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torrent

10^{16} Weave New Materials

Special Feature 1 :

CMSI International Symposium

Tokyo Satellite Workshop
Nagoya Satellite Workshop
Kobe Satellite Workshop

Special Feature 2 : Collaboration between SPIRE

Field 1 × Field 2, Field 2 × Field 5

The 4th CMSI Poster Award

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

Special Feature 1

CMSI International Symposium 2013

Extending the power of computational materials sciences with K-computer

The first CMSI International Symposium was held on October 21 and 22, 2013 at the Ito International Research Center at The University of Tokyo. The theme was "Extending the power of computational materials sciences with K-computer." The conference was held approximately one year after shared use of the K computer began on September 28, 2012. The program centered on presentations of the achievements of research conducted using the K computer, and the discussion focused on the prospects for the new age of materials science ushered in by massively parallel computers.

Achievements of one year of shared use of the K Computer

The Symposium was held along with the following three satellite workshops:
1) CMSI Tokyo Satellite Workshop 2013: Novel Electronic Structure Calculation Method
2) CMSI Nagoya Satellite Workshop 2013: Large-Scale Molecular Simulation for Understanding Molecular Mechanisms
3) CMSI Kobe Satellite Workshop 2013: Recent Progress in Tensor Network Algorithms

Workshops 1) and 2) featured researchers from Japan and other countries who spoke about the achievements of, respectively, RSDFT, a real-space first principles density functional theory (DFT) calculation software program that opened up the development of massively parallel computing in computational materials science through the use of the K computer, and MODYLAS, a software program for conducting molecular dynamics simulations for large-scale molecular systems, and the workshops were held to discuss the future prospects for these programs. Workshop 3) differed from the other two in that it dealt with the field of computational materials science overall and focused on efforts to promote integration with the field of

mathematical science and the establishment of the fundamental building blocks for creating new algorithms. For more information on the individual workshops, see the separate report for each workshop.

The first day of the conference began with a keynote address from Professor Keiji Morokuma (Kyoto University). This was followed by presentations on research achievements by CMSI research group representatives. The second day featured three parallel sessions that were designed to share and go deeper into the issues and achievements raised in the satellite workshops and the presentations by 11 invited speakers from overseas. Through a happy accident of good timing, the symposium was held just after the announcement that the Nobel Prize in Chemistry 2013 had been awarded jointly to Martin Karplus, Michael Levitt and Arieh Warshel "for the development of multiscale models for complex chemical systems" — in other words, for the development of the so-called QM/MM hybrid method. At the beginning of his keynote address, Professor Morokuma spoke about the award-winning research and shared some anecdotes relating to Professor Karplus. Subsequently, he talked about a recent research achievement of his own group, the identification of numerous new reaction mechanisms following an exhaustive search of transition states, and discussed the power that supercomputers have given to computational materials science. It was a very impressive presentation. The invited speakers who talked about research issues in the individual sessions gave presentations on the impressive achievements in state-of-the-art research, and these were followed by lively debates and exchanges of information.

How will software development change?

One of the important research topics in computational materials science is the development of new calculation theories and calculation models that can expand the scope of applicable targets and phenomena. The QM/MM hybrid method was first proposed in the 1970s, but (it is my impression that) it was not until the mid-1990s that it rapidly came into widespread use. This is because of the contributions of many researchers that resulted in improved calculation methods and software, as well as because of increased computer performance. In addition, the development of the field of life science meant that, for the purpose of identifying the functions of biomolecules, there was an increased demand for "observation" through simulations of the structure and dynamics of molecules inside living organisms (in aqueous solutions) that are difficult to observe through experimentation. As shown by this and other examples, a number of conditions must be met in order for a calculation model to be recognized as useful and to come into widespread use. But in many cases if one waits to begin research until these conditions are met, it will be too late. The revolutionary computation performance achieved by the K computer is expected to serve as the catalyst for producing next-generation calculation models and software, but continuous efforts based on a long-term perspective and an organization to support

G. Klimeck

these efforts will be indispensable in order to make this a reality.

One of the missions of CMSI is to disseminate and promote the software that is developed in projects. To this end, CMSI puts a great deal of effort into promoting activities such as the use of the MateriApps portal site, the holding of software workshops, software distribution and so on. In this context, the presentation on nanoHUB by Professor Gerhard Klimeck (Purdue University) was impressive. nanoHUB was developed between 2002 and 2010 as a project of the U. S. National Science Foundation (NSF). It is a system designed to enable the sharing in cyberspace of simulation software, presentation tools, teaching tools and so on in the fields of nano science and nanotechnology, and it is already in use worldwide. As an evolution of this type of system, I imagined

V. Schauer (left) and J. Enkovaara (right, CSC-IT Center for Science, Finland), discussing during the coffee break

(although possibly I am getting too far ahead of myself here) that we are approaching the point at which a system will be developed wherein, after it has been decided what should be calculated, the input data will be (semi-)automatically generated and then numerous / large-scale calculations will be executed through cloud computing, and subsequently the vast quantity of calculation results will be (semi-)automatically output in the form of academic papers and reports. (If this day comes, academic papers that are based on calculations alone may come to have no meaning.) Even if such a time comes, the development of new calculation models and calculation programs for these models will still be needed, and this will continue to be an important task. Apart from theoretical work, however, the development of calculation models and programs may be conducted by software companies, or if the market is not large enough, this may be done by volunteer groups of specialists in the fields of information science, mathematical science and computational materials science and the results released as freeware.

(Kazuo Kitaura : Graduate School of System Informatics, Kobe University)

Prgoram

10/21 Monday

10:00 -18:00 • Keynote : Keiji Morokuma (Kyoto Univ.)
• Invited Talk : Shiro Sakai (The Univ. of Tokyo)
• CMSI Priority Research Topics using the K computer
18:00 -20:00 • Banquet (Event: KAGURA by KARAS and Hideo)

10/22 Tuesday

Special Topics "New Science Developed by New Massively Parallel Computation Approach"

9:00 -12:20 • Invited Talks :
Glen Evenbly (Caltech), Weitao Yang (Duke Univ.),
Gerhard Klimeck (Purdue University)
12:20 -15:00 • Parallel Sessions:
Recent Progress in Tensor Network Algorithms
Large MD Simulation
Novel Electronic Structure Method
15:15 -17:15 • Invited Talks:
Jan Rossmeisl (CAMD), Blazej Grabowski (MPIE)

Tokyo Nagoya Kobe

Interview with Foreign Researchers

We asked some foreign researchers who attended the satellite workshops about their impression of the workshops and Japanese young researchers.

Volker Schauer

University of Stuttgart, Germany

Q1: Please tell us about your research briefly.
In my research, I create algorithms in order to calculate the electronic structure of clusters of atoms with the finite element method. In general such localized basis functions provide advantages in the efficiency on modern parallel hardware architectures.

Q2: How did you feel when you attended the satellite workshop in Tokyo?
The satellite meeting was an excellent chance to share my research ideas with other young international researchers, working on similar topics.
Especially the speakers and topics were thereby well choosen to give a nice overview over the newly developing real space methods in electronic structure calculations - so I enjoyed the seminar very much.

Q3: What is your impression about young researchers in Japan during your stay?
Young researchers seem to find an excellent accademic environment in Japan, which provides various opportunities, as for example it is done by the CMSI.

