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Torrent

10^{16} Weave New Materials

Interview with
Kazuya Ishimura, Developer of SMASH

CMSI Kobe Branch

K Computer News

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

Interview with Kazuya Ishimura, Developer of SMASH

Interviewee:

Kazuya Ishimura

CMSI Molecular Science Division Researcher,
Theoretical and Computational
Chemistry Initiative (TCCI),
Institute for Molecular Science,
National Institutes of Natural Sciences

Interviewer:

Yasushi Shibuta

Associate Professor,
Department of Materials Engineering,
Graduate School of Engineering,
The University of Tokyo

On September 1, 2014, a new player emerged in the world of quantum chemistry calculations, in the form of a new program that was released on the Internet under an open source license. Its name: Scalable Molecular Analysis Solver for High performance computing systems, or SMASH for short. The field of quantum chemistry calculations already has programs such as Gaussian and GAMESS that hold a major share of the market, and these programs have continued to evolve by incorporating the knowledge and experience of researchers and engineers around the world. That makes it particularly surprising that SMASH was developed and ultimately released through the tireless efforts and passion of a single researcher. That researcher is Kazuya Ishimura, and in this issue we spotlight the work that led to the achievement of SMASH.

Quantum chemistry calculations in the many-core era

As suggested by its official name (Scalable Molecular Analysis Solver for High performance computing systems), SMASH is characterized by the ability to perform electron state and structural optimization calculations as routine work on computers ranging from PC clusters (made up of PCs equipped with scalar CPUs) up to the K computer. In quantum chemistry calculations, approximations based on chemistry and physics knowledge are introduced to the Schrödinger equation — which cannot be solved analytically with the exception of hydrogen and some other atoms — in order to determine the electron distribution of molecules. Specifically, by entering the atomic orbitals (electron distribution of the atom) and coordinates and performing Hartree-Fock calculations (the most basic calculations), it is possible to determine the molecular orbitals (distribution of electrons in the molecule) (Fig.1). The quantity of calculations generally increases in direct proportion to the cube (or, in the case of highly precise calculations, the fifth power or more) of the number of atoms. For this reason, acceleration and parallelization of calculations are essential.

SMASH combines the Pople-Hehre method, which rotates the coordinate axis and reduces the quantity of calculations, with the McMurchie-Davidson method, which uses a recurrence equations to efficiently determine high orbital angular momentum terms. This makes it possible to perform the high-speed atomic orbital 2-electron integral calculations that are performed in almost all quantum chemistry calculations. In addition, redundant coordinates that use bond length, angle and torsion angle information are introduced to reduce the number of geometry optimization cycles, resulting in a more utilitarian program. In actual large-scale parallel calculations on 100,000 CPU cores of the K computer using SMASH, a 50,000 times increase in speed and execution efficiency of 13% were achieved in B3LYP energy calculations for a bilayer graphene molecule $(C_{150}H_{30})_2$ consisting of 360 atoms (Fig.2). In terms of single-node calculation performance, the Hartree-Fock energy calculation for Taxol ($C_{47}H_{51}NO_{14}$) molecule was 40% faster compared with GAMESS.

SMASH represents a ray of light in the large-scale parallel computation of the electron state of enormous molecules, which up to now has been considered to be very difficult. There are high hopes that it will become a basic tool for pursuing efficient development in the many-core era. So what led Dr. Ishimura to decide to tackle the development of a large-scale parallel quantum chemistry calculation program with such enormous potential all by himself?

