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Torrent

10^{16} Weave New Materials

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

K computer

CMSI Division Researchers

The Young Leaders who are Creating the Computational Materials Science of Tomorrow

CMSI has introduced a new Division Researcher program. Division Researchers have various roles and missions, but the goal of all activities is the promotion and development of computational materials science. In this issue, we focus on how this position came to be created and how the roles of Division Researchers were determined. We will also hear from new researchers who have begun actual activities as Division Researchers to get a sense of their determination and objectives.

Turning the Headwaters of Materials Science into a "Torrent" of Innovations

The Computational Materials Science Initiative (CMSI) is a research network made up of computational science researchers in the three fields of condensed matter physics, molecular science and materials science. CMSI has received a grant from the Ministry of Education, Culture, Sports, Science and Technology to promote research in Field 2 "New Materials and Energy Creation" of the High Performance Computing Infrastructure (HPCI) strategy program. The goal of computational materials science is to link theory and experiment to open new doors in science and technology. The computational materials science is a young science, in which new techniques in advanced computing are being developed and whose diverse research topics range from single molecules to practical materials. The aim is to use supercomputers — led by the K Computer, the world's fastest supercomputer — to expand and deepen the headwaters of materials science into a torrent of innovations in material functions and energy conversion.

What distinguishes the CMSI strategy program is that, in addition to state-of-the-art research and development of specific "hot topics," creating a research and development infrastructure for the next generation of computational materials science is one of the major objectives. To this end, CMSI holds symposiums, workshops, hands-on training sessions, collaborations with experimental researchers and so on to form networks among the people interested in this field, in particular young researchers. CMSI also supports the activities of these researchers whose goal is the formation of a new research and development infrastructure in all areas including computer use, program development, program use and so on. Research achievements as well as personnel, software and simulation data are featured in the CMSI newsletter and on the CMSI website and so on as part of the effort to create a center that can communicate CMSI activities and achievements to the world.

Recently CMSI has introduced a unique program, the "Division Researcher" program, for the individuals engaged in activities to promote and develop the field of computational materials science.

The Need for a New Research and Development System that Can Respond to Trends in Hardware Development

All matter is made up of atoms and molecules. The goal of computational materials science is to determine the behavior of matter as collections of atoms and molecules, and to use computers to solve basic equations that describe this behavior and predict the properties possessed by these materials. Researchers strive to verify experimental results and gain an understanding of the mechanisms by which functions are manifested, and then apply the results in material design.

The computers that are used for simulations are made up primarily of central processing units (CPUs) that perform calculations, memory units that store data and results, and communication units (network) that link the CPUs and the memory units. In order to conduct simulations of physical systems in a larger scale or perform at higher speed calculations that formerly took a great deal of time, supercomputers made up of a network of multiple CPUs and memory units are used. As the pace of acceleration of CPU operating speed has slowed, in recent years the clear trend in large computers has been toward multicore computers and parallel processing. For example, the K Computer has 640,000 computing cores. To make effective use of this type of ultra-parallel computer, revolutionary algorithms and software not achievable through the simple extension of existing technologies must be developed. Until the beginning of the 21st century, increases in computing performance were effected primarily by increasing the operating speed of the individual cores, and it was possible to reap the benefits of improved hardware performance without greatly modifying existing programs. In this sense, it was a time in which one merely had to wait and speeds would increase. But the new trends in computing hardware require a qualitatively different research structure from those of the past.

Up to now, software for determining state-of-the-art physicochemical phenomena was almost exclusively developed and maintained on an individual laboratory basis. However, software designed for use on large-scale computers requires a great deal of time and effort for research and development, and improving the program becomes a more complex process. For this reason, software that is useful and can be used by many researchers, and that will contribute to the promotion and development of computational materials science, will need to be maintained and developed organizationally to ensure that the program continues to be passed on to future researchers. It was in an effort to resolve this issue that the "Division Researcher" program was created.

Role and Mission of Division Researchers

In recruiting and hiring researchers, CMSI makes a clear distinction between "Priority Area Researchers," who use the K Computer to work on specific key issues in computational materials science, and "Division Researchers," who work to promote and develop the field of computational materials science itself. Priority Area Researchers endeavor to solve the most urgent problems for which results are needed currently. In contrast, the role of Division Researchers is to find solutions to crucial problems that must be resolved to make progress in next-generation computational materials science, and to pursue infrastructure-building. Their main role is to develop the new methodologies and basic technologies that will be widely used in the field of computational materials science; develop and disseminate important software applications that are expected to be used by many users in the field of computational materials science; develop simulation code by applying the advanced parallelization and speed-up techniques, and conduct computational materials science research using such a code; and build a public release environment to enable many users including both laboratory researchers and company researchers to use research achievements. The goal of all of these missions is to disseminate and expand

the academic achievements of state-of-the-art computational materials science research, and ensure that they are returned to society in order to enable computational materials science to be used as a tool for resolving the immediate problems faced by people in their daily lives.

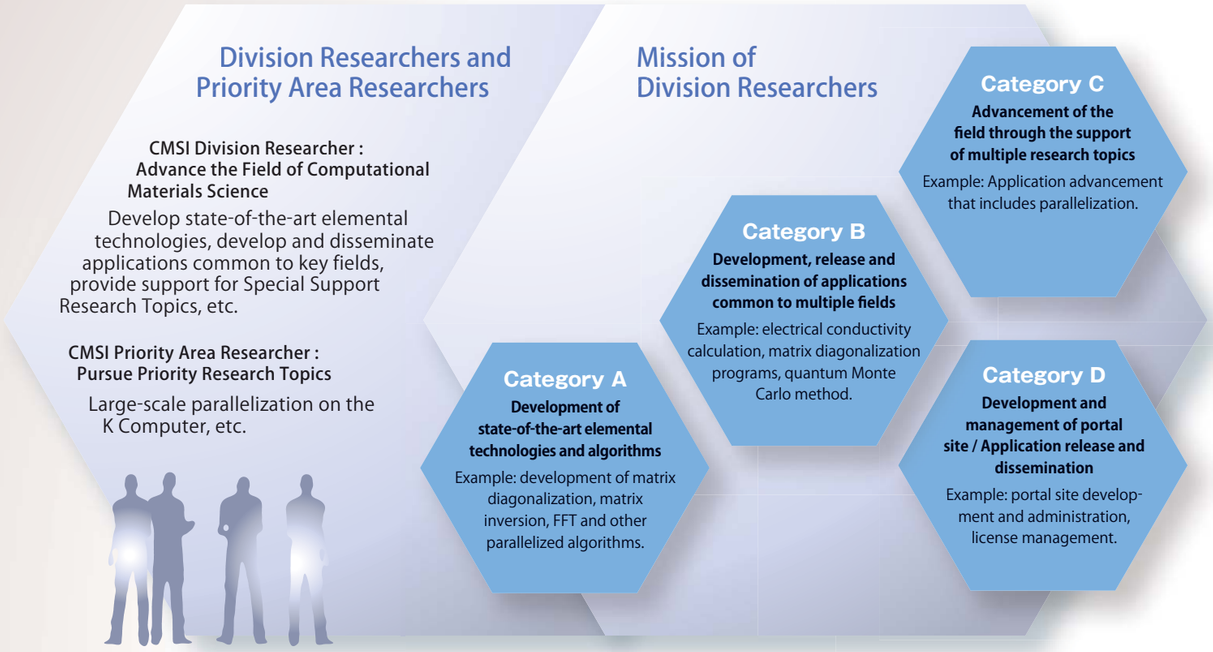
CMSI research topics include explication of the mechanism by which the functions of superconductors and other materials are manifested; generation and storage of next-generation energy, an issue that is expected to become more and more important in the coming years; research to achieve breakthroughs in semiconductor devices, whose rate of speed increase is beginning to plateau; elucidation of molecular control mechanisms for viruses and other threats to humanity; and magnetic materials and structural materials that offer equivalent performance without using scarce elements. All of these areas are ones in which progress is needed to ensure that human beings are able to live lives of abundance here on earth. Computational materials science links theory and experiment in these areas, and Division Researchers in each category (see figure below) conduct research to ensure that achievements in these areas will contribute to academic and social development.

