-front about asking you to give them your programs. When that happens, I worry about what might happen to a program I designed all by myself after I hand it over. Conversely, when you release software publicly, you can set conditions: I'm making the software available under these conditions and I expect you to observe those conditions when you use it.

Ishimura: These days I think even people who conduct experiments perform a lot of calculations. But I doubt that they're users of the kind of programs that will be developed under this Initiative. This will change if someday there are people in the field of experimentation who need a supercomputer because the PC clusters in the laboratory are insufficient.

Tsuneyuki: Programs like Gaussian and GAMESS have a lot of functions, so I wonder if it will be OK even without a supercomputer. As long as you're going to release the program, there's no sense in releasing one that has the exact same functions. It has to have functions that no existing software has.

Ishimura: One example would be switch to massively parallel computing. It would be hard to make an effective approach with existing software. I wonder if you could do it through parallelization and increasing the speed.

Udagawa: Occasionally I'm in communication with people in the field of nuclear physics, and they tell me they sometimes find programs with algorithms for analyzing the structure of atomic nuclei useful. However, different languages are used in different fields, so something needs to be done about that as well.

Tsuneyuki: In your fields, are there any examples of software being released overseas?

Ishimura: There are many examples of that in Europe and the United States. I imagine it's because program development and release is taken into consideration when conducting evaluations.

Tsuneyuki: Japan is behind other countries when it comes to software development. So I hope this project provides the opportunity to release software. Japanese developers have released lots of freeware games. I wonder where they come up with those ideas.

Sato: Surely they do it to see the reaction to their work.

Todo: I wonder if the reaction is enough of an incentive for software release.

Ishimura: I doubt that I'd have the time to do that while doing my post-doctoral research. I might be able to if I could see many career paths other than that of researcher, but I doubt that all of us will be able to get an academic position.

Ohba: I think these days companies have extremely high expectations when it comes to computer simulations.

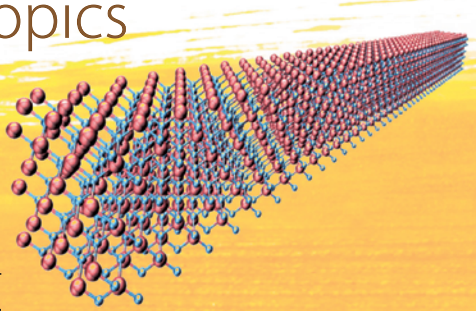
Todo: Still, it's not like there's a market for people who have used computers in their work. People search for them in their area of specialty. What I'd like to see is for the Initiative to publicize to companies that are looking for computation personnel the fact that

Kazufumi Sato
3rd-year Ph.D candidate,
Laboratory of Materials Modeling,
Division of Materials Science and Engineering,
Graduate School of Engineering Research,
Hokkaido University

CMSI Research Topics

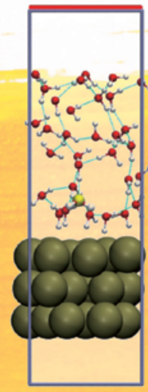
Next-generation advanced device science

As semiconductor device miniaturization approaches its physical limits, research is being promoted into nanoscale devices that use the quantum effect. Next-generation supercomputers will be used to perform simulations that incorporate the quantum effect that controls nanoscale phenomena in order to develop guidelines for designing new devices.



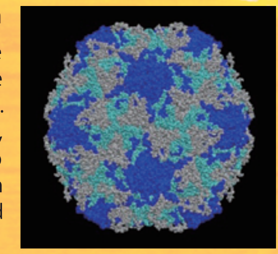
Energy Conversion

Unprecedented large-scale simulations will be conducted to identify the basic processes of fuel cells, methane hydrate and so on, in order to discover materials that are suitable for use in energy conversion and storage.



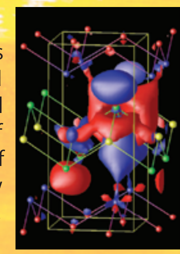
Molecular Function and Matter Transformation

The structure and functions of nanoscale molecules and molecular ensembles will be studied with a view to controlling these functions. For example, all-atom simulations of viruses, which are molecular ensembles, will help researchers identify the molecular mechanism responsible for infection and immunity and lead to the development of antiviral agents.