Mikael Lund

Lund University, Sweden

Q1: Please tell us about your research briefly.
In the statistical mechanical group at Department of Theoretical Chemistry in Lund, we study materials such clay, cement, and cellulose fibres. We are also interested in more bio-oriented applications such as protein-protein interactions. Our main tools are Monte Carlo and atomistic molecular dynamics simulations as well as classical polymer density functional theory.

Q2: How did you feel when you attended the satellite workshop in Nagoya?
Due to the relatively small number of people at the Nagoya meeting, the discussions were informal and much more lively than at bigger conferences. This, combined with a diverse range of speakers of all ages and from different disciplines, made this meeting a very awarding experience for me and led to a collaboration with Kyoto University.

Q3: What is your impression about young researchers in Japan during your stay?
This was my first time in Japan and to be honest I didn't quite know what to expect other than high scientific quality. From the two meetings I attended I was very impressed by the level of research by the young researchers — especially the concerted efforts to maximize performance on the K computer.

Glen B. Evenbly

California Institute of Technology, USA

Q1: Please tell us about your research briefly.
My research is focused on the development and application of tensor network methods for the efficient simulation of quantum many body systems. In particular, I do a lot of work with a class of tensor network known as the multi-scale entanglement renormalization ansatz, and study its application to quantum critical systems.

Q2: How did you feel when you attended the satellite workshop in Kobe?
The Kobe meeting was attended by a variety of recognized figures from the tensor network community, both locally and from abroad. It was interesting to learn of the latest developments happening in tensor networks.

Q3: What is your impression about young researchers in Japan during your stay?
The young researchers I met in Kobe seemed enthusiastic and eager to learn, I had good experiences discussing my research with them, and learning of their own research.

Vladimir Kazeev

ETH Zurich, Switzerland

Q1: Please tell us about your research briefly.
I study the possibility of finding and representing solutions of large-scale problems in terms of relatively few parameters with the use of so-called tensor decompositions. The aim is achieving highly adaptive representations of this kind in computations and grounding them mathematically.

Q2: How did you feel when you attended the satellite workshop in Kobe?
The meeting was very inspiring in terms of the location, scope and participants. In the heart of the Japanese high-performance computing facilities. On important current topics in the numerical simulation of quantum systems. With experts of the field and eager young researchers.

Q3: What is your impression about young researchers in Japan during your stay?
The work presented by young researchers demonstrates a high scientific level and remarkable diligence. Also, I particularly appreciated the effort they made to let us enjoy an internationally-friendly professional environment on the Japanese soil.

CMSI Tokyo Satellite Workshop 2013

Novel Electronic Structure Calculation Method

Implementing a new method for calculating electron states

This satellite workshop was held over two days, October 18 and 19, 2013, at the Faculty of Engineering Building 6 on The University of Tokyo Hongo Campus. The gaussian base method is widely used, particularly in the field of quantum chemistry, as a way of implementing non-empirical electron state calculation methods, while the plane wave base method is widely used in the field of solid state physics. In addition to these two mainstream methods, new methods such as the real-space finite difference method, the finite element method and the wavelet base method have been used increasingly in recent years to implement electron state calculations. One reason for this is the need to accommodate the massively parallel use of computers. For example, unavoidably fast Fourier transformation is needed for the band calculation codes for solids that use the plane wave base method, and there have been concerns regarding whether this can be accommodated by massively parallel computers. Moreover, gaussian functions and the plane wave base method are tightly constrained by the boundary conditions for the calculations, and this was a major restriction when modeling surfaces, interfaces and even more complex materials.

This satellite workshop featured presentations on the real-space finite difference method, the finite element method and the wavelet base method by six researchers from Japan and three researchers from overseas. The goal was to discuss the characteristics of each method and deepen understanding, and with any luck to appropriate technologies that can be used in each code. The presentations on the real-space finite difference method were given by myself, Tomoya Ono, Masashi Noda and Shunsuke Sato from Japan, and by Jussi Enkovaara, one of the developers of the GPAW package, from overseas. The presentations on the finite element method were given by Eiji Tsuchida from Japan and Volker Schauer from overseas. The presentations on the wavelet base method were given by Hideo Sekino from Japan and Luigi Genovese, one of the developers of BigDFT, from overseas. The workshop made clear that each of these methods has elements that overcome the aforementioned problems, and moreover that they all possessed adaptivity, something that previous methods did not offer.

L. Genovese (CEA Grenoble, France), giving his invited talk

The path to all-electron calculation

Adaptivity is a technique in which calculation points can be concentrated in locations with dramatic changes in functions, for example near the atomic nucleus, while calculation points are only sparsely distributed in areas that experience more gradual change. Promoting the use of this technique makes it easy to handle things extending to the electrons in the core, in other words enabling "all-electron calculation." The concrete implementation of this technique is being promoted in the finite element method and the wavelet base method. It is known that gaussian functions do not form a complete system in mathematical terms, and the base functions tend to become linearly dependent on one another, so it is difficult to increase the precision of the system. The presentation by Sekino, in which he said that "wavelets may become a new base function for quantum chemistry calculations that form a complete system," was impressive.

The current mainstream methods — gaussian functions and the plane wave base method — were developed at a time when computers themselves were in the process of being born and maturing. Compared to that time, modern computers have been completely transformed. Algorithms that were developed in the early stages are becoming incompatible with the most recent computer architectures. Even so, it is not possible for us to switch over to other methods immediately. Even the simple implementation of a new technique requires enormous amounts of time and labor. It has been said that the introduction of Python succeeded in reducing the development time for GPAW and other packages. But undoubtedly there are some people who are reluctant to spend the time needed to become familiar with the use of Python. As computers evolve to have greater and greater complexity, the costs of program development will increase greatly as well, and this is a frequent topic of debate in efforts to achieve exabyte computing. This satellite workshop served to make us consider this issue once again. To be honest, however, the answer to the question of what should ultimately be done about it has not yet been discovered.

(Jun-ichi Iwata: Graduate School of Engineering, The University of Tokyo)

CMSI Nagoya Satellite Workshop 2013

Large-Scale Molecular Simulations for Understanding Molecular Mechanisms

Researchers from Japan and other countries introduce the latest development trends

The satellite workshop of the CMSI International Symposium held in Nagoya October 17 - 19, 2013 featured presentations on the latest research achievements by up-and-coming young researchers involved in state-of-the-art research in Japan and other countries, on such topics as molecular dynamics (MD) and QM/MM researches using massively parallel computers and the study of protein, lipid membrane and other biomolecules. Researchers at home and abroad who are developing the software needed to execute calculations for these large-scale systems also explained the latest trends in software development.

The venue for the workshop was the Nagoya Urban Institute, located on the 14th floor of a high-rise building adjacent to Kanayama Station. It was an impressive setting that afforded a panoramic view of Ise Bay. As the venue can be accessed directly from Chubu International Airport (Centrair) on the Meitetsu train line without the need to change trains, and it is also not far from JR Nagoya Station, it was undoubtedly convenient for not only the invited overseas guests as well as the researchers who came from other parts of Japan to attend.

