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Torrent

10^{16} Weave New Materials

Special Issue Software Development in CMSI

CONQUEST Aims for Global Domination

Interview with David Bowler and Tsuyoshi Miyazaki, developers of CONQUEST

Torrent [tɔ:rənt]:
The Newsletter of the Computational Materials Science Initiative (CMSI)

Software Development in CMSI

The K computer has been made available for general use since last September. Besides the development of algorithms, the development of community code is also essential for making effective use of this leading edge computer. In this issue we look at the current state of software development in the field of computational materials science, as well as introducing initiatives to develop open source programs that have already started within CMSI, and the order-N first-principles software CONQUEST being developed under an international joint project, aiming to define the direction that future software development should take.

Improved computer performance and advances in algorithms

In the 66 years between the emergence of the world's first general-purpose electronic computer, ENIAC, in 1946, the computational performance of leading edge supercomputers has progressed by a factor of more than 50 trillion. Since the TOP500 list (http://top500.org/) has started in 1993, performance has improved by a factor of about 270,000 in just 19 years. Thanks to the overwhelming evolution of these computers, it is becoming possible to conduct highly accurate simulations of large-scale systems that were unthinkable in the past, such as first-principles calculations with systems of one million atoms, or molecular dynamics simulations with systems of ten million atoms.

In condensed matter physics, molecular science, and materials science, which are the research field of CMSI, various other approaches have come to be used including quantum chemical calculation, Monte Carlo method, exact diagonalization of matrices, as well as multiscale and hybrid approaches combining several methods. One of the main characteristics of simulations in "computational materials science," which covers these fields, is the focus on the equilibrium state or steady state of systems with strong correlations, rather than the temporal evolution of systems that can be obtained from a specific initial state. Or when researchers are considering non-equilibrium states, very long simulations from femtoseconds to picoseconds and nanoseconds are required. Furthermore, the systems to be simulated are not necessarily three-dimensional. In simulations of strongly correlated quantum many-body systems, non-local operations are often used as a means to incorporate the effects of quantum correlation accurately and efficiently, or to arrive at equilibrium state with as few iterations as possible. Consequently, huge computation and network communication capacity are required.

To make full use of leading edge computers like the K computer and to make advances in next generation materials science, development of the performance of computers themselves is not sufficient. In order to efficiently solve the fundamental equations of materials science, advances in computational science theory—in other words algorithms—have played an extremely important role. Some representative examples are the fast Fourier transform (FFT), the Monte Carlo method and other means of quickly solving given equations. In addition, the development of the approximation techniques that can reduce the computational cost without spoiling the accuracy, such as the fast multipole method (Torrent No.2), the divide-and-conquer method (Torrent No.5) and the order-*N* method mentioned in this issue as well as the methods designed for modern computer architecture such as the real-space method (Torrent No.3) should also be mentioned.

The current state of the computational materials science

In the field of computational materials science, new methods are being proposed daily, and researchers are constantly testing them in applications. It is not unusual that just a single researcher or a very small group pursue the whole cycle of identifying an effective model for explaining a phenomenon seen in an actual material, developing algorithms based on various ideas, programming, conducting simulations, analyzing the results, and providing feedback to the effective model. In fields close to experiments and applications, gigantic application programs such as GAUSSIAN for quantum chemistry calculations (see the column on page 5) are widely used, but this is the exception, and many research groups use their own individual programs. When users within a group move on, for example when graduate students graduate, the existence of the programs will be forgotten totally.

The existence of many individual codes means that the input parameters used for calculation and the output of simulation results are frequently done in different formats, too. As a result, it is difficult to save and search data in a standardized way. In addition, this is becoming a significant obstacle to analysis and coupled calculations (hybrid calculations combining two or more different application programs) using tools developed by other researchers.