Background and difficulties faced in the development of SMASH

Dr. Ishimura has been researching quantum chemistry calculations ever since his graduation research days, and he developed the program based on GAMESS. In the process, he has steadily acquired more and more experience in algorithms and program development. His codes of 2-electron integral calculations and the second-order Møller-Plesset perturbation theory (one type of electron correlation calculations) were formally incorporated into GAMESS. But one day, when he tried introducing OpenMP into GAMESS in order to achieve higher parallel performance,

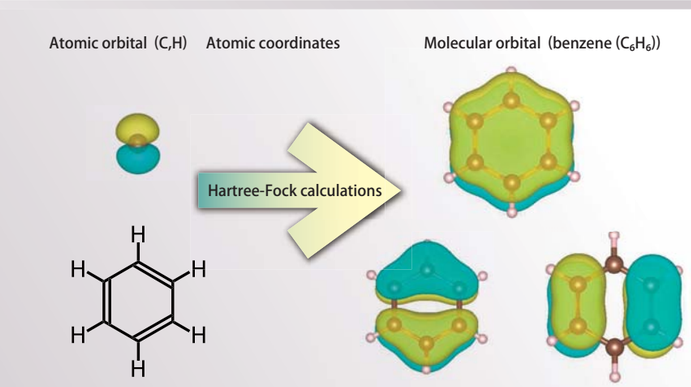
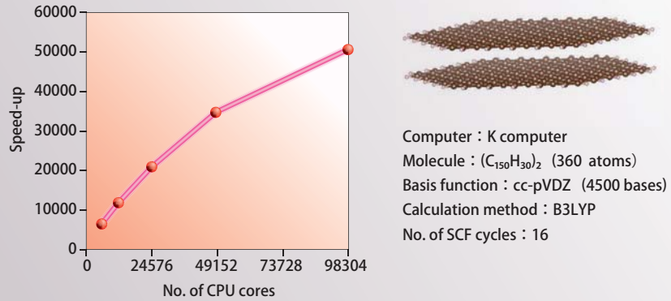


Fig. 1 Quantum chemistry calculations (schematic)

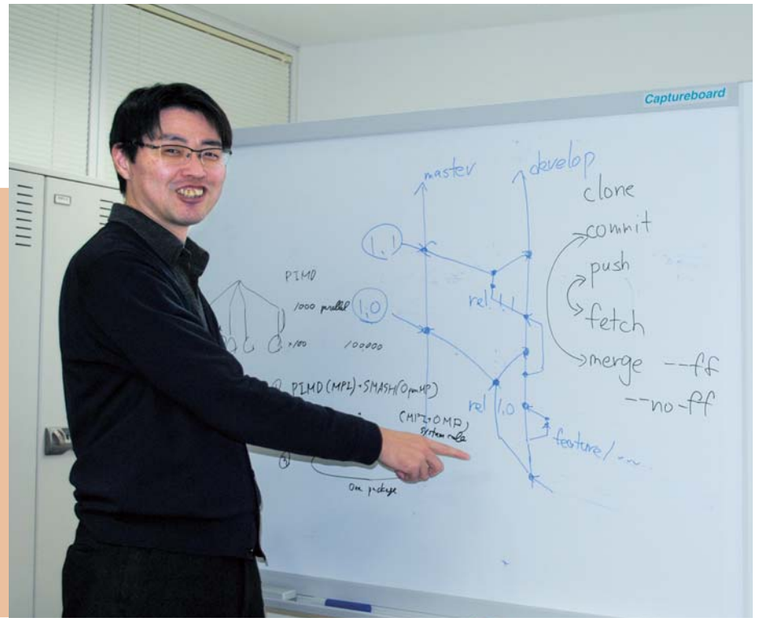


No. of CPU cores	6144	12288	24576	49152	98304
Execution time (seconds)	1267.4	674.5	377.0	224.6	154.2

Fig. 2 Parallel efficiency of DFT energy calculation: bilayer graphene

Kazuya Ishimura

Received a Doctorate of Science from the Graduate University for Advanced Studies and then worked on the development of large-scale parallelization and high-speed algorithm programs for quantum chemistry calculations at Toyota Central R&D Labs., Inc. and Kobe University. The 2-electron integral calculation code that he developed has been incorporated into the GAMESS quantum chemistry calculation program and is still used today as a default routine. Hobby: playing badminton.



he found that major changes were needed, ranging from variable assingments to the basic framework of the program. Ultimately, it became a code that could only perform specific calculations, and naturally it could not be incorporated into the main GAMESS program. Dr. Ishimura became keenly aware of the necessity of the program, which can be performed efficiently in the era of many-core computers. He also realized that there were limits to what could be achieved by development based on existing programs. "So I thought it would ultimately be faster for me to develop a program by myself, from the ground up," Dr. Ishimura says. And so he began the full-fledged development of a large-scale parallel quantum chemistry calculation program.