This satellite workshop featured three invited guests from overseas countries. Qiang Cui (University of Wisconsin, U.S.A.) is conducting intensive research into the chemical reactions of biomolecules using QM/MM calculations. Mikael Lund (Lund University, Sweden) is conducting large-scale simulations of protein molecule mixing using a unique coarse graining model that considers pH. Tzu Ray Shan (Sandia National Laboratories, U.S.A.) was one of the members of the team that developed Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS), the well-known general molecular dynamics calculation software for parallel computing use. (Weitao Yang, who is well-known for his work on the density functional theory, participated in the international symposium at The University of Tokyo only.) The speakers from Japan were Mitsunori Ikeguchi (Yokohama City University), who has pursued extremely intensive research into proteins and other biologically relevant molecules; Nobuyuki Matsubayashi (Kyoto University); Hideaki Takahashi (Tohoku University); Takefumi Yamashita (The University of Tokyo); Wataru Shinoda (Nagoya Universiry), who is working to develop coarse graining models; Tatsuya Ishiyama (Tohoku University), who conducts wide-ranging research on interfacial systems; and Kazushi Fujimoto (Ritsumeikan University).

Attendants of the workshop. In front row, from left: Kojima, Ikeguchi, Andoh, Junk, Yamada, Ishiyama. In back row, from left: Yoshii, Hayashi, Matubayasi, Lund, Shan, Cui, Shinoda, Okamoto, Takahashi

M. Lund, giving his invited talk

All of the participants are engaged in cutting-edge research that makes use of the breadth of latitude afforded by massively parallel machines and broadens the horizons of research, and the discussions at the workshop were lively.

Current state of increased speed and use of massively parallel computing for MD calculations

One of the main topics of the workshop was increased speed and the use of massively parallel computing for molecular dynamics calculations. Jaewoon Jung spoke about the GENESIS program being developed at RIKEN, Tzu Ray Shan spoke about LAMMPS, which was developed by Sandia National Laboratories in the United States, and Yoshimichi Andoh spoke about MODYLAS, which was developed mainly by the Okazaki Laboratory at Nagoya University. The workshop was an excellent opportunity to learn about the current state of performance and other aspects of state-of-the-art MD calculation software that is designed for massively parallel computing. In addition, Kenji Yasuoka gave a very interesting talk on efforts to increase the speed of MD calculations using special purpose computers, which also touched on the history of development.

On both of the evenings during the period of the workshop, the participants took the opportunity to enjoy themselves and deepen friendship while sampling Nagoya regional specialties that included the famous tebasaki (chicken wings) in the area around Kanayama Station.

(Noriyuki Yoshii, Nagoya University)

CMSI Kobe Satellite Workshop 2013

Recent Progress in Tensor Network Algorithms

Tensor network—a new framework for computational science

A variety of calculation methods are used in computational materials science simulations, including the first-principles density-functional method and the molecular dynamics method. These algorithms have been developed and improved in order to quickly and accurately solve Schroedinger equations for electron states and Newtonian equations that describe molecular motion. There are also known algorithms that can be applied to a wider range of general problems, rather than to specific problems and basic equations. It might be more appropriate to call the Monte Carlo method, for example, "framework" that is used to solve complex problems on a computer in a realistic amount of time, rather than calling it "calculation methods."

Tensor networks have attracted a great deal of attention in recent years as one such framework. To rigorously express the state of a system that obeys quantum mechanics, an exponentially large number of variables with respect to the size (volume) of the system are needed. Even the world-largest supercomputer would be completely inadequate in terms of memory capacity and calculation capability. In the meantime, in an actual system the enormous number of variables would not all be equally important. Tensor networks are able to express the state of the system as the product of low rank tensors (generalization of matrices), which enables these networks to express accurately and at a low cost only the sections that contribute to the properties of the system.

In the K computer tour

"Identifying only what is important in the midst of enormous degrees of freedom and describing the essence of a system" is an approach that is common to all science.

Kobe, a place of interchange between disciplines

The CMSI International Workshop 2013 "Recent Progress in Tensor Network Algorithms" was one of the satellite workshops held as part of the CMSI International Symposium 2013. The workshop was held for three days, October 16-18, 2013, at the RIKEN Advanced Institute for Computational Science (AICS) in Kobe, Japan. AICS is where the K computer is located, and it is the place where the CMSI Kobe Division as well as the divisions of five strategic fields are concentrated. It is therefore the most appropriate venue for a workshop such as this that transcends the boundaries between different fields.

The workshop featured presentations ranging from basic tensor network theory to applications in a wide variety of fields such as quantum chemistry calculations, strongly-correlated quantum systems, phase transition and critical phenomena, photo-induced phase transition, the relationship between black holes and tensor network renormalization groups, machine learning, data mining and wavelets. The specific topics included entanglement (quantum correlations) in the ground state of many-body quantum systems, matrix product states, density matrix renormalization groups, Projected Entangled Pair State (PEPS) and Multi-scale Entanglement Renormalization (MERA). There were also many intriguing lectures from a computer science perspective, on topics such as optimization of the computational cost of simulations, detailed analysis of tensor network accuracy, large-scale parallelization using the K computer, and the development of tensor network libraries.

The workshop was attended by more than 40 persons, greatly exceeding the number of participants that had initially been expected. There were ten participants from overseas including some who were invited speakers, and each day there was an air of excitement in the AICS seminar room on the first floor where the lectures were held. A significant period of time had been allotted for questions and answers after each lecture, but even afterward during the break periods the spirited debate continued. In between the sessions, participants also visited the K computer (Fig.2) and enjoyed lunch in the Kobe Kachoen (flower and bird) Park, and there was also a get-together where participants could establish closer relationships as they enjoyed the view of the Akashi Kaikyo Bridge at night.

V. Kazeev (center) in his invited talk, and G. Evenbly (right)

Tensor networks are a new type of algorithm that has experienced rapid development since the beginning of this century. Both the lecturers and the participants at the workshop were overwhelmingly young, and most of the invited speakers were young researchers in their 20s or 30s. In the poster session, established researchers could be seen posing questions to young researchers in order to take the discussion to a deeper level. The workshop was one that was filled with a sense of purpose that spanned the boundaries between generations and disciplines, and aimed at the further development of this new method. Especially, the workds by G. Chan, "a new framework for quantum mechanics, second only to Feynman's path integral," and R.Orús, "a new language and component for computational science" expressed in their invited talks have left a strong impression on our mind.

(Synge Todo: Graduate School of Science/ISSP, The University of Tokyo)

What We have Learned from Cooperative Phenomena in Complex Biological Systems

Chisa Kamada
Team Member, Planning & Coordination Group,
HPCI Program for Computational Life Sciences, RIKEN

Field 1 and Field 2 Joint Symposium

A symposium entitled "HPCI SPIRE Program Field 1 × Field 2 Symposium in Nagoya University Computational studies of complex biomolecular systems to understand the role of intermolecular interactions" was held on Tuesday, December 17, 2013 in the lecture hall of the IB Building at Nagoya University.