Expanding the Division Researcher Activities Throughout the World

The research institutions with which Division Researchers are affiliated include the CMSI Divisions in the areas of condensed matter physics, molecular science and materials science (Institute for Solid State Physics, The University of Tokyo / Institute for Molecular Science, National Institutes of Natural Sciences / Institute for Materials Research, Tohoku University), the Molecular Science Sub-Division (Graduate School of Arts and Sciences, The University of Tokyo), the Materials Science Sub-Division (AIST Kansai, National Institute of Advanced Industrial Science and Technology) and Industry-Government-Academia Cooperation Divisions (National Institute of Advanced Industrial Science and Technology / National Institute for Materials Science). Moreover, the CMSI Kobe Branch that was established in April 2011 in the Advanced Institute for Computational Science was set up to integrate all of these fields. In addition to Division Researchers, it will have specially appointed CMSI faculty to lead activities to promote individual fields and conduct overall coordination.

Division Researcher activities will not be limited to the individual institutions with which they are affiliated. Researchers will be active in all fields of computational materials science and an effort will be made to promote the integration of the condensed matter physics, molecular science and materials science. In addition, technical workshops for young CMSI researchers will be held once every two months. These workshops will feature lectures on the elemental techniques needed for large-scale computing, discussion of the issues faced in each field, exchanges of views regarding the ideal supercomputer in the future and so on. Technical workshops will be planned and conducted by the Division Researchers themselves.

These Division Researcher activities will enhance communication among the young researchers who are the future of computational materials science, with the goal of extending it throughout the entire world.



1st CMSI Young Researcher Technical Workshop

The first Young Researcher Technical Workshop was held on July 7-8, 2011. This was the first event to be held at the new CMSI Kobe Branch and served as an opportunity for young CMSI researchers to gather at the Advanced Institute for Computational Science to discuss technology-related issues.

The first day featured presentations by seven young CMSI researchers who have already begun experimental use of the K Computer. They spoke about cutting-edge large-scale computing techniques and problem-solving approaches, including the problems they had encountered in coding. The attendees asked many expertise-related questions. The invited speaker, Yutaka Ishikawa, a professor in the Graduate School of Information Science and Technology at the University of Tokyo, gave a presentation entitled "The Path to Exascale Computing," in which he gave the attendees a real sense that the move to develop the next supercomputer was already underway.

In the evening, the poster session was held at a different venue. Presenters and attendees could be seen engaged in animated discussions, and the debate spilled over into the roundtable discussion. Many of the young researchers were meeting each other for the first time, but the common ground of computational materials science enabled them to speak freely to one another, resulting in a very lively session.

The second day featured a presentation by Naoki Kawashima, a professor in the Institute for Solid State Physics at the University of Tokyo, entitled "The Achievements We Anticipate from Division Researchers." This was followed by a session featuring self-introductions from the new Division Researchers who will work to advance the field, in which they presented the content of their research up to now and spoke of their future ambitions. Shinji Tsuneyuki, Representative Director of CMSI, also spoke about his hopes for the activities of the Division Researchers. The meeting served to reaffirm the activities and mission of CMSI.

Takahisa Kouno, Yusuke Konishi, Kazuhito Shida and Takehiro Yonehara will plan the second and subsequent Young Researcher Technical Workshops as organizers of this fiscal year. The Technical Workshops, organized and held by the young researchers themselves, will be a valuable activity for the achievement of dramatic progress in computational materials science, integrating the fields of condensed matter physics, molecular science and materials science.

Profiles of Division Researchers

Here are the Division Researchers who adopted in research at CMSI up through August 31,2011.

Nobuyuki Kawagashira

Condensed Matter Physics Division Researcher
Institute for Solid State Physics, The University of Tokyo

Majored in computer science at the University of Tsukuba. General linguistics and bioinformatics at the different doctoral courses and research institutions.

Motivation for applying for the position
I wanted to use my knowledge in the areas such as UNIX, databases and web development.

Mission / Role
To assist in computational materials science research using information processing technologies.

Ambition
I want to use the web and social networking services to create an information community for computational materials science researchers.

Takahisa Kouno

Condensed Matter Physics Division Researcher
School of Engineering, Nagoya Institute of Technology

Majored in electrical and electronics engineering at Yamaguchi University. Engaged in research into GRID computing at Graduate School of Engineering, Nagoya Institute of Technology.

Motivation for applying for the position
I applied because I was interested in large-scale parallel computing and wanted to work on application development.

Mission / Role
To conduct tuning for order-N real-space DFT parallel code and multi-scale hybrid quantum-classical code.

Ambition
I want to conduct research into hybrid parallel programming that utilizes both MPI and OpenMP as well as other large-scale parallel programming technologies to help develop applications for next-generation supercomputers.

Yoshitake Sakae

Molecular Science Division Researcher
Graduate School of Science, Nagoya University

Majored in functional molecular science at the Graduate University for Advanced Studies and received his Ph.D. Engaged in research into enzyme reactions through quantum chemistry calculations at Graduate School of Science, Hiroshima University.

Motivation for applying for the position
I wanted to continue application development.

Mission / Role
To develop the REM additional function software. This software will enable various existing molecular simulation programs to be used to search for molecular structures in an efficient manner.

Ambition
I want to improve REM functions and develop new structural search techniques, and to work on the development of molecular force fields that will enable highly advanced simulations.

Shun Sakuraba

Molecular Science Division Researcher
Institute for Chemical Research, Kyoto University

Majored in computational biology at the Graduate School of Frontier Science, the University of Tokyo and received his Ph.D. Engaged in the development of ermod, the solvation free energy calculation software based on solution theory, at the Institute for Chemical Research at Kyoto University.