Basic Science of Novel Quantum States / New Materials

Researchers will study cutting-edge basic issues relating to condensed matter physics and quantum chemistry in order to discover novel quantum states, elucidate the dynamics of electron systems, predict quantum finestructure of molecules and study the emergence of new functionalities through fluctuations and dynamics.



there are certain people with those skills. I hope that kind of process becomes established.

How Can We Train People to Use Next-Generation Supercomputers?

Ishimura: At the Institute for Molecular Science, I worked on a supercomputer with several hundred cores, and at the Toyota Central R&D Labs I worked on one with 2,000 cores. But each time the number of cores increases by one decimal place, it takes two years until you're able to master it. From PC clusters to the several thousand core level, and then from there to existing supercomputers, and from there to next-generation supercomputers. Even if you teach students to go from zero to PC clusters in class, how to train students who are able to master computers from that point on is a major issue.
Tsuneyuki: Up until recently, the environment didn't exist in which you could conduct parallel computing with more than 10,000 cores. At that level, even a computer science specialist would find it tough going.
Todo: In my own experience, people can study on their own and master something on the order of 1,000 cores. But beyond that, currently support from a computer vender is absolutely necessary to optimize a program.
Tsuneyuki: Another objective of CMSI is to build a support system for parallelization. We could invite a parallelization specialist from a private company to come. Or if there was someone specializing in computer science who was also interested in applied computing, we could recruit that person.
Udagawa: If someone is interested in performing calculations with 10,000 cores, is it easy for that person to get training?
Tsuneyuki: There's a forum for discussion of what problems should be computed on the next-generation computer (popularly known as "K Computer"). The forum will decide the priority between the problems. I think it would be great if there was a mechanism by which, if young people have an idea for something they want the computer to solve, they could apply and we could say, "That's a great idea! Why don't you do it?" In the near future, we're planning to have a workshop for finalizing the report of the year's achievements and the schedule for the next fiscal year. So you could make proposals at that workshop.
Ishimura: Undoubtedly there are people who would like to have the opportunity to get vendor support for training in 1,000 or 10,000 core computing. It would also be good for there to be a forum where people could speak more freely than at an academic conference. Where they could ask questions freely and where they could talk about failures as well as successes. Experience is essential for parallelization, so I think sharing and accumulating experiences would be very helpful.

Tsuneyuki: But even if we got a vendor to optimize the program of a specific group, the knowledge would not be communicated outside that group. I wonder if there's a way to raise the level of the field as a whole.
Ishimura: I think we should discuss with one another at informal workshops and get vendors to share their experiences as well, so that everyone's level would be improved.
Sato: It may be essential for achievements derived through computation to be released. There's still little acknowledgement of computation. When you say you do computations, you get a surprised reaction from people. I'd like people to have a clearer understanding of the fact that computation can make a major contribution in many research fields.
Ohba: Companies have a need for computation in many areas. For that reason, I think that when they access the Initiative's website, they should be able to find out how to perform computations and find seeds about joint research projects. It would be good if the website could provide that kind of information
Tsuneyuki: I hope we can put out a newsletter that's something like a "research cafeteria." There would be lots of things on the shelves and people could come and pick up the things they found interesting. Something like that.
Ohba: That would be great — a resource that would make people think, "It sounds like I could find some interesting seeds there." Or "I had heard that the professor was trying to do that; I wonder how it went after that." "If he's managed to make a go of it, I'd like to use it." I hope it becomes a source of information that can fulfill those kinds of demands.
Tsuneyuki: I think whether or not Japan is able to develop the next generation of K Computer will depend on whether achievements are produced by CMSI. We also need to begin the discussion about the type of next-generation supercomputer that should be built once we've mastered K Computer.
Todo: The first sections of K Computer were shipped today. We'll have to do our best to keep moving forward as well.