In HPCI SPIRE Field 1, various symposiums and seminars have been held to foster better understanding of the HPCI and computer simulations in life sciences and disseminate our research outcomes and activities for researchers (including those who work in private sector companies) and the general public by dividing the country into six blocks: Hokkaido/-Tohoku, Kanto, Chubu, Kansai, Chugoku and Kyushu/Okinawa. For this symposium, Professor Motonori Ota of the Graduate School of Information Science at Nagoya University, a Field 1 member, served as facilitator. As Nagoya University has many researchers who are studying biomolecules in Field 2, Professor Ota suggested the idea of holding a joint symposium with Field 2. In response, Professor Masaki Sasai of the Graduate School of Engineering at Nagoya University, a Field 2 member, also agreed to serve as facilitator, and the symposium was held by collaboration t between Field 1 and Field 2.

Exploration of life phenomena and the role of high-performance computing

The keywords for the symposium were complex systems, interaction and high-performance computing. At the opening session, Professor Ota stated the main point of the symposium as follows: "The interaction between molecules holds the first key to the understanding of cooperative phenomena in complex biomolecular systems." He followed this up by saying, "An issue we should be resolved is understand how increasing amount of data and its calculation by high performance computing link to qualitative understanding of life phenomena." Each of the speakers also gave presentations on various research topics that were in line with this basic theme of the symposium.*

To me, the presentations were fresh and inspiring. This was because of the effort to identify the truth in the very minuscale movements (or perhaps we should refer to them as behavior) of hemoglobins and nucleosomes and so on, which we all learned about in biology classes in junior high and high school, and because of the diverse approaches of many researchers studying the same research topic. Hemoglobin, for instance, is known to transport oxygen in the blood with binding iron (heme). However, a close look at this mechanism reveals that, once the first heme subunit binds oxygen molecule, binding the second, third and fourth oxygen molecules gets progressively easier and easier. Conversely as well, when the oxygen is released, a cooperative phenomenon known as the allosteric mechanism appears and causes the oxygen to be separated in order the first time, the second time and so on. Extremely complex calculations are needed to understand these microscopic mechanisms, making us realize again the major role played by high-performance computing.

Collaboration between computer simulations and experiments

Another impressive point in the symposium was the explanation given by Visiting Professor Yuichiro Maeda (Structural Biology Research Center, Nagoya University), Ota's collaborative researcher, during the question and answer period following Professor Ota's presentation. The catalyst for the decision of these two professors to begin collaborative research was the fact that, in order to pursue their research, they needed to go back and forth between conducting experimental measurements in order to investigate the structural dynamics and then combining these results with the results of computer calculations. "Collaboration between computer simulations and experiments" is a phrase that is frequently used by researchers in conversation with one another during projects, but I was able to get a clearer picture of it after listening to a description of the process in a debate setting.

There were spirited question and answer sessions after each of the presentations. At the closing session, Professor Sasai summed up the symposium as follows: "Although Field 1 and Field 2 both target biomolecules, the background is different in these two fields. However, I think it is meaningful for us to experience a wide variety of different research styles." I felt strongly that, as in the case of the cooperative phenomenon of biomolecules, it is important for us in our research as well to continue to pursue activities that go beyond disciplinary boundaries.

* Summaries of the lectures presented at the symposium are available on the Field 1 website.
http://www.kobe.riken.jp/stpr1-life/index.html

HPCI SPIRE Program Field 1 × Field 2 Symposium in Nagoya University

Computational studies of complex biomolecular systems to understand the role of intermolecular interactions Speakers

"Alteration of dynamical nature of actin capping protein induced by CARMIL"

Motonori Ota

Professor, Graduate School of Information Science, Nagoya University<Field 1>

"Morphological diversity of biomembranes"

Hiroshi Noguchi

Associate Professor, Institute for Solid State Physics, The University of Tokyo<Field 2>

"Structural transition control mechanisms for large biological supramolecules"

Akio Kitao

Associate Professor, Institute of Molecular and Cellular Biosciences, The University of Tokyo<Field 2>

"Structure prediction and molecular simulations for membrane proteins"

Yuji Sugita

Chief Scientist, Theoretical Molecular Science Laboratory, RIKEN<Field 1>

"Development of supramolecule modeling pipeline"

Tsuyoshi Shirai

Professor, Department of Computer Bioscience, Nagahama Institute of Bio-science and Technology

"Stability of nucleosomes containing histone variants"

Hidetoshi Kono

Group Leader, Molecular Modeling and Simulation Group, Japan Atomic Energy Agency<Field 2>

"SCLS computer systems open to life scientists"

Chisa Kamada

Team Member, HPCI Program for Computational Life Sciences, RIKEN<Field 1>

"Electrostatical allosteric mechanisms common in molecular machines and intrinsically disordered proteins"

Mitsunori Takano

Professor, Graduate School of Advanced Science and Engineering, Waseda University

"Statistical approaches to the relaxation and reactions in proteins"

Masataka Nagaoka

Professor, Graduate School of Information Science, Nagoya University<Field 2>

"Working principle of actomyosin motors "

Masaki Sasai

Professor, Graduate School of Engineering, Nagoya University<Field 2>

The SCLS motto: "Go find a punchline! "

The name SCLS stands for Supercomputational Life Science. At SCLS, researchers simulate the complex, diverse behavior of living systems to reveal important principles of human health and disease, with the ultimate goal of enabling discovery of new medicines.

"Just as a joke isn' t funny without the punchline, science needs more than results — it needs the equivalent of a "punchline" to complete it," says Director Toshio Yanagida. In response to his enthusiastic encouragement, all project members work hard day after day.

Aiming for Breakthroughs through Interdisciplinary Exchange

Atsuko Irie
Assistant Technical Staff,
Institute of Particle and Nuclear Studies, High Energy Accelerator Research Organization

Increasing collaboration between SPIRE Field 2 and Field 5

It has been three years since the HPCI SPIRE (Strategic Programs for Innovative Research) program began. During this period, an annual Interdisciplinary Exchange Workshop where researchers in Field 2 "New materials and energy creation" and Field 5 "The origin of matter and the universe" can discuss issues common to both fields has been held. In the area of research support as well, a cooperative organization is being built. The targets of Field 2 research are solid state science, molecular science and materials science, while the targets of Field 5 research are elementary particles, atomic nuclei and space. Despite the fact that these two fields appear at first glance to be different in terms of both targets and the scale of the research, why is progress being made on collaboration between these two SPIRE fields?

Field 2 and Field 5 differ in terms of the components making up the system that is the target of the research. However, the physical laws that are used to describe the various properties and changes are very similar. For this reason, the fields face many of the same issues in terms of theory and calculation methods. Collaboration between the two fields is aimed at discussing these common issues and cooperating with one another to resolve them.