Motivation for applying for the position
I wanted to continue to refine ermod, so I applied to be a Division Researcher at CMSI.

Mission / Role
To improve the parallel efficiency of ermod to expand the range of application to multi-component heterogeneous solution systems, and to promote the software through activities such as user workshops.

Ambition
I would like to expand "what can be solved using small calculations," both theoretically and computationally (although I realize that this is paradoxical as a for CMSI researcher).

Yusuke Konishi

Industry-Government-Academia Cooperation DivisionResearcher
Nanosystem Research Institute, National Institute of Advanced Industrial Science and Technology (AIST)

Majored in physics at the University of Tokyo and received his Ph.D. (science). Engaged in research into photoinduced phase transition at the Institute of Materials Structure Science of the High Energy Accelerator Research Organization (KEK).

Motivation for applying for the position
I applied because I would be able to conduct research in the fields of condensed matter physics and computational physics.

Mission / Role
To pursue research into nanostructure formation in semiconductors and so on using first principles, the Monte Carlo method, molecular dynamics and other approaches, and to work on the CMSI public relations activities.

Ambition
I'd like to pursue various types of work while valuing cooperative relationships with other people.

Masato Kobayashi

Molecular Science Division Researcher
Faculty of Science and Engineering, Waseda University

Majored in quantum chemistry at Waseda University and received his Ph.D (science). Since 2008, has been working on application development for the K Computer as a doctoral research fellow at the Grand Challenge to Next-Generation Integrated Nano-science.

Motivation for applying for the position
I applied because I wanted to continue to develop software for the K Computer in order to do my part to invigorate the field of computer science and make it pervasive throughout society.

Mission / Role
To work on the advancement of additional function software, primarily hybrid parallelization and speeding up of the DC software for linear scaling quantum chemical calculation.

Ambition
I want to deepen interchange with many people both within CMSI and outside, without being limited to a certain field or existing frameworks such as computing, experimentation or theory.

Kazuhito Shida

Materials Science Division Researcher
Institute for Materials Research, Tohoku University

Majored in information science at the Japan Advanced Institute of Science and Technology. Engaged in research into physical property calculation using the Monte Carlo Method at Tohoku University.

Motivation for applying for the position
In my student days, I also used what was at the time a state-of-the-art parallel supercomputer, so I was very interested in seeing what progress had been made in the more than ten years since that time.

Mission / Role
To transplant to the K Computer and optimize programs such as TOMBO, a first principles electronic state calculation program that uses a proprietary all-electron mixed-basis approach developed by the Institute for Materials Research, in order to achieve physical property calculations for materials on an unprecedented scale and gain new knowledge in the field of material science.

Ambition
My current goal is to do as much as I can to try to eliminate the gap between the research up to now (the Monte Carlo method in material science) and the state-of-the-art parallel computing of the K Computer.

Ambition
My ultimate goal is to answer the question, "What is life?"

Ryota Jono

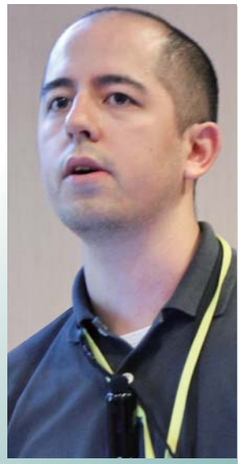
Molecular Science Division Researcher
School of Engineering, The University of Tokyo

Majored in biotechnology at School of Agricultural and Life Sciences, The University of Tokyo and received his Ph.D (agriculture). Agricultural and Life Sciences Engaged in research into solvation structure using molecular dynamics and charge-separated states using quantum chemistry.

Motivation for applying for the position
I wanted to expand the research for charge-separated states of photosynthesis and solar-cells from the standpoint of "energy creation" using the K Computer.

Mission / Role
To simulate the process of electron transfer from the charge separation to the redox reaction in order to propose guidelines to enhance the efficiency of photo-energy conversion.

Daniel J.Sindhikara



Molecular Science Division Researcher
Institute for Molecular Science, National Institutes of Natural Sciences

Majored in physics at the University of Florida. After receiving his Ph.D., began conducting research into molecular recognition at the Institute for Molecular Science.

Motivation for applying for the position
I had been involved in research on the next-generation supercomputer project at the Institute for Molecular Science, and I wanted to continue that research.

Mission / Role
My mission is the application of 3D-RISM and development of analysis tools. Specifically I am developing use of 3D-RISM for drug design. Currently, I am modelling the binding of Tamiflu to Neuraminidase.

Ambition
Ultimately, I'd like to bring 3D-RISM drug design to the point of complete automation. Under the course of the research, I'd like to create tools that can be used in general applications in addition to drug design.

Kanako Yoshizawa

Condensed Matter Physics Division Researcher
Institute for Solid State Physics, The University of Tokyo

Majored in physics at Graduate School of Science and Technology, The Sophia University and received her Doctorate of Science. Engaged in research into physics theory at the Institute for Solid State Physics, The University of Tokyo.

Motivation for applying for the position
The use of large-scale parallel computing will be indispensable for progress in research from this point on. So I'd like to participate in the supercomputer project.

Mission / Role
Optimization of the TAPP/QMAS plane wave basis first principles calculation code. The plane wave basis DFT code is one of the most basic in first principles calculations, and several software programs have been developed in Japan as well. We plan to either choose one of them or combine them and add functions to create a software program that can compete with the major software programs overseas.

Ambition
I'd like to work on the development of packages that are convenient and highly expandable and can be used by many researchers. And I'd like to link this to the discovery of a new type of physics that uses the new generation of high-speed computers.

Masashi Noda

Molecular Science Division Researcher
Institute for Molecular Science, National Institutes of Natural Sciences

Majored in material engineering at the School of Engineering, The University of Tokyo and received his Ph.D (engineering). Engaged in research into optical response of nanostructures based on large-scale computing at the Institute for Molecular Science.

Motivation for applying for the position
Up to now, I've been engaged in numerical calculation type research into electronic dynamics based on large-scale computing. I'd like to expand this research into ultra-parallel large-scale computing using the K Computer.

Mission / Role
To conduct tuning of real-time, real-space electronic dynamics programs on the K Computer, and also develop ordinary numerical calculation algorithms and help with research into other topics.

Ambition
I'd like to conduct large-scale optical response calculations for energy transfer and solar cells in order to gain an understanding of natural phenomena, and also acquire basic knowledge relating to device development.

Takehiro Yonehara

Molecular Science Division Researcher
Graduate School of Arts and Sciences, The University of Tokyo

Majored in theoretical chemistry at the Graduate School of Science, Kyoto University and received his Ph.D (science). Engaged in research into molecular nonlinear science at the Graduate School of Arts and Sciences, The University of Tokyo.

Motivation for applying for the position
I wanted to participate in cutting-edge molecular science that goes beyond theoretical predictions of dynamics, such as creating new molecular phases that do not exist in the natural world and controlling their reactions.