(Recorded September 29, 2010)

"K" News

Work is progressing on the construction of the next-generation supercomputer (popularly known as "K Computer") on Port Island in Kobe. The supercomputer is expected to be completed in the fall of 2012. On September 29, 2010, the first eight computer racks were delivered. With these eight racks, the new supercomputer is already more than twice as fast as the Earth Simulator, the world's fastest computer at a time in the past. When completed, the new supercomputer will link more than 800 racks and is expected to achieve a speed of 10 petaflops (ten quadrillion calculations per second).

Photo: RIKEN

CMSI Calendar

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

● **September 30, 2010**
1st CMSI Symposium: "Turning the Headwaters of Basic Science into a Torrent of Innovations in Functional Materials and Energy Conversion"
Venue: Tetsumon Memorial Hall, The University of Tokyo

The first CMSI Symposium held to commemorate the official start of the CMSI Program was attended by some 170 persons, including not only representatives from the central CMSI institutions but also representatives from industrial, government and academic organizations throughout Japan.
The opening address for the symposium was given by Professor Shinji Tsuneyuki, the director of CMSI. Professor Tsuneyuki predicted that next-generation supercomputing would produce many dramatic achievements, and he noted that the many researchers from the fields of condensed matter physics, molecular research and material research who had come together at CMSI were committed to achieving breakthroughs based on the philosophy that "more is different." These words were greeted by enthusiastic applause from the assembled participants.
Professor Hideo Hosono of the Tokyo Institute of Technology, the foremost researcher in the area of iron-based superconductive materials, expressed his hopes for the achievements of CMSI, saying that experimenters would respond to achievements in computational science and this would spur research overall. Science journalist Akira Ozeki, a member of the editorial committee of the Asahi Shimbun newspaper, expressed his strong support for the initiative, placing it in the context of current trends by saying, "A dialogue between science and society is indispensable for determining and supporting science and technology policy. What's more, scientific knowledge is becoming a source of Japanese culture."
The second half of the symposium featured presentations on major research topics on new materials and energy creation: quantum simulations for next-generation semiconductor devices, all-atom calculation of a virus in order to develop antiviral agents, fuel cell and methane hydrate research, a determination of material properties and internal structure, and basic issues in physics and chemistry that constitute the "headwaters" for various applied research projects. Each of these topics can be expected to open up new frontiers in research.
The symposium ended with encouraging words from Professor Kiyoyuki Terakura of the Japan Advanced Institute of Science and Technology, who noted that, "It is often said that the period up until the start of the project is when the dream is alive. In this case, I hope you continue to hold fast to your dream even after the project begins."

● **November 11 - 12, 2010**
CMSI Workshop: "Basic Science of Novel Quantum States and New Materials"
Venue: Okazaki Conference Center, National Institutes of Natural Sciences

● **January 5 - 7, 2011**
Joint Workshop of Institute for Solid State Physics, CMSI and Next-Generation Functional nanomaterials for Information Technology: "Computational Materials Science: Challenges and Prospects"
Venue: Lecture Hall, Institute for Solid State Physics, The University of Tokyo

● **January 17, 2011**
Next Generation Supercomputing Symposium 2010 and 1st Joint Five-field Strategic Program Workshop
Venue: Nichii Gakkan Co. Kobe Port Island Center

● **February 4 - 5, 2011**
1st Seminar of the CMSI Computational Molecular Science Division
Venue: Okazaki Conference Center, National Institutes of Natural Sciences

● **February 7, 2011**
CMSI Symposium on Industry-Government-Academic Collaboration
Venue: Akihabara Convention Hall

● **February 18, 2011**
1st CMSI Seminar on Industry-Government-Academic Collaboration
Venue: Akihabara Convention Hall

● **February 22 - 23, 2011**
5th Open Symposium on Next-Generation Integrated Nanoscience Simulation Software (Support)
Venue: Lecture Hall, Konan University Port Island Campus

● **March 8 - 12, 2011**
18th Computational Materials Design (CMD®) Workshop (Support)
Venue: International Institute for Advanced Studies
Organized by: Institute for Nanoscience Design, Osaka University, etc.