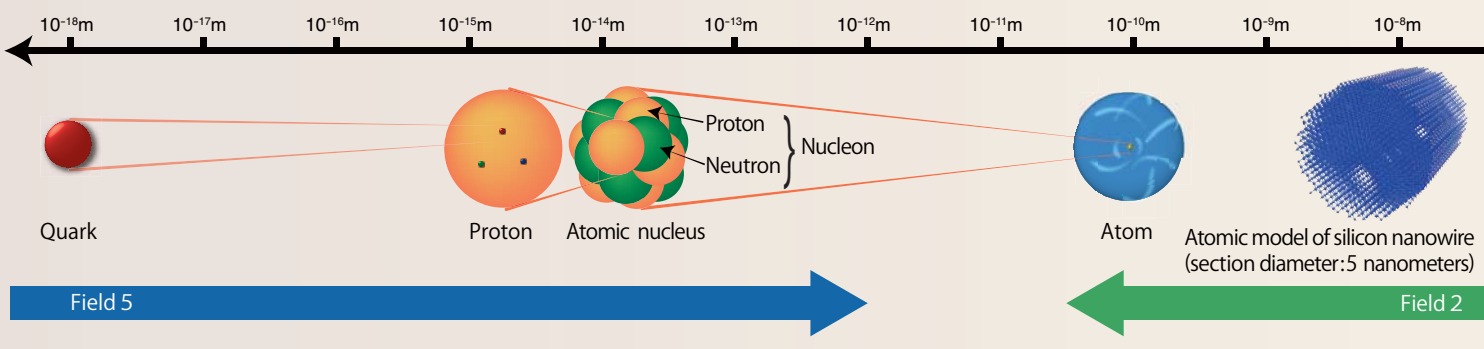
A look back at history reveals that exchanges between materials science researchers and elementary particle and nuclear science researchers has produced many breakthroughs in the past. Famous among these is the example of Professor Yoichiro Nambu, recipient of the 2008 Nobel Prize in Physics, for whom the Bardeen - Cooper - Schrieffer (BCS) theory that explains the physical phenomenon of superconductivity led to the idea for spontaneous symmetry breaking, the breakthrough for which he was awarded the Nobel Prize.

One example of a specific issue that is common to both Field 2 and Field 5 is quantum nature, a universal aspect of fields in the micro realm. In Field 2, researchers study electrons and ions in materials, while in Field 5 researchers study the protons, neutrons and other particles that make up atomic nuclei, as well as the quarks and gluons that make up those particles. Within the many research endeavors, there are actually many issues that these fields have in common, such as the development of rigorous calculation methods and approximate means methods for quantum many-body systems and the construction of models and so on. There are also commonalities in terms of the gravity simulations used in space and the molecular dynamics simulations used in materials science. Molecular dynamics calculations are used for elementary particle lattice QCD calculations and atomic nuclei collision phenomena as well. The common attributes of issues such as these are not limited to Field 2 and Field 5, but to understand the common elements that are based on physics, it is essential to first deepen collaboration between these two SPIRE fields that are separated only by low barriers.

Interdisciplinary Exchange Workshop

The third Field 2 × Field 5 Interdisciplinary Exchange Workshop was held November 13 and 14, 2013 at the Institute for Molecular Science in the National Institutes of Natural Sciences, located in the city of Okazaki. The workshop featured 16 pairs of presentations, and 40 participants engaged in spirited discussion. The topic was "Dynamics calculations for quantum many-body systems." In the background of this topic is the fact that it has recently become possible in materials science research to observe the course of chemical reactions in units of femtoseconds (10^{-15} second) and attoseconds (10^{-18} second). In order to do this, it is necessary to calculate the quantum dynamics of electrons and ions in a time domain. In nuclear physics, on the other hand, simulations of nuclei collisions using time-dependent mean field theory have been developed since the 1970s. Presentations at the Interdisciplinary Exchange Workshop centered on photoelectron dynamics calculations and mixed classical and quantum dynamics calculations from the fields of molecular science and materials science, and quantum dynamics calculations relating to photoresponse and collision phenomena from the nuclear field.

At previous Interdisciplinary Exchange Workshops, there were many presentations based on large-scale calculations, and there were also presentations from the fields of mathematical science and computer science.



"This time, the presentations were not necessarily limited to large-scale calculations, and there was an awareness of the need to search for seeds for which large-scale calculations will be needed in the future," says Professor Kazuhiro Yabana of Tsukuba University, who served as facilitator for the workshop. "For this reason, the emphasis was on physics as well as calculations." Associate Professor Katsuyuki Nobusada of the Institute for Molecular Science, who also served as facilitator, said in his greeting at the start of the workshop that he hoped that the participants "would seize the opportunity to perform large-scale calculations in the future."

Research support

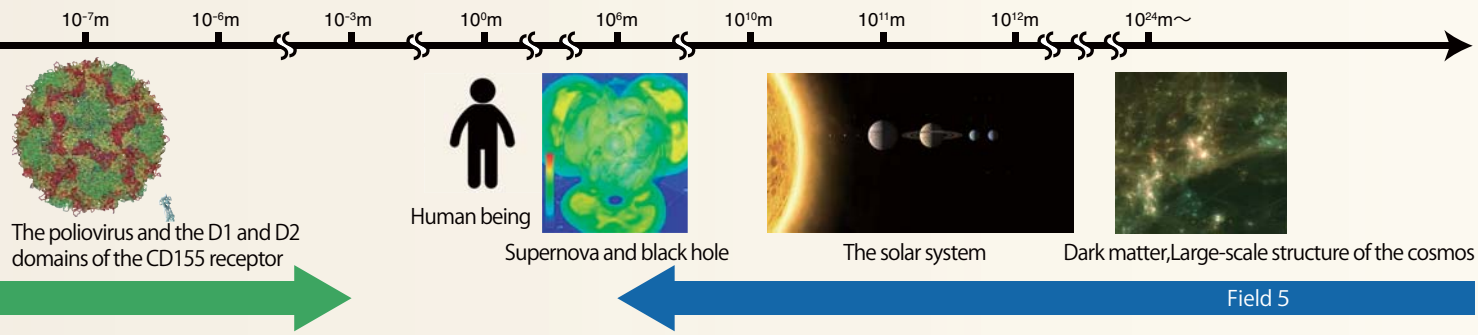
The Interdisciplinary Exchange Workshop also featured presentations regarding research support. Researcher Kazuya Ishimura provided a report and information regarding the CMSI young researcher technical workshops???, which are held to share information and technologies such as programming, tuning and so on, and the "TOKKUN!" CMSI application advancement training camp. In SPIRE Field 5, a user support* team made up of researchers in the elementary particle, atomic nuclei and space fields and computational science researchers has been organized. If there is a request from a researcher somewhere in Japan in the field of elementary particle, atomic nuclei or space, the team members who are knowledgeable about the content of the request propose solutions and provide advice. In the past, the team has handled issues relating to efficient parallel computing algorithms, requests for recommendations of visualization software, routines for solving differential equations, the development of special diagonalization routines and so on. In the future, SPIRE Field 5 researchers will attend SPIRE Field 2 workshops and other events, and requests for assistance from Field 2 researchers will be accommodated in Field 5 user support activities. In this way, the researchers will establish closer relationships in the area of research support as well. Collaboration between SPIRE Field 2 and Field 5 may once again produce breakthroughs in these fields such as the one produced by Professor Nambu. We look forward to the achievements of their activities in the future.