When most people hear the phrase "program development," they undoubtedly picture someone pounding on a keyboard from dawn to dusk. But most of Dr. Ishimura's time is taken up by work with pencil and paper. For him, the process of developing the algorithm through comprehensive consideration of such aspects as developing the form of equations to speed up the program, figuring out the arrangement of multidimensional arrays, designing loops, introducing appropriate approximations and so on is critical. Writing the program itself was not that difficult. On the other hand, even though he was developing SMASH from scratch, he had no idea how it would be evaluated, and that caused him unease and anxiety. The main algorithms had already been published in academic papers, and SMASH was developed to substantiate and make it possible for anyone to freely use those algrorithms. In that sense, developing the program was not an end but a means. So no matter how much time he spent on it as a means to an end, it would be difficult to perceive any output that could be considered an achievement.

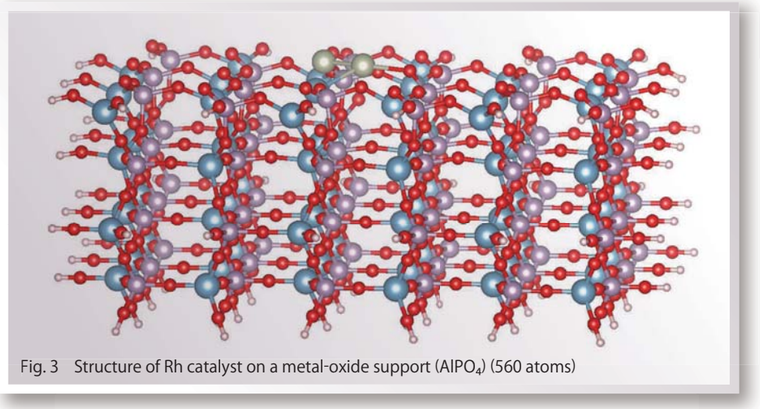


Fig. 3 Structure of Rh catalyst on a metal-oxide support ($AlPO_4$) (560 atoms)

New Encounters and Progress

For a long time, Dr. Ishimura worked all by himself to develop SMASH, and now, slowly but surely, his efforts have begun to bear fruit. Since last year when he released the program, he has been contacted by researchers and developers in many fields who want to use SMASH to start performing quantum chemistry calculations or incorporate some of the functions of the SMASH program in the development of their own programs. Unexpectedly, he also received inquiries from people in the field of computer science regarding the details of the program from a computer specialist's standpoint. Because he had decided to distribute under an open source license and had made the program simple to execute, in a mere six months he had succeeded in attracting people in a wide range of fields and producing new seeds for future growth. Dr. Ishimura has great expectations for the power of SMASH users. "With SMASH, you can use just a bit of the program, or you can plunge in and get deeply involved," he says. "There are a lot of things that need to be done to prepare for a post-K computer world. I'd love for anyone who is interested to get involved in development, and I'm ready and willing to collaborate on a variety of levels."

Meanwhile, SMASH is steadily meeting expectations in terms of quantum chemistry calculation needs. For example, Dr. Ishimura is collaborating with the "Elements Strategy Initiative" of the Ministry of Education, Culture, Sports, Science and Technology, using a quantum chemistry approach to search for alternative metals for automobile exhaust catalysts. In quantum chemistry calculations for metal-oxide supported catalysts, it is thought that a size of at least several nanometers will be needed to ensure that cluster size will have no effect on the properties of the support and catalyst. Dr. Ishimura has already performed electronic state calculations for a Rh catalyst on an $AlPO_4$ support consisting of 560 atoms (Fig.3). If more and more of this type of research is accumulated and that combined with computer support enables alternative metal catalysts to be designed, it will greatly reduce the experimental cost involved in catalyst development, and this will make a tremendous contribution to the automobile industry in particular. It is only natural that there are such high hopes for SMASH, which makes possible large-scale parallel quantum chemistry calculations.