Mission / Role
To create a bridge between various theoretical science computing techniques that have developed, and a space that can be shared with people from other fields of computational science.

Ambition
I'd like to communicate in various ways the theories and computation skills that I have absorbed, and to contribute to scientific advancement through work in the field of computational science.

The Expected Conditions for CMSI Division Researchers from Experimental Chemistry

Haruo Inoue
Professor, Center for Priority Area, Tokyo Metropolitan University

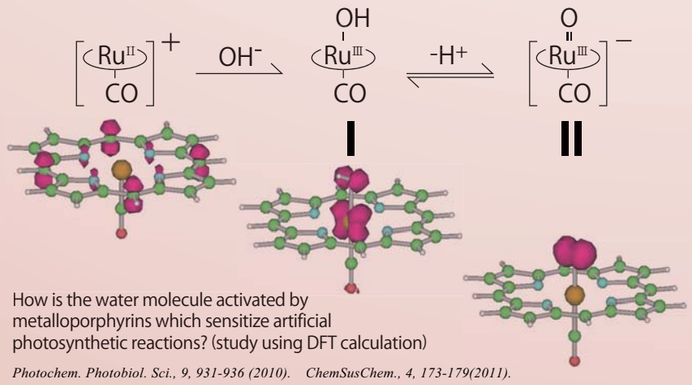
I would like to begin by discussing artificial photosynthesis, a research area in which I am currently engaged. Artificial photosynthesis is a system having a mechanism, by which sunlight and water as electron source are used to reduce materials to produce high-energy ones such as hydrogen and carbohydrates. Unlike solar cells, the artificial photosynthesis could extract desired amount of energy when needed. The reduction processes with water as the electron source would not produce any pollutants at all. From the viewpoint of materials circulation as well, this method is thought to provide an ideal next-generation energy system.

Nevertheless, a challenge to even partly mimic the ingenious mechanisms of the natural system is not so easy. In natural photosynthesis, multiple photons are harvested in antenna system, and the photons are efficiently utilized to activate the oxygen-evolving complex into a highly oxidized form that enables the oxygen evolution. The highly oxidized state is amazingly maintained during the reaction of four-electron oxidation of water. In our research, we are focusing our attention on one-photon excitation of the artificial system that induces two-electron oxidation reactions. In recent years, there has been a major breakthrough, and the actual realization of artificial photosynthesis with water is now almost on the corner. We are now working on the elucidation of the reaction mechanism in molecular level. How the water molecule is activated in the one-photon/two-electron oxidation reaction should be the central subject to be clarified. Theoretical calculation using the density-functional approach has been a very powerful tool in the study.

Japan is one of the leading countries in the world in the area of theoretical chemistry. Nevertheless, if theoreticians alone try to approach any scientific subjects only from a theoretical viewpoint, the results may tend to lack a "reality" of state of the arts in experimental science. In order to not merely develop techniques of calculation but to verify and make them into universal tools, I think researchers, who can step back a bit from the techniques themselves and take a so-called "interpreter's" perspective, would be indispensable for the key-points. The Division Researchers at CMSI who pursue research in multiple research groups on the cutting edge of the corresponding field would be expected not to merely share information and to have communication among the groups and other fields, but would develop into this new type of researcher.

In the future, what if — for example — the framework would expand, so researchers would not only remain at CMSI but also take up residence at an experimental chemist's laboratory for three months or so in response to a proposal? Actually, theoretical calculations of electronic states on a very high level are already being carried out at experimental chemistry laboratories. The greater progress would be expected in experimental analysis than is now being done, if the support of theoretical chemists could be obtained at the initial stages of calculation. Conversely, the opportunity to learn the essence of experimental chemistry through such a "give-and-take" manner with experimental chemists would be a great stimulus to theoretical chemists as well. Furthermore, it would undoubtedly open up new fields of study.

The mechanisms at each level of time and space axis on an actual material are now going to be elucidated, and then those mechanisms would be correlated with each other and be generalized to lead to prediction and design of new materials. Experimental chemists, too, have high hopes for the future advances of computational materials science.
(August 11, 2011 at the Advanced Institute for Computational Science)



How is the water molecule activated by metalloporphyrins which sensitize artificial photosynthetic reactions? (study using DFT calculation)

Photochem. Photobiol. Sci., 9, 931-936 (2010). ChemSusChem., 4, 173-179(2011).

Interview with RSDFT Developer Junichi Iwata

Subject
Junichi Iwata
Lecturer, Graduate School of Engineering, The University of Tokyo

Interviewer
Yoshimi Kubota
2nd year Ph.D candidate majoring in earth and planetary science Graduate School of Science, The University of Tokyo

RSDFT stands for the "Real-Space Density-Functional Theory" calculation method. It is an application for performing first-principles calculations of various material properties without depending on empirical adjustment parameters. RSDFT is an attempt to conduct first-principles calculations on a scale of 100,000 atoms using the K Computer. We talked to Junichi Iwata of the University of Tokyo, the person who has been the driving force behind the development project, to ask what "first-principles calculations" are and the distinguishing characteristics of RSDFT.

What are First-principles Calculations?

Various materials are present around us. Their properties, such as color and hardness, are many and varied. How are these properties determined? Condensed matter physics researchers investigate the behavior of electrons and atomic nuclei in order to understand the nature (physical properties) of materials. In such microscopic level, however, it is difficult to understand all of the behavior of electrons and nuclei through experimentation alone. For this reason, numerical calculations or numerical experiments play an important role.

First-principles calculation is a method of performing such the crucial role. "First principle" means "the most basic principles, ones that cannot be deduced from other principles or hypotheses and so on." The term is also used in philosophy and other disciplines in addition to physics. Dr. Iwata made clear that there are subtle differences in what is meant by "first principles" depending on the field of research.

"In condensed matter physics, 'first principles' refers to the fundamental laws of quantum mechanics. Calculations that use these fundamental laws as a starting point and include no empirical parameters, except the fundamental physical constants such as electron mass and charge, for the purposes of adjustment with experimental results, are referred to as first-principles calculations.

The ultimate goal of condensed matter physics is to predict the properties of all of the materials that may exist in the world, based on the first principles of quantum mechanics. However, it is practically impossible to perform all calculations starting from the first principles without any approximation. Depending on the target of researches and the scale of the system being considered, the fundamental equation must be transformed into more sophisticated one suitable for practical calculations, and approximation must be applied to get results with required accuracy as fast as possible."

Even calculations that are generally referred to as first-principles calculations are of various types, depending on the basic equation and the degree of approximation. The Real-Space Density-Functional Theory (RSDFT) that Dr. Iwata has been developing is a program for performing first-principles calculations in quantum mechanics for systems with many electrons and atomic nuclei, based on the density-functional theory that was awarded the Nobel Prize for chemistry in 1998. First-principles calculations predict physical properties more reliable than methods in which empirical parameters are introduced. However, the first-principles calculations are disadvantageous in that they are only capable of handling a small number of atoms (it is said that they can handle at most several hundred to a thousand atoms). Dr. Iwata says that RSDFT makes it possible to perform calculations for systems consisting of 100,000 atoms.