(Assistance: Kazuhiro Yabana, University of Tsukuba

* User support
For more information on user support offered in SPIRE Field 5, go to:
http://www.jicfus.jp/field5/en/promotion/user/

HPCI SPIRE (Strategic Programs for Innovative Research)
Field 5: The origin of matter and the universe

The history of the universe is thought to have begun approximately 13.8 billion years ago in an ultra-high temperature and ultra-high density state known as the Big Bang. Subsequently, as the temperature decreased, baryons such as protons and neutrons were produced from quarks. Then the protons and neutrons bonded together to produce light atomic nuclei.
Dark matter of an unknown nature is also present in the universe, in quantities that are far more abundant than those of the baryons. The universe is thought to have formed initially when the dark matter came together to form structures as a result of gravity, and ordinary baryon materials were attracted to these structures to form the stars and the Milky Way, at which point the universe assumed its present form. While there is active star birth in the Milky Way, stars also become extinct as a result of gravitational collapse, supernova explosions and so on. Heavier atomic nuclei are produced through this process.
In this way, there is a close relationship between the generation of materials and the formation of the structure of the universe. The goal of HPCI SPIRE Field 5 "The origin of matter and the universe" is to use computational science to achieve an integrated understanding of the origin and structure of the universe and the formation of matter — from elementary particles through atomic nuclei, stars and the Milky Way — throughout the history of the universe that began with the Big Bang.



4th Graduate Interview

Graduate :

Hiroko Kashima

Kobe Steel, Ltd.

Aluminum & Copper Business Department, Technology Division, Analytical Technology Research Office,

Kashima majored in Mechanical and System Engineering in the Graduate School of Science and Technology at Kyoto Institute of Technology. She joined Kobe Steel after receiving her Master's degree for research into simulation of solidification structure formation in convection flows using the phase-field method.

In Her Second Year on the Front Lines of Manufacturing

Interviewer :

Yasushi Shibuta

Lecturer, Department of Materials Engineering, Graduate School of Engineering, The University of Tokyo

Designing not only strength but sensory appeal as well

Shibuta : What kind of work are you presently engaged in?

Kashima : I'm in the Analytical Technology Research Office in the Aluminum & Copper Business Department. I'm working on the design of structures that are more effective in terms of both strength and cost using aluminum materials, as well as developing formation methods, all from a material manufacturer's perspective. Recently I've been working on the strength design for aluminum cans (the so-called "bottle cans," which are cans shaped like a bottle).

Shibuta : When you design an aluminum can, what is the most important thing that is needed?

Kashima : The problem of how to make it light. For example, even just making the can wall thinner in 1.0μm increments makes it quite a bit lighter. But on the other hand it has to maintain enough strength to withstand the weight of around 200kg from above. We try to design structures that can maintain both of these things and are also advantageous in terms of cost.

Shibuta : Apart from light weight, what else are you focusing on?

Kashima : Well, for example, there is a diamond-cut can whose body is formed using the famous "Miura map fold" method used in the development of satellite panels. This structure is resistant to pressure in the axial direction, and when the can is opened, the pressure is released and the Miura map fold surface texture is emphasized. The loud POP! that you hear when you open the can defines the image of the product. I think it's really interesting that not only the strength but also the sensory appeal is produced by the structural design.

Shibuta : Do you use analysis techniques, meaning simulations, in the design process?

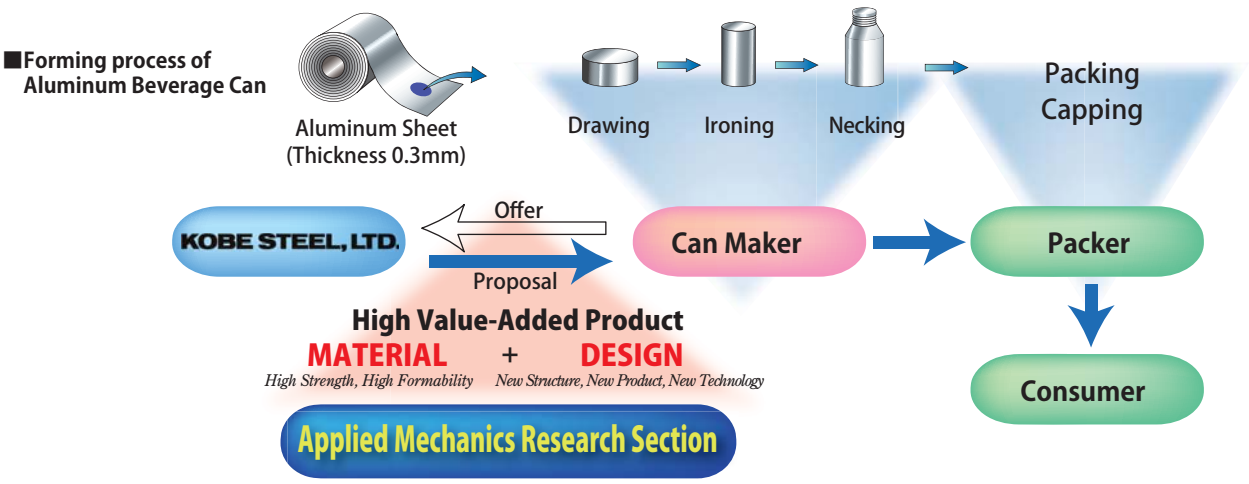
Kashima : We use both experimentation and analysis. For analysis. we conduct structural analysis using the finite element method and perform optimization calculations for the topology and so on. And we perform strength tests for the structures that we've actually designed to test whether or not the axial strength meets the required standards.

Shibuta : What are the advantages of introducing simulations?

Kashima : Currently finite element analysis for aluminum cans can be conducted in about five to six hours, and it's possible to predict the strength of an object within a realistic period of time.

Shibuta : In university research, we sometimes use the fact that we've conducted large-scale calculations on the order of several weeks to several months as a selling point. But when you're developing a product at a company and you have a limited amount of time before the deadline, it's more important to produce the desired result within a realistic period of time. Conversely, is there also the problem that you need the help of computers even if it takes time?

Kashima : To give just one example, there was a problem in which variations in strength were produced in the rolling process due to anisotropy in crystal orientation, and one section of the can would crumple when the can was subjected to internal pressure. Highly precise control of the material structure is needed to resolve this problem, so we have to put a lot of work into exper-



iments based on metallurgical tests. Currently I'm in charge of the strength design aspects. But as a material manufacturer, I think that it would be advantageous if it were possible to perform computer analysis seamlessly for everything from optimal control of the material structure through structural design, to be able to actively control the material structure so it meets the desired objectives.

The clear realization that material science is the foundation of manufacturing led to a career path at a manufacturer

Shibuta : You mentioned control of the material structure. As I understand it, you were engaged in research on a related topic in your student days.

Kashima : Yes. I conducted research into simulations of solidification structure formation within convection flows in the laboratory of Professor Tomohiro Takagi at the Kyoto Institute of Technology.

Shibuta : Can you go into a bit more detail about the content of the research?

Kashima : I used the phase-field method to analyze the growth of solidification structures taking into account the convection flow that are produced during the casting process, and the dynamic effect of the convection flow on the fragmentation of dendrites (the dendritic crystals that branch out in multiple directions). To be more specific, I used the Navier-Stokes equation that is a basic equation for fluids, and the phase-field equation to perform coupled numerical analysis.

Shibuta : The phase-field method is a method that has been widely introduced for free boundary problems, as an analysis method that expresses changes in complex interface shapes in terms of the evolution over time of the distribution of order parameters. Did you develop the code by yourself?

Kashima : I used code that had been developed in our laboratory, modifying it so it would fit my model. That's how I learned how to program. Now we use mostly packages, but the things that I learned in my student days are really proving useful in my work now.