Application SPEC Sheet [SMASH]	
Code Name	SMASH
Method / Algorithm	Quantum chemistry calculations (Hartree-Fock, DFT, MP2 methods)
Overview / Features of Code	It is capable of calculating energies and coordinates of nano-sized molecular systems with high parallel efficiency. The input format and the program strucutre are simple. It is easy to extract frequently used routines, such as 1- and 2-electron integral calclations.
Materials for Simulation	Molecules and clusters which consist of up to 1,000 atoms
Development Leader	Kazuya Ishimura
Developers / Developing Institutions	Theoretical and Computational Chemistry Initiative, Institute for Molecular Science
Development Period	3 years
Development Language / Number of Lines of Source Code	Fortran90/95, 75,000 lines
Operating Environment	K computer, FX10, Intel CPU machines (Intel, GNU, PGI compilers)
Parallelization Method	MPI and OpenMP
Status of Parallelization	50,000 times speed-up on 100,000 CPU cores
Software Release	Distributed at http://smash-qc.sourceforge.net/ under the Apache 2.0 open source license
Related / Competing Applications	Gaussian, GAMESS, NWChem, NTChem, GELLAN

Researcher Training in the Post-K Computer Era

Up to now, Dr. Ishimura has developed SMASH all by himself. But in a post-K computer era, he thinks program development will have to be a team effort. To that end, he is actively providing opportunities to train young people. At a Young Researcher Technical Workshop that Dr. Ishimura organized two years ago, the participants were divided into groups, and each group applied a different fine-tuning to the program based on the profiler data from programs brought in by the participants. The workshop produced visible achievements: reportedly some 20% of the participants achieved a 30% or better performance in computing time as a result of fine-tuning and algorithm review. On the other hand, many of the participants faced the same problems and were stuck on the same points. Accordingly, Dr. Ishimura did not merely seek to improve the skill level of the individual participants but instead provided an environment in which they could pool their knowledge of compiling and fine-tuning. In this way, he focused on working to improve the overall level of the young people in the field.

There are many similarities between developing a software program and training the next generation of young people. Much of the work is done in the background, and a lot of time and effort is required before visible results are produced. It may be because Dr. Ishimura has had the experience of working steadily to develop a software program that he is able to train the next generation using what is, in a sense, a natural process. "It would make me happy if young people would study SMASH just as I once used GAMESS to study the basics of quantum chemistry calculations," he says. One senses that there is a weight behind these words.

And the acronym SMASH? That comes from the world of badminton, Dr. Ishimura's hobby, which he still practices once a week. Like the shuttlecock in the SMASH logo, we hope SMASH will fly swiftly across the front lines of the post-K computer era.

◆Interviewer's Postscript

Yasushi Shibuta

Through this interview, I realized that there are many points in common between program development, in which enormous amounts of time and effort are required before visible results can be obtained, and the training of the next generation of researchers. As a young university professor, I struggle daily with the question regarding the education of undergraduate and graduate students. It was very inspiring and a great opportunity for me to see the tireless efforts and passion devoted to program development by Dr. Ishimura.

6th Visiting Our Graduates

Graduate :
Shunsuke Kirino
Research and Development Office
ACCESS Co., Ltd.

Received his Ph.D for research conducted at the Institute for Solid State Physics of The University of Tokyo, using the time-dependent density-matrix renormalization group method to conduct condensed matter theory research into nonequilibrium transport phenomena in a quantum dot system, dielectric breakdown of Mott insulators and other topics. Joined ACCESS Co., Ltd. in 2011.

Using Programming Technology Accumulated Through Research

For this sixth installment of "Visiting Our Graduates," Ayaka Kuroki, a Ph.D candidate at Graduate School of Engineering in The University of Tokyo, visited Shunsuke Kirino, who works as a software engineer at ACCESS Co., Ltd. Kirino is in his fourth year at the company and is currently a technology leader leading a team of young people who are working on new projects.