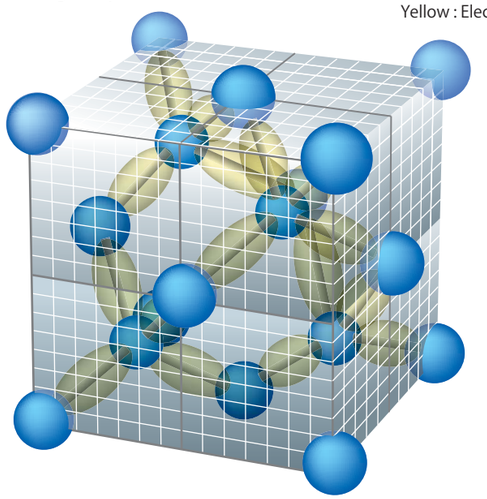
What is a Program RSDFT?

In order to determine physical properties, it is crucially important to calculate the electron states. To examine the materials around us, it is sufficient to consider only systems made up of valence electrons (outer electrons) and ions (aggregates of core electrons and atomic nuclei). RSDFT uses the density-functional theory to calculate valence-electron states. Density-functional theory can calculate the energy ground state of electrons (expressed as a wave function) using only the density distribution of electrons. As these calculations are simpler than solving the Schrödinger equation, they are suitable for solving many-electron systems. "RSDFT is designed to solve the Kohn-Sham equation, the fundamental equation in density-functional theory, in the most efficient manner possible on supercomputers," says Dr. Iwata. RSDFT is characterized by the approach that the Kohn-Sham equation, which is a partial differential equation mathematically, are solved as a finite-difference equation numerically.

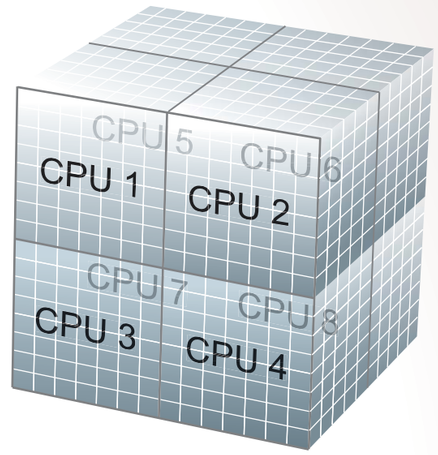
In the first-principles calculations for up to several hundred atoms that have been performed up to now, great success has been achieved with calculation techniques that express wave functions as superposition of simple plane-wave basis and use fast Fourier transformation (FFT). However, as computers become larger in size and massively parallel in

Fig.1 Discretization and parallelization for the purpose of conducting real-space calculations

Silicon crystal unit cells
Blue : Silicon atomic nuclei
Yellow : Electron density distribution



Electrons (yellow) are present in a continuous distribution around silicon atomic nuclei (blue) arranged in a space. In the real-space method, this continuous electron density distribution is depicted as points on a discrete mesh.



The real-space mesh is divided into large blocks. A different CPU handles each block, and adjacent CPUs communicate with one another and execute calculations in a coordinated manner.

nature, FFT requires enormous amounts of communication time, and as a result this has become a bottleneck for massively parallel computing. But with RSDFT, Dr. Iwata has developed a technique for calculating wave functions using the real-space method, which in theory was known to be able to draw out sufficient performance from parallel computers. In the real-space method, the space is represented as a discrete three-dimensional mesh, and numerical calculations are performed to determine wave function values at each point on that mesh. Moreover, the mesh space is divided into several blocks, and each block is calculated by different CPUs. In other words, the actual space that has been divided into blocks is mapped onto the computer that has been divided into compute nodes in the same manner (Fig.1). This allows the work to be allocated in an efficient manner and enables parallel computing with little waste. The calculation of wave functions with the real-space method eliminates the need to use FFT, thereby resolving the communication problem.

Interchange with Computer Scientists Resulted in Dramatic Progress

RSDFT has another advantage with respect to increasing calculation efficiency: the Gram-Schmidt orthogonalization algorithm. Orthogonalization of wave functions is an indispensable calculation. However, the computational cost of the orthogonalization is proportional to the third power the system size, and therefore the simulation of large physical systems resulted in an explosive increase of the computational time. "The problem was solved by replacing the algorithm based on the inner product of vectors with an algorithm based on the matrix product, which can be computed highly efficiently" says Dr. Iwata. Borrowing the wisdom of computer science made it possible to dramatically increase calculation efficiency.

Junichi Iwata

Studied techniques for programming electric circuits and the like in his student days, but became interested in physics (especially quantum mechanics) in the course of pursuing independent study to substantiate calculation techniques. In graduate school, went on to work in a nuclear theory laboratory, and was awarded his Ph.D for research into the optical response of electron systems using the time-dependent density-functional method. Began research into parallel computing in 2005. Also began teaching computer science as a CMSI lecturer in August 2011. Interests include eating ramen, playing mah-jongg and jumping.

The development of RSDFT was a continuation of the PACS-CS (Parallel Array Computer System for Computational Sciences) development project at the University of Tsukuba. At monthly joint meetings with computer science researchers, Dr. Iwata explained what he wanted to accomplish with RSDFT. "I explained many times what I wanted to do, and they gave me various kinds of advice," recalls Dr. Iwata. "Initially I found it is difficult to understand the computer science jargon, but after repeating the face-to-face meetings several times, we became to be able to talk smoothly without any problems. In addition to the Gram-Schmidt algorithm, I was able to learn the latest theories in computer science, outside of my expertise. That was also helpful for developing the program." Close communication with computer science researchers appears to have been the key of the success.

At the same time, the one-to two-year period during which Dr. Iwata was focused on developing RSDFT was also a frustrating time for him. Dr. Iwata's main duty is physics research. Because so much of his time was taken up with software development, he was unable to do the work that he should do as a researcher, producing data and publishing the achievements in the form of academic papers. While he was working to develop RSDFT, he battled uncertainty with regard to whether or not he was doing the right thing. How did he keep up his motivation? "I knew that when I completed, I'd be able to calculate anything. I believed that it would surely have a major impact. And I'm a person with a great deal of patience." Dr. Iwata's inherent tenacity enabled him to get through the periods in which no achievements were produced. However, currently in Japan it appears that researchers are not held in high regard for developing software alone. "Someday I'd like to change that," says Dr.Iwata, aware of his position as a member of the CMSI project.