Shibuta : Did you have any opportunities to present the results of your research when you were a student?

Kashima : Yes. I had presentations at international conferences overseas twice and at conferences in Japan many times. In the beginning, I did not like to make presentations in front of people, but in the course of presenting over and over again I got over my dislike for the most part. And it turned out to be a great opportunity. Also, it was good stimulation to have the opportunity to speak with professors who are conducting cutting-edge research.

Shibuta : What left the deepest impression on you through the research you conducted in your student days?

Kashima : When we conducted actual simulations of structure formation in cast structure solidification, I realized how wide-ranging the impact that materials science has on everything in terms of the most basic aspects of manufacturing. That was when I decided to apply for a job at materials manufacturers after I graduated.

A child who 'loved to take things apart'

Shibuta : Why did you decide to major in mechanical engineering at college?

Kashima : I liked building things even when I was a little girl. So I guess I've always been interested in "manufacturing."

Shibuta : What kind of things did you build?

Kashima : It wasn't so much building as wondering how things were constructed and liking to take them apart. For example, I disassembled my alarm clock. And then I couldn't put it back together again. (Laugh)

Shibuta : So you were a classic example of a mechanically minded person. (Laugh) Was the influence of your family a big factor?

Kashima : It was the influence of my father. He also liked to take various things apart. I used to enjoy watching him do that.

Shibuta : What were you interested in when you actually began majoring in mechanical engineering at college?

Kashima : When I listened to lectures at the college, I also became interested in fluid dynamics. I was fascinated that you can use the Navier-Stokes equation, a basic equation, to visualize phenomenon like currents that you can't see, using computational fluid dynamics (CFD).

Shibuta : I see. That aspect is definitely intriguing.

Kashima : In my student days, I was able to conduct research into material structure from the standpoint of both fluid dynamics and material mechanics. That was a tremendous experience for me.

Shibuta : As your sphere of activity has expanded from the university to a company setting, you've been able to truly experience how your interest grows broader as it is combined with various types of knowledge and experience, and that must give you a lot of self-confidence. What are your goals for the future?

Kashima : I want to actively participate in exhibitions and international conferences overseas, and engage in design and development from a global perspective.

Shibuta : We're looking forward to the results of your wide-ranging endeavors.

(January 20, 2014 at Kobe Corporate Research Laboratories, Kobe Steel, Ltd.) (Photo: Tomohiro Takaki, Kyoto Institute of Technology)


Research Center for Computational Science


Fujitsu PRIMERGY RX300S7 342nodes

Institute for Molecular Science, National Institute of Natural Sciences

Hisashi Okumura
Associate Professor, Research Center for Computational Science,
Institute for Molecular Science, National Institute of Natural Sciences

The Molecular Science Division pursues research into large-scale computing in the field of molecular science, under the direction of Director Kazuo Takatsuka. It also collaborates with experimental researchers and industry to conduct personnel training and other activities to advance the field. Hisashi Okumura introduces the CMSI Molecular Science Division, located in the Institute for Molecular Science, and the Research Center for Computational Science, which conducts supercomputer use and maintenance.

Emphasizing the training of young researchers and researcher interchange

The Theoretical and Computational Chemistry Initiative (TCCI) is located within the Institute for Molecular Science at the National Institute of Natural Sciences. The Institute for Molecular Science is a world-famous research institute that conducts research in chemistry and the fields of physics and materials science that are closely related to chemistry. The FY2014 University Ranking published in April 2013 by the Asahi Shimbun Newspaper includes rankings for the frequency with which academic papers from various institutions were cited by the Thomson Reuters Corporation in 2007 - 2011. The Institute for Molecular Science was ranked number one in Japan in the fields of chemistry and materials science and number two in Japan overall.

The Institute for Molecular Science Computer Center, the predecessor of the Research Center for Computational Science at the National Institute of Natural Sciences, was established in May 1977 as a research facility for the Institute for Molecular Science. In January 1979, it began a shared use service using a Hitachi M-180. Currently the Center has a system with a total of 326.2 TFlops, made up of the Fujitsu PRIMERGY, Fujitsu PRIMEHPC FX10 and SGI UV2000. In the past 35 years, the Center has achieved a seven-digit improvement in computing performance. These computing resources are made available to researchers throughout the country on a shared use basis. The number of users has been increasing during the past five years; in FY 2012, there were 213 groups and 807 individual users. 20% of the computing resources are provided within the CMSI use framework to researchers who are involved in CMSI. In addition to the computing hardware, molecular simulations and quantum chemistry calculation software are also provided for shared use, and these are made available to CMSI researchers as well. The Center's fast, large-scale computing environment is used for research in the fields of molecular science, physics and bioscience, and a diverse array of research projects are underway based on molecular theory, condensed matter theory and biomedical simulations.

The Research Center for Computational Science does not simply provide a computing environment. It also invests a great deal of energy in the training of young researchers and fostering the exchange of information and interchange among researchers. Every winter, together with TCCI, the Center jointly sponsors the Molecular Simulation School and Quantum Chemistry Winter School, featuring lectures by professors who are engaged in advanced research activities in the fields of molecular simulation and quantum chemistry. These Schools have earned a reputation as excellent venues for the training of graduate students and young researchers. Every January, the Center also holds a Research Center for Computational Science Workshop, in which active researchers from the fields of molecular science and a wide range of related fields such as condensed matter physics and material science are invited as lecturers, to discuss issues that need to be resolved in the areas of both theory and computational science and the methodologies that will be needed.

Fumiyasu Mizutani

Mizutani majored in physics at Aichi University of Education, but fate brought him to the National Institute for Physiological Sciences, located on the same campus as the Institute for Molecular Science. He joined the Institute for Molecular Science in 1995. This is his 30th year of being fascinated by computers.

"Ensuring easy operation for users even if the system changes"

The Research Center for Computational Science has a total staff of 16: Director Shinji Saito, Professorr Masahiro Ehara, one associate professor (myself), five assistant professors, six technical staff members, and two office assistants. The technical staff members support the diverse activities of TCCI and the Research Center for Computational Science. Fumiyasu Mizutani, who has supported the operations of

the Research Center for Computational Science for many years, provided an introduction to the Center and spoke about the challenges and rewards of the work, both of which he is made keenly aware of on a daily basis.

"The main supercomputer at the Research Center for Computational Science has changed from one made by Hitachi to one made by NEC, and further to one made by Fujitsu. Moreover, the Center was quick to realize the importance of parallel computing, and it introduced subsystems made by IBM and SGI. For that reason, some people joke that it's like a computer museum, but that's because it's always had a climate in which it wasn't mired in the past but always made an active effort to introduce whatever technology was best at the time. But the tradeoff was that the Center couldn't make users suffer inconvenience as a result, and that made things rough for the operation side. For example, the molecular orbital method application named Gaussian that is used frequently is provided with a tool that allows you to enter a job simply by specifying the input file, and it's designed so users won't have to be concerned about differences between systems. As you can see, part of our day-to-day work activities is searching for areas for technical development, and I find that kind of thing very rewarding.

In order to make things convenient for CMSI users, as part of the FY 2012 supercomputer upgrade we introduced the first machine of commercial version of the K computer, Fujitsu PRIMEHPC FX10, as a development server. Not only in ordinary use but for system upgrades as well, we reflect the opinions of the molecular science community. So I hope people will continue to actively share their views with us."