Interviewer :
Ayaka Kuroki
3rd year Ph.D student majoring in chemical systems engineering
Graduate School of Engineering,
The University of Tokyo

Majoring in theoretical chemistry and computational chemistry. Became attracted to the work of a researcher and gained experience in museum administration and exhibit creation at the university museum, and was also involved in creating scientific content as a visual designer, working to communicate the language of researchers to a wide variety of people.

Learning the Joy of Programming at Graduate School

Kuroki : As I understand it, you went from conducting research in theoretical condensed matter physics to working as a software engineer. Were you always good at programming?

Kirino : Actually, up until my first year in the Master's program, I had done almost no programming. In my laboratory there was an expert in a numerical calculation method known as the density-matrix renormalization group, and that person became my teacher.

Kuroki : Was it then that you began to be interested in programming?

Kirino : Yes. I found it really interesting to be able to use the computer to accomplish things that I had not been able to do up to that time. In the context of physics, you could say I devised and mastered a new calculation, or I became aware of a new phenomenon.

Kuroki : Was there something along the way that made you realize that becoming an engineer was one of your options?

Kirino : It wasn't a sudden shift. It was the fact that I became interested in programming. It was after I'd been programming for about two years, at the beginning of the second year of my doctoral program.

Kuroki : Are the programming language and libraries that you used in your research different from the ones you're using in your work?

Kirino : Yes, they're completely different. But ultimately they're basically the same in terms of figuring out how to make the program faster and more concise. So what I did before is proving to be very useful.

Naturally, it's on a large scale, and when you have other people working with you, readability is the most important factor. And supposedly the maintenance costs in the course of ongoing use — revising the software, adding functions and so on — are greater than the initial cost of creating the software. So it's crucial to reduce maintenance costs, and for that purpose the code has to be designed well — it has to be easy to read and easy to revise.

Creating the "Behind the Scenes" Part of the System

Kuroki : Could you tell us a little about your current job?

Kirino : The products made by ACCESS are data network solutions for browsers, information appliances, smartphones, electronic publishing systems and so on. For example, we create chat and teleconferencing functions for company use, billing functions, and server system functions for smartphone notification, which are available to multiple applications as common functions. Recent sensor device innovations are increasingly focusing on sensor connectivity with the cloud, so we are readying services that process information received from sensors as available common functions.

A single system is normally made up of multiple components that work together. For example, a smartphone application has a component for receiving transmissions from smartphones, and it transfers the received data to and from another component, where it's subjected to some type of processing and then a response is issued. We create these kinds of "behind the scenes" components.

Kuroki : "Behind the scenes?"

Kirino : Yes. In the case of a chat tool for company use, we determine the specifications for data transmission and receipt — for example, the type of information we display on the user interface or the right timing for sending notifications, etc. — and then we create the program.

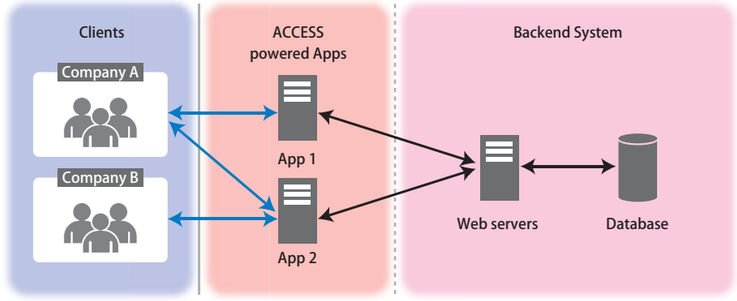
Kuroki : It seems very systematic. So even though you use the term "user interface," you're not trying to predict human behavior.

Kirino : No, we create the components for machines to talk to one another. These aren't the components that the user comes into direct contact with, so in that sense it's behind the scenes.

Right now I'm in the research and development department, so I'm working to build and operate systems for common use that employ various types of in-house applications. The functions that are used in common within the company — for example, user management and sending email and so on — are designed to be common components that eliminate the need to develop components for every single application. And, actually, right now more and more people are gradually beginning to use the system that we've developed. So I feel it's particularly rewarding to design a program that works behind the scenes.