Fig.2 Structural changes in transistors as a result of miniaturization

Use of a three-dimensional structure enables increased control of the current between source and drain by the gate electrode

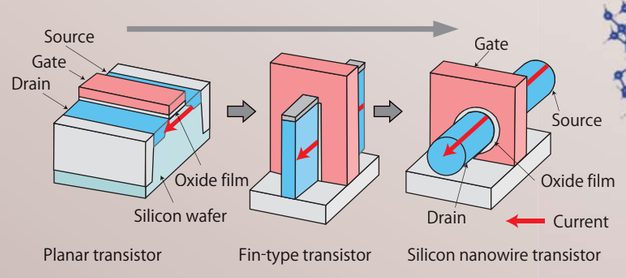
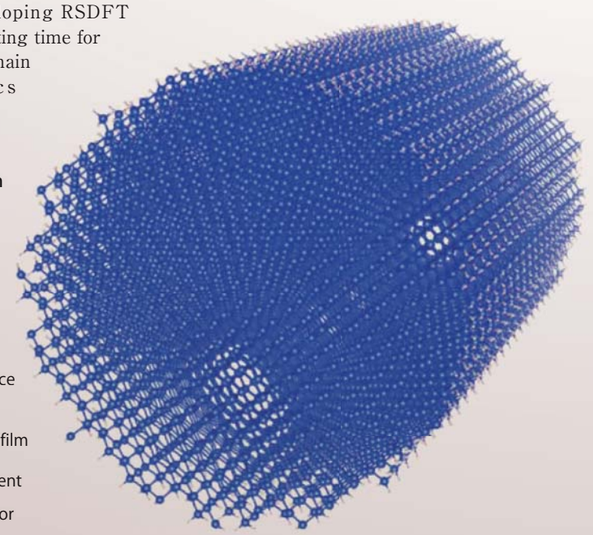


Fig.3 Atomistic model of a silicon nanowire (section diameter: 5 nanometers)



Application to Next-generation Semiconductor Device

The K Computer makes it possible to execute first-principles calculations on the scale of several tens of thousands to 100,000 atoms. What can be studied? In their simulations of 100,000 atoms, Dr. Iwata and his colleagues are targeting semiconductor devices. Semiconductor devices are an indispensable part of the PCs, cell phones and other electronic devices that we use in our daily lives. Miniaturization of these devices has been pursued in order to reduce power consumption and achieve faster speeds. When a device has been reduced down to the size of several nanometers, however, the quantum mechanics behavior of the electrons comes to have a direct impact on performance, and it is difficult to establish a detailed design approach to such devices through experimentation alone. For this reason, there are great expectations for first principle computing.

The field-effect transistors that have been used in semiconductor devices have a structure in which an oxide film and a metal object called a gate are placed on top of a flat silicon wafer. The voltage of the gate electrode is turned on and off to control whether or not the current flows in the silicon, making the device function as a switch. However, if the device is made too small (on the level of several nanometers), there is a tiny bit of current leakage even when the current flow is off, and therefore transistors are nearing the point at which miniaturization is no longer feasible. For this reason, nanowire transistors with cylindrical or square column shapes rather than the conventional two-dimensional laminated structure have been proposed as the next generation of semiconductor devices. Nanowire transistors will have a structure in which the oxide film and gate metal enclose a wire made of silicon (silicon nanowire)(Fig.2). In actual silicon nanowire transistors, the cross-sectional diameter is expected to be 10-20 nanometers, and the distance that current will flow is expected to be 5-10 nanometers (Fig.3). The transistor will be made from 100,000 silicon atoms, that is exactly the size which can be calculated using the K Computer. Dr. Iwata speaks enthusiastically about these devices, saying "I want to perform calculations on the K Computer to clarify the physical properties of nanowire transistors in order to develop these transistors for actual use."

Besides semiconductor devices, biomolecules also have been focused as another target of RSDFT. The use of RSDFT will enable simulation of a entire molecule in the case of a simple protein. Since RSDFT can be applied not only to solids but to liquids and gases as well, it is expected to have applications for a wide variety of materials.

Research assistance provided by Shinya Kyogoku
(Graduate School of Engineering, the University of Tokyo)
Pictures provided by Kuniyuki Kakushima
(Tokyo Institute of Technology)

Yoshimi Kubota

◆ **Interviewer's Postscript**

Dr. Iwata is currently pursuing joint research with the aim of adding molecular dynamics and other new computing functions to RSDFT. Reportedly he has earned the solid trust of the joint developers and software users involved in the project. I was very impressed by the fact that during this interview he used the blackboard and slide references to carefully explain the mathematical expressions and technical terms to me. I look forward to following Dr. Iwata's future career as a computer science educator both at CMSI and elsewhere.

【Number One in the World for Software, Too?】

In June 2011, we received some wonderful news. At the 26th International Supercomputing Conference (ISC'11 - see pg.15), the K Computer was ranked number one in the world in the Top 500 ranking of computer processing performance for its world's highest performance of 8.162 petaflops. This November, the winner of the IEEE Gordon Bell Prize, the world's highest award for software development, will be announced. The IEEE Gordon Bell Prize has been called the Nobel Prize of the supercomputer world, and it is awarded for breakthroughs in parallel computing during the year. RSDFT has been nominated for this prize and is currently a finalist. We hope the outcome brings recognition as world number one in the area of software as well.

Application Spec Sheet **[RSDFT]**

Code Name	HP-RSDFT
Method / Algorithm	Real-space finite-difference pseudopotential method/ Conjugate gradient method
Overview / Features of Code	Can perform first principle electron state calculations based on density-functional theory, using the real-space finite-difference pseudopotential method. Suitable for massively parallel computing, as fast Fourier transformation is not required. The amount of computation is proportional to the system size to the third power, but most of the calculations are matrix product calculations, so calculations can be executed with extremely high efficiency.
Materials for Simulation	Metals, semiconductors, surfaces / interfaces, defects, nanostructures
Development Leader	Atsushi Oshiyama
Developers / Developing Institutions	Junichi Iwata, etc. / The University of Tsukuba, The University of Tokyo, RIKEN etc
Development Period	Development began in FY 2006
Development Language / No. of Lines of Source Code	Fortran, 50,000 lines
Operating Environment	PACS-CS, Tsukuba T2K, SGI Altix, K Computer (Linux)
Parallelization Method	Hybrid parallelization (MPI and OpenMP)
Parallelization Status	Max. 12,288 cores (K Computer), peak performance ratio 10 - 30%
Software Release	Conditional release planned (FY 2012)
Related / Competing Applications	RRSPACE (Osaka University), PARSEC (University of Minnesota) etc., first principle computing
Other Functions	Can handle not only periodic boundary conditions but isolated system boundary conditions (molecules, etc.) as well

CMSI Calendar

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

● August 11-12, 2011
2nd Symposium of the Theoretical and Computational Chemistry Initiative (TCCI)
Venue : Advanced Institute for Computational Science

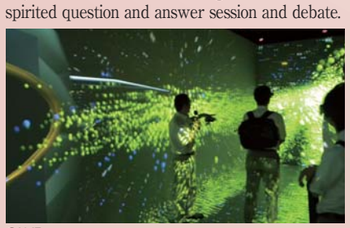
TCCI was established in February 2011 as the molecular science division of CMSI. A workshop was held as the 2nd TCCI Symposium following the 1st Symposium that was held in February of this year. Some 100 researchers came together in the fierce heat of summer for presentations on research progress and the state of program development for the K Computer.