The capabilities of the technical staff are crucial for accomplishing the various tasks at the Research Center for Computational Science. As team leader, Mizutani in particular not only serves as the facilitator for the technical staff, he also has a thorough knowledge of all work activities, and he is essential to the operations of the Center. He hopes that the teaching staff and the technical staff will continue to maintain close collaboration as they provide a large-scale high-speed computing environment, while at the same time playing a role in the development of computational molecular science through the training of personnel in the fields of theory and computational science and promoting research interchange.

Center and laboratory staff
In back row, from left : Ono, Sawa (Technical Staff), Iwahashi (Technical Staff), Mori, Matsuo (Technical Staff), Tashiro, Ito (Assistant Professor), Ishida (Assistant Professor), Mizutani (Technical Staff)
In middle row, from left : Toya (Office Staff), Ishihara (Office Staff), Kawaguchi, Kondo, Imoto, Nagaya (Technical Staff)
In front row, from left : Naito (Technical Staff), Ehara (Professor), Fukuda (Assistant Professor), Saito (Center Director), Okumura (Associate Professor)
(In the background is the Laboratories building of IMS)

Message from the Director of the Molecular Science Divisions

Kazuo Takatsuka

Recently I have become concerned about the "dream" of research. A dream is something that you hope for, something that you pursue step by step in order to achieve. From that process, new dreams and challenges are born. A "never-ending" dream is not one that is distant. It's more that, as you move one step closer to it, a new dream appears. It's similar to the hierarchical structure of natural phenomena. Recently I realized that a great many of the questions that I was burning to solve in my younger days have been answered. But at the edge of the horizon, there was always the next mountain that I wanted to climb. The K computer, too, was once a calculation environment that existed only in our dreams. Now that it has been achieved, it would be a pity if the dreams of young researchers and students rapidly faded away and became something that was strangely realistic. Once you are able to perform calculations and visualize things, is that really the end? Are your goals achieved once the numbers have emerged? Surely that cannot really be true. Surely there must be even bigger dreams.

CMSI Calendar

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

●On-line Lecture: Advanced Computational Science B
Date : 10 April – 24 July, 2014
※Every Thursday during the above term.
※Up-to 20 sites available
※Please check the latest info on CMSI Web

●CMSI Kobe Hands-on: FMO Tutorial
Date : April, 2014 – date not fixed
Venue : CMSI Kobe
※To be held once a month between May 2014 and February 2015.)
※Please check the latest info on CMSI Web

●CMSI Kashiwa Hands-on
Date : To be held once a month between April and February 2015
Venue : ISSP, The University of Tokyo

●ISSP International Workshop "New Horizon of Strongly Correlated Physics" (NHSCP2014)
Date : 16 June – 4 July, 2014
*Symposium: 25-27 June, 2014
Venue : ISSP, The University of Tokyo

●1st Research Filed Summer School 2014
Date : August, 2014 – date not fixed
Venue : Kobe

●CMD®25
Date : September 1-5, 2014
Venue : International Institute for Advanced Studies

●TCCI Winter College (Molecular Simulation)
Date : 14-17 October, 2014
Venue: Institute for Molecular Science , Okazaki Conference Center (OCC)

●5th TCCI Joint Workshop (Steering Committee)
Date : October 17-18, 2014
Venue : Institute for Molecular Science, Okazaki Conference Center (OCC)

●CMRI Symposium
Date : November, 2014 – date not fixed
Venue : IMR, Tohoku University

●4th CMSI Symposium
Date : 8-10 December, 2014
Venue : IMR, Tohoku University

●TCCI Winter College (quantum chemistry)
Date : 15-16 December, 2014
Venue : Institute for Molecular Science , Okazaki Conference Center (OCC)

●ACCMS-VO9 International Meeting
Date : 20-22 December, 2014 (tentative)
Venue : Okinawa

●CMD®26
Date : February 23-27, 2015
Venue : G Building, School of Engineering Science, Osaka University

The 4th CMSI Poster Award

Of the research presentations at the 4th CMSI Workshop (held in conjunction with joint research using the Institute for Solid State Physics supercomputer) on December 10-13, 2013, the following presentations were selected to be recipients of the Awards.

CMSI Poster Award

Hiroshi Watanabe

Institute for Solid State Physics, The University of Tokyo

Research Topic: Making Invisible Visible: Visualization of Bubbles

Appropriate visualization of calculation results is important, as it helps to achieve an intuitive understanding of physical phenomena and may even trigger the discovery of new phenomena. In large scale computing, however, the amount of data is enormous, making the data difficult to handle. Data formats that enable the data to be compressed without losing any vital information can be devised to make the data lighter and facilitate analysis and visualization.

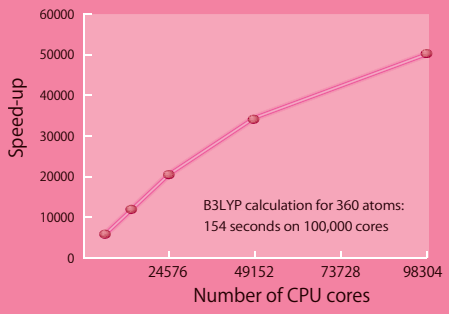
CMSI Young Researcher Encouragement Award (Oral presentation)

Kazuya Ishimura

Institute for Molecular Science, National Institutes of Natural Sciences

Research Topic: The Search for New Structures and Functions of Nanosize Molecules: Efficient Development of Massively Parallel Computing Programs

A massively parallel quantum chemistry calculation program was developed and demonstration calculations were executed using a 100,000 CPU core of the K Computer. The achievement of high parallel performance and execution performance has made it possible to perform nanosize molecule calculations as routine work. In order to improve the efficiency of development in Field 2, preparations are underway to compile a library of calculations that can be shared and make it publicly available as an open source resource.



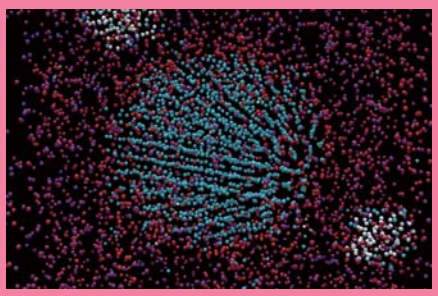
CMSI Visual Award (Oral presentation)

Takuma Yagasaki

Okayama University

Research Topic: Molecular Dynamics Calculations for the Methane Hydrate Decomposition Process

As dissociation of methane hydrate proceeds in liquid water, methane molecules are released into the surrounding area and bubbles are formed. Analysis conducted using the K Computer revealed that these methane bubbles accelerate the hydrate decomposition. This mechanism may be useful to utilize gas hydrates as an energy storage material.



Torrent No.9 March 2014

Cover : What would happen if the moon does not exists? If a huge meteorite did not fall? Scientists enjoy various "if"s. Simulation enables us to shape those "if"s. Well, what would happen if you are absorbed in hydrate with methane? You scenery could be like this. (CG: Masakazu Matsumoto, Okayama Univ.)

Torrent : The Newsletter of the Computational Materials Science Initiative (CMSI) No.9, March 2014

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

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