Kuroki : Have you never dreamed of playing a more center-stage role?

Kirino : In a sense, I think I began this work by deciding that a "behind the scenes" role would be better. That's my individual preference anyway, but there are many areas in which the technology is more interesting behind the scenes. For example, making it possible for the program to handle large-scale requests, to accept massive quantities of data for search, to continue running even if a single server crashes, and so on.



Outline of building a server system.

Becoming a Technology Leader in the Third Year After Joining the Company

Kuroki : Have you learned a lot since you joined the company?

Kirino : Yes. I'm programming on the server side now, and I have never worked with servers when I was in graduate school. After I joined the company, I went through training, and then I started working on an e-book project, and I studied it there. After two and a half years, I switched to my current project, and I studied a lot of things there as well.

Kuroki : So you're learning about new technologies and new research as well.

Kirino : That's definitely necessary. It's hard to keep up with the cutting edge of computer science, but by the time you get to the doctoral program stage, you realize that there are a lot of very important things written in academic papers, so you have to read them to catch up.

Kuroki : What's the age range of the people in your company?

Kirino : There are four members in my team, and I'm the oldest. The team members range in age from 31 to 26. It was about the same at my previous team.

Kuroki : I understand you're the team leader.

Kirino : When my current project was first launched, I was appointed as the leader. The environment at my company encourages even young people to be free to do what they want, and I think I was very lucky to be able to join the project as a leader even though I was only in my third year at the company. Right now I'm trying to figure out what type of work to have the other three members of the team do, by trying to draw them out about what kind of work they really want to do, and working to raise their skill level by assigning tasks that are slightly above their technical level and so on. I'm finding that it's not that easy. My former team leader was very good at creating the appropriate degree of distance between himself and the team members, and he sensed when I was feeling frustrated. It's really important to be motivated to do your work.

I Want to Create Something that Many People Feel is Useful

Kuroki : Now that you're able to program and you can do various kinds of work, what do you think you want to do from this point on?

Kirino : I keep saying "behind the scenes," but the truth is that I'd like to create products that are used by a lot of people. That was also my motivation for joining this company. For instance, the development of a smartphone browser meant that people no longer needed to carry around a PC to be able to access the Internet from anywhere. Recently, the appearance of smartphones and a wide variety of applications has changed the way people communicate. I'd like to create something like that, something that changes the way people live and work. I want to create something that is seen as useful by as many people as possible.

Kuroki : Are the products that you're creating in your current job things that can be used by people overseas as well?

Kirino : I don't really sense any national boundaries in the world of the Internet. But in products there are some things that are rooted in the user's culture, so I think we have to be knowledgeable about culture as well.

CMSI Kobe Branch

Tatsuya Sakashita

Researcher, CMSI Condensed Matter Physics Division
Center of Computational Materials Science at the Institute for Solid State Physics, the University of Tokyo

The CMSI Kobe Branch is located at RIKEN Advanced Institute for Computational Science (AICS), which is the home of the K computer, and serves as the center of activity for researchers using the K computer, including researchers in the fields of condensed matter physics, molecular science, and materials science. Here, Tatsuya Sakashita talks about the activities carried out at the Kobe Branch.

The Closest Research Center to the K Computer

Under the Institute for Solid State Physics at the University of Tokyo, the CMSI Kobe Branch was established in April 2011 as a branch of the Center of Computational Materials Science. The branch occupies a room having closest proximity to the K computer on the 5th floor of AICS, which is located on Kobe Port Island.

While it is now possible to log in and use the K computer from anywhere, only researchers in AICS had access during its initial trial period that lasted until September 2012. At the time of my appointment there, CMSI researchers from all over Japan congregated at the CMSI Kobe Branch and were immersed in research work day and night.

The CMSI Kobe Branch has work spaces for seven visiting researchers and a fourteen-seat conference space equipped with a large monitor and videoconferencing system that is freely available to all those in residence. This space has been used for computational materials science seminars and has served as a receiving site for CMSI distance learning (refer to Torrent No.8) and seminars. CMSI Kobe Hands-on and TOKKUN! (application advancement training camp) introduced below have also been held here.