● **March 9 - 10, 2011**
HPC Industrial Use School Nanotech Course (Support)
Venue: Institute of Industrial Science, The University of Tokyo
Organized by: Industrial Committee for Super-computing Promotion

Messages from CMSI Division Directors

Tetsuo Mori

Director, CMSI Materials Science Division

Institute for Materials Research, Tohoku University

Graduate School of Engineering, Hokkaido University

Most of the practical materials studied in material science are manufactured by means of nonequilibrium processes. Their internal structure is non-uniform. This means that, for example, the phenomena that determine material strength have a pronounced nonlinearity, and therefore it is difficult even to give a quantitative description of the phenomena themselves, to say nothing of determining the physical properties that lie behind the phenomena. For this reason, experiments usually precede theoretical and computational researches. However, advances in computational materials science will be indispensable in order to make effective use of limited resources and develop materials with great precision.

Japan is one of the world leaders in the development of steel and other materials. The expectations placed on computational material science to provide the break-throughs needed to carry on this tradition are considerable.

Computational materials science in the next generation will be innovated and developed by today's young people. A great deal of knowledge will be gained from people in different fields such as condensed matter physics and molecular science as a result of the CMSI project, and unique material science techniques will be systematized based on this knowledge. Young researchers must play a central role throughout this entire process. The goal of the Institute for Materials Research, Tohoku University, is to work with these young researchers and serve as a center for establishing next-generation computational materials science.

Naoki Kawashima

Director, CMSI Condensed Matter Physics Division

Institute for Solid State Physics, The University of Tokyo

The Institute for Solid State Physics at the University of Tokyo has assisted the development of state-of-the-art parallel computing in the computational materials science community through the use of shared supercomputers.

Many of these shared supercomputer users have employed original programs created by individuals and laboratories, producing many important achievements through this kind of "handicraft cottage industry style" approach. This tradition will undoubtedly be carried on in the future as well. At the same time, however, with the increase in parallel computing there have also been increased efforts to create programs that skillfully make use of computer capabilities.

With the establishment of CMSI, the Institute for Solid State Physics aims to play an active role in developing technologies for large-scale parallel computing and the accumulation, release and dissemination of software assets, in addition to its existing projects. For this purpose, we are currently considering the establishment of a Computational Materials Science Research Center (tentative name) as a new organization within the Institute. This would make it possible to create a toolbox to support next-generation "handicraft" research in the future.

Kazuo Takatsuka

Director, CMSI Molecular Science Division

Institute for Molecular Science, National Institutes of Natural Sciences

Graduate School of Arts and Sciences, The University of Tokyo

Computers are magnificent tools. However, whether or not they are actually useful is dependent on the person using them. The human brain is made up of a complex network of neurons. When people are linked together, the networks of multiple brains are connected, forming a higher order of network. Moreover, the network within each individual brain is also stimulated. The connection distance (correlation range) is also extended. Thanks to the establishment of CMSI, my brain, which has been focused on molecular science, now has a correlation with condensed matter physics and materials science as well, so the reception distance is longer and the coverage area for receiving communications is wider. I find this tremendously exciting.

Students studying at a university know very little about companies before they begin looking for a job. (It could also be said that they know next to nothing about society.) However, the people who are already employed by companies may also have forgotten what they were like when they were young and energetic and racing toward the future. The goal of CMSI is to help form networks that link students, universities, research institutes and companies with one another. Here, too, we hope that these networks will lengthen and expand correlation ranges and coverage areas.

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Next-generation Supercomputer Strategy Program Field 2 "New Materials and Energy Creation"

Computational Materials Science Initiative

Office Institute for Solid State Physics, The University of Tokyo
Kashiwanoha 5-1-5, Kashiwa, Chiba 277-8581, Japan

TEL: (+81) 4-7136-3279 FAX: (+81) 4-7136-3441 http://cms-initiative.jp ISSN 2185-8845

Computational Materials Science Initiative

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