In their initial remarks, the guest speakers expressed their hopes for rapid achievements of a kind that would only be possible with the K Computer. Lectures by the invited speakers included those by representatives chosen from among the Priority Area Researchers, researchers working on core applications for the Next-Generation Integrated Nanoscience Project leading the development of programs for the K Computer, and researchers affiliated with the RIKEN Advanced Institute for Computational Science (AICS). These included lectures by Ryo Maezono, associate professor at Japan Advanced Institute of Science and Technology, on the topic of condensed matter physics, and Toshiyuki Koyama, professor at Nagoya Institute of Technology, on the topic of materials science.

In addition, Professor Haruo Inoue of Tokyo Metropolitan University, who is also an artificial photosynthesis researcher in charge of research on "Chemical Conversion of Light Energy" in the PRESTO project of the Japan Science and Technology Agency (JST), gave a special lecture entitled "The Goal of Artificial Photosynthesis," in which he reported that considerable progress has been made in understanding the basic process by which photosynthesis can be achieved artificially.

Many attendees participated in the tour of the Cave Automatic Virtual Environment (CAVE), a multi-screen 3D immersive display system, that was led by Professor Akira Kageyama of Kobe University, serving to indicate the great level of interest in CAVE. The social gathering that began in the evening was also extremely well attended, with more than half of those present participating. At the gathering, AICS Director Kimihiko Hirao offered words of encouragement and expressed his great hopes for the achievements to be produced by TCCI.

The poster session in the afternoon on the second day was held in a small lounge but featured a spirited question and answer session and debate.



CAVE tour

Presentation

Poster Session

Photos : Kazuhiro Takemura (The University of Tokyo), Yoshitake Sakae (Nagoya University)

● Field 2×Field 5 Interdisciplinary Exchange Workshop
Date : July 26, 2011
Venue : Center for Computational Sciences, University of Tsukuba

● Magnetism Division, Element Strategies Working Group
Date : July 29, 2011
Venue : Faculty of Science, The University of Tokyo (Hongo Campus)

● 15th Molecular Simulation Summer School
Date : September 9 - 11, 2011
Venue : Ushimado Marine Laboratory, Faculty of Science, Okayama University

● Center of Computational Materials Science 1st Symposium
Date : September 12 - 13, 2011
Venue : Institute for Solid State Physics, The University of Tokyo

● CMD® Workshop (organized by CMSI and Osaka University)
With Tutorial Course
- 19th September 5 - 9, 2011
  Venue : Cybermedia Center, Osaka University
- CMD® Workshop in the Philippines (supported by De La Salle University)
  Date : October 11 - 12, 2011
- CMD® Workshop in Vietnam (supported by Vietnam National University, Ho Chi Minh City)
  Date : December 8 - 10, 2011
- CMD® Workshop in Thailand (cosponsor not yet finalized)
  Date : Mid-February, 2012 (planned)
- 20th March 6 - 10, 2012
  Venue : International Institute for Advanced Studies (Kyoto)

● 2nd CMSI Young Researcher Technical Workshop (held concurrently with panel discussion on "Considering the Next Supercomputer After the K Computer")
Date : September 14, 2011
Venue : Institute for Solid State Physics, The University of Tokyo

- 3rd CMSI Young Researcher Technical Workshop
  Date : November 25, 2011
  Venue : Komaba Campus, The University of Tokyo
- 4th CMSI Young Researcher Technical Workshop
  Date : February 1, 2012
  Venue : Institute for Materials Research, Tohoku University
- 5th CMSI Young Researcher Technical Workshop
  Date : Early March, 2012 (planned)
  Venue : Not yet decided

● 3rd Joint Research Interchange Forum, HPCI Strategy Program
Date : October 3, 2011
Venue : Advanced Institute for Computational Science

● TCCI Interchange Symposium with Experimental Chemistry
Date : November 10 - 11, 2011
Venue : Fukui Institute for Fundamental Chemistry, Kyoto University

● Battery Division, Element Strategies Working Group
Date : November 9, 2011
Venue : Koshiba Hall, The University of Tokyo

● Catalyst Division, Element Strategies Working Group
Date : November 12, 2011
Venue : Fukui Institute for Fundamental Chemistry

● TCCI Industry-Academia Cooperation Symposium
Date : November 24, 2011
Venue : Nomura Conference Plaza, Nihonbashi

● Computational Materials Science Symposium
Date : December 6 - 7, 2011
Venue : Institute for Materials Research, Tohoku University

● TCCI Winter College
(Molecular Simulation)
Date : December 12 - 16, 2011
Venue : Okazaki Conference Center, National Institutes of Natural Sciences
(Quantum Chemistry)
Date : December 19 - 20, 2011
Venue : Okazaki Conference Center, National Institutes of Natural Sciences

● Materials Science • MPI Workshop
Date : December 12, 2011, January (planned), February (planned)
Venue : Nakanoshima Center, Osaka University (December)

● CMSI Joint Seminar
Date : January 30 - 31, 2012
Venue : Institute for Materials Research, Tohoku University

● Industry-Government-Academia Cooperation Symposium
Date : Early February, 2012 (planned)
Venue : Not yet decided

● Quantum Chemistry Massively Parallel Computing Workshop
Date : February 13 - 17, 2012
Venue : Okazaki Conference Center, National Institutes of Natural Sciences

K Computer News

ISC'11 Report

From "K" to "Exa"

Haruhiko Matsuo
Project Researcher
Graduate School of Engineering,
the University of Tokyo

The International Supercomputing Conference (ISC) '11 was held June 19~23 in Hamburg, Germany. Haruhiko Matsuo attended the conference and experienced for himself the transition from the K Computer to exascale supercomputers that is already underway on the front lines of computer science throughout the world.

The ISC is the world's largest international conference and exhibition devoted to supercomputing, storage and networks. Held annually since 1986, the event features the announcement of one of the two annual updates to the Top 500 rankings. I attended this year's conference because, as a researcher, I wanted to investigate the worldwide trends in this field.

The first day had a festival eve atmosphere and featured tutorials, workshops and the like. From the second day on, the main event was held. As in the case of a regular academic conference, it consisted of an international conference plus an exhibition. However, the conference was characterized by the participation of many top-level high-performance computing (HPC) vendors such as NVIDIA and SGI as presenters, giving it a strong business color as opposed to an academic atmosphere. Because it was not skewed to the academic side of things, I felt it gave attendees a glimpse of the actual supercomputers that will appear in the near future.

On the first day, I attended an MPI / OpenMP hybrid programming tutorial. It was a high-level tutorial that afforded the opportunity to gain hands-on knowledge in hybrid programming.