Hands-on Workshops and TOKKUN! for Application Promotion and Advancement

CMSI not only conducts leading research on computational materials science through large-scale simulations on the K computer, but also actively publicizes its achievements in application development to promote these applications both domestically and overseas (refer to the article on MateriApps in Torrent No.8). As a part of these efforts, CMSI has held a monthly workshop (Kobe Hands-on) at the CMSI Kobe Branch. In these workshops, participants use cluster workstations provided for both visualization and post-processing of computational data from the K computer to learn operational procedures while actually running programs.

To date, the workshops have covered various applications developed at CMSI, including ALPS, OpenMX, xTAPP, Rokko, feram, FMO in GAMESS, FU, MODYLAS, and SMASH, as well as a version control system, which is now an essential tool for software development. With each installment, the workshops have become richer in content for beginners, intermediates, and experts (developers) with varying levels of difficulty and purpose. The workshops also have a benefit for developers in that they are able to attract new users to their applications and receive feedback, including suggestions on the need to add functionality and to make the software more user-friendly. The events have also provided opportunities for developers to integrate applications that have been developed independently.

TOKKUN! is a training camp at which participants can bring their own programs and perform tuning at the serial and parallel levels for successful application to the general use category of the K computer. Participants in TOKKUN! receive advice from CMSI division researchers, system engineers from Fujitsu, and researchers from the Research Organization for Information Science and Technology. This camp also offers a great opportunity to learn from experts while discussing programming with other participants in a relaxed atmosphere. Discussions on how to use applications developed at CMSI, including OpenMX, FMO, and MODYLAS, were introduced in the last installment of TOKKUN!

Members of Kobe branch: Yae Matsushita, Kazuo Kitaura, Taisuke Ozaki, Tatsuya Sakashita, Yuki Yamashita (from left to right).

Integrating Fields through Large-Scale Parallel Computing

In addition to the above events, the CMSI Kobe Branch has hosted Informational Exchange Workshops on K computer and HPCI Supercomputer Use for sharing experiences in performance tuning and application use, CMD® Workshops, and CMSI Young Researcher Technical Workshops as well as the CMSI International Workshops 2013 and 2014 (refer to Torrent No.9) that took up the topic of tensor networks in an event closely connected with particle physics, nuclear physics, and astrophysics. In addition, press seminars for presenting results of simulations on the K computer to a general audience and TCCI (Theoretical and Computational Chemistry Initiative) seminars were planned and carried out with AICS.

As supercomputers enter an age of massively parallel computing, collaboration among researchers of hardware, software, physics, chemistry, and mathematics, among other fields, will be essential to develop methods of high-speed, high accurate calculations and to create user-friendly software. AICS is the first research institute in Japan to gather researchers of so many disciplines in one location. We will continue to develop the CMSI Kobe Branch as a new testing ground for integrating fields through large-scale parallel computing by promoting exchange with neighboring researchers in computational science, including the AICS research teams, and utilizing the nationwide CMSI human resource network in computational materials science.

Message from the Director of the CMSI Kobe Branch

Taisuke Ozaki

In his best-selling book entitled Capital in the Twenty-First Century, Thomas Piketty predicts that the rich will only get richer in a capitalist society. While I only have a superficial understanding of his work, it seems to me that the same situation is occurring in the development of simulation software. In Japan, software development tends to be considered a side business, and I have heard few successes of producing de facto standard software in scientific and engineering fields of Japan. The development of de facto standard software normally takes a period of twenty years or more, and once relative merits of software imperceptibly appear, information and personnel become consolidated and development progresses at an accelerated pace. Any distinctions that emerge at this time are already past the stage of correction and can lead to a gulf that takes more than ten years to bridge. At CMSI, we precisely assess the situation, discuss what needs to be done to develop software, and take suitable steps to aid our developers. It is our hope that these actions will bear fruit in the development of world-leading software.