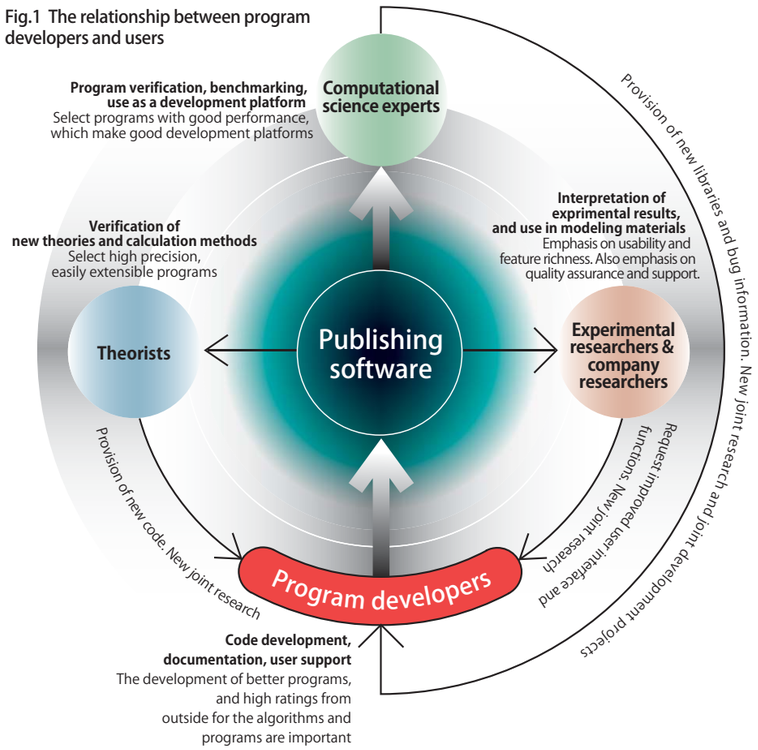
Meanwhile, the cost of developing and upgrading applications is beginning to increase. This applies for example to hybrid parallelization to utilize massively parallel computers and multicore architecture which are currently the mainstream, cache tuning, and optimization of communications for a specific network topology. In order to make effective use of large-scale computers such as the K computer, it is becoming imperative to undertake software development in an organized fashion that goes beyond individuals. Furthermore, cooperation with specialists in computer science and numeric calculation in addition to the field of computational science is becoming increasingly important.

What "publishing software" means?

The Division Researcher program run by CMSI is different from the ordinary doctoral research fellow program (see Torrent No.3). Rather than staying within a specific research group, the mission of participants is to promote the field of computational materials science overall, in other words, developing advanced component technology and establishing the basic technology crucial for next-generation computational materials science. As such, it is a totally unprecedented and unique program. Correspondingly, in order to foster programs themselves in the field as a whole, it is necessary to promote publishing software.

The open source programs referred to here are programs with source code that users can download from the web and so on with comparatively lax terms of use (license). Users can compile and execute the programs themselves, and publish the results of simulations. Open source programs (in the narrow sense) do not include programs that require a joint research agreement, or that are only distributed in

Fig.1 The relationship between program developers and users



binary format. Although the terms of use differ slightly according to the program, users may be able to alter the source code or incorporate their own program in accordance with the calculation required, or they may be able to make modifications to the code and redistribute it. Well known examples are the Linux OS, the Emacs editor, and the GCC compiler.

There are various types of users in the field of computational materials science. Theorists may use the programs as platforms for verifying new theories and approximations, or for trying out new ideas, while experimental researchers and researchers in corporations will use them for interpreting experimental results and modeling real materials. For computational science experts, open source software should be useful for verifying the output results of their own programs, benchmarking computing speed, and as modules for coupled calculations. Meanwhile, the requirements for open source software differ according to the use to which they are put. They include ease of use, richness of feature, speed, accuracy, and so on (Fig.1).

The necessity of community code

Software where the source code is simply made available on the web cannot be called an open source program. In order for it to be used by a wide range of users, first the code must work correctly, and it must have an easy-to-use user interface such as a GUI, as well as documentation in Japanese or English such as manuals for installing and using it, and tutorials for typical users. In addition, user support using email