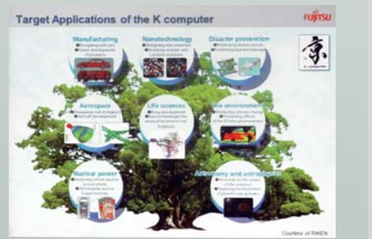
On the second day, the Top 500 ranking was announced, and I was surprised to

hear that the K Computer had jumped to the number one position. In Japan, people tend to focus only on the flops value (a performance indicator consisting of how many times per second the computer can perform floating point number calculations). But it appears that it was features such as the low power consumption and long continuous running time that had a greater impact

and resulted in the high evaluation.

On the third day, I was able to hear a debate on the exascale supercomputing environment between Dr. David Kirk of NVIDIA and Dr. Thomas Sterling, a giant in the field of parallel architecture. There were also various other interesting presentations, too numerous to mention.

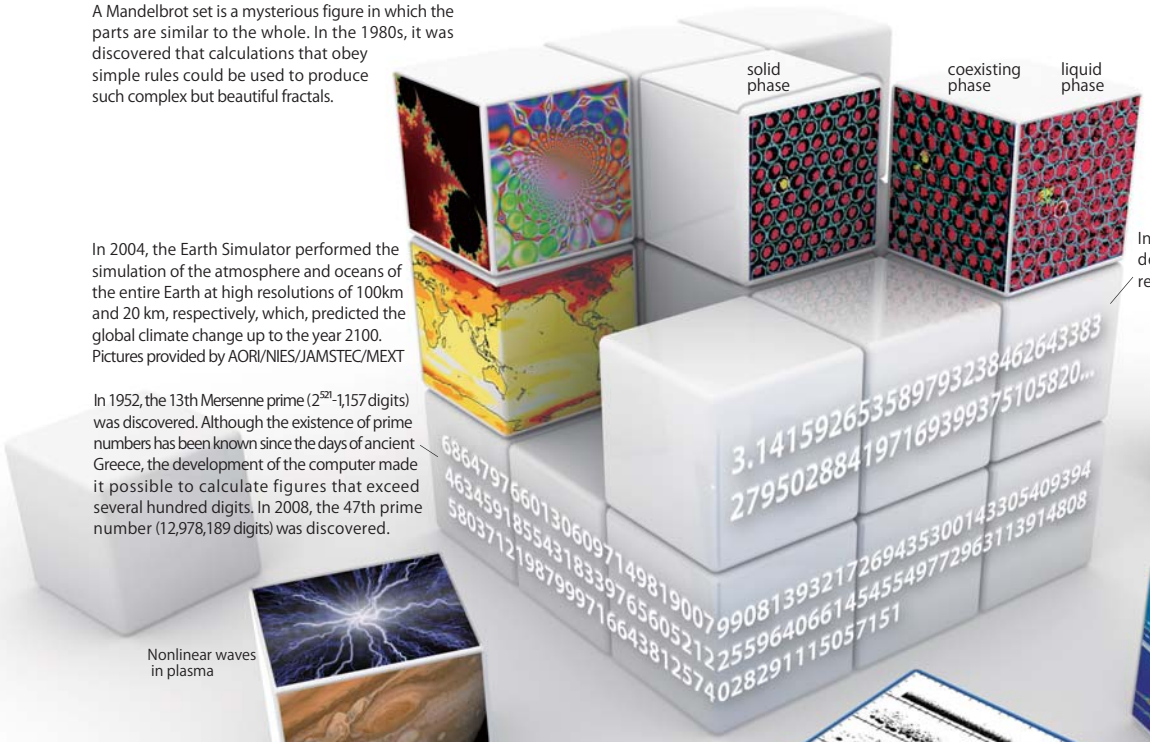
What impressed me most as a result of attending ISC'11 was the fact that next-generation supercomputing is already on the exascale level. Up until very recently, the K Computer was referred to as the next-generation supercomputer, so once again I was astonished at the rapidity of the generational transition in supercomputing. Also, by being able to actually hear the voices of people from top supercomputer vendors and others near that level, I was able to get some solid leads in my investigation into what the trends in the world of supercomputers will be in the near future.



Great Monuments Built by Computers

The uses of computer simulations are not limited to verifying conjectured hypotheses and elucidating the results of real-life laboratory experiments. Creative numerical experiments can sometimes produce results that surpass the expectations of human beings and even give birth to completely new fields of research.

A Mandelbrot set is a mysterious figure in which the parts are similar to the whole. In the 1980s, it was discovered that calculations that obey simple rules could be used to produce such complex but beautiful fractals.



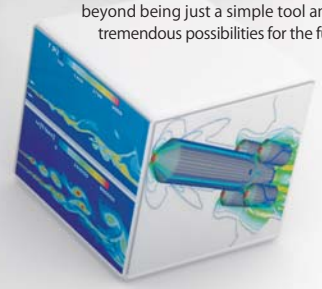
In 2004, the Earth Simulator performed the simulation of the atmosphere and oceans of the entire Earth at high resolutions of 100km and 20 km, respectively, which, predicted the global climate change up to the year 2100.
Pictures provided by AORI/NIES/JAMSTEC/MEXT

In 1952, the 13th Mersenne prime (2^{521}-1,157 digits) was discovered. Although the existence of prime numbers has been known since the days of ancient Greece, the development of the computer made it possible to calculate figures that exceed several hundred digits. In 2008, the 47th prime number (12,978,189 digits) was discovered.

The Alder Transition (1957 - 1960). It was discovered through simulations that a phase transition between the solid phase and the liquid phase occurs in particle systems with only pure hard-core repulsions.
Pictures provided by Hiroyasu Toyoki

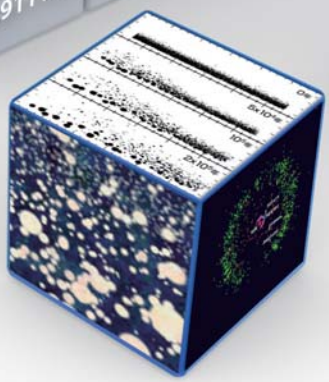
In 1943, ENIAC calculated the value of π to 2,037 decimal places. The number of decimal places reached 5 trillion in 2010.

In 1997, Deep Blue became the first computer to defeat a human world chess champion opponent, demonstrating that the computer had developed beyond being just a simple tool and held tremendous possibilities for the future.



The numerical wind tunnel (NWT) created the basis for computer fluid dynamics simulations of airplanes and space transport vehicles.
Pictures provided by JAXA

The nonlinear lattice experiment conducted by Fermi, Pasta and Ulam (1953). The discovery of the quasi-periodic behavior seen in interacting particles was subsequently developed into solitary wave (soliton) and chaos research. (The image shows solitary waves found in nature.)
Pictures provided by NASA



The GRAPE, a special-purpose computer for astronomical simulation, calculates the gravity interactions of multiple astronomical bodies. In 1997, it was discovered that multiple protoplanets grow in a dominant fashion in the course of the formation of solar systems.
Pictures provided by Eiichiro Kokubo

Torrent : The Newsletter of the Computational Materials Science Initiative (CMSI) No.3, September 2011

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