K Computer News

"Flagship-2020 Project," a project aiming at development of the post-K supercomputer which becomes succession of the K computer, has started. It is planned that the post-K supercomputer will have many-core architecture using general-purpose CPUs, and realize exa-scale computing* by around 2020. Development of application software for the post-K has also started. For that purpose, 9 top priority research topics have been set from the wide field from basic science to the disaster prevention/environmental problems. For the 5th priority research topic "Development of New Technology for Highly-efficient Energy Creation, Conversion/Storage, and Use," 9 institutions (representative: Institute for Molecular Science) have been selected. For the 7th priority research topic "Creation of New Functional Devices and High-Performance Materials for Next-Generation Industry," 9 institutions (representative: Institute for Solid State Physics) have been selected. From now on, the development of next-generation application software for computational materials science will be advanced in cooperation with computer scientists.

* "Exa" stands for 18th power of 10, 100 times of K.

Profiles of Division Researchers

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

Swastibarata Bhattacharyya

Materials Science Division Researcher

Department of Physics, Yokohama National University

I did my masters in physics from Indian Institute of Technology Guwahati. I received my PhD in the field of material science from Indian Institute of Science, Bangalore. At present, I am working on first principles mapping onto phase field model at Department of Physics, Yokohama National University, Japan.

Ambition

To learn and contribute to the first-principles all-electron mixed basis program TOMBO.

Motivation for applying for the position

To learn development of first principles based theory and code that will be used to study materials properties.

Mission/Role

Phase field methods are very effective in studying the evolution of microstructures in various materials. We want to bridge this empirical method to the first principles based atomistic methods.

Sankar Kumar Deb Nath

Materials Science Division Researcher

Institute for Materials Research, Tohoku University

I obtained Ph.D. from the department of Mechanical Engineering, Bangladesh University of Engineering and Technology, Dhaka, Bangladesh on the mechanics of composite materials. Majored in multi-scale modelling in mechanics of solids and liquids, atomistic simulations of physics and chemistry related problems. Currently I am working on the phase field modelling of Cu, Al and Cu-Al alloys using molecular dynamics simulation.

Ambition

My aim is to investigate the thermodynamic properties of the solid-liquid interface of Cu, Al and Cu-Al alloys.

Motivation for applying for the position

Dendrite structures are formed during the solidification of pure and alloy materials due to the anisotropy of the phase change of the solid-liquid interface. Detailed investigation of the physical and thermodynamic properties of the solid liquid interface are needed by the atomistic approach like molecular dynamic simulations to study the anisotropy of the solid-liquid interface during solidification using the large scale phase field modelling.

Mission/Role

The anisotropy of the solid-liquid interfacial properties of Cu, Al and Cu-Al alloys such as kinetic coefficient, melting point, interfacial free energy etc. will be determined from the project.

Sergi Ruiz-Barragan

Molecular Science Division Researcher

Japan Atomic Energy Agency

Graduated in Chemistry at University of Girona and received the Doctorate in the same university with a exited states and non-stationary processes thesis. Current research with path integrals and QM/MM Molecular dynamics in Shiga's group at JAEA.

Ambition

Provide a new program for doing molecular dynamics and path integrals at the same time that I improve my conception of the molecular movement.

Motivation for applying for the position

Develop new methods for studying dynamics. Chemist is not a static science and I think that we need to understand correctly the movement of atoms and molecules to improve the reaction and obtain greener ways to produce some products.

Mission/Role

To improve the path integral code for QM/MM and use it for study some reactions with the solvent for understand the temperature and the isotope effects in reactions.

Torrent No.11 March 2015

Cover : "A picture is worth a thousand words," it is often said. If you want to explain the results of a simulation, using an image makes it easy for your listeners to understand (particularly when your English is not fluent). But if you simply create a detailed drawing, your listeners may focus on parts of the image that are unrelated to the point you are trying to make, leading to needless misunderstandings. So you should consider your mode of expression carefully. This image shows how methane bubbles accelerate the breakdown of a methane hydrate crystal (which has been color-coded to indicate the distance from the center of gravity), resulting in irregularities on the crystalline surface. The water molecules have been omitted. (CG: Masakazu Matsumoto, Okayama Univ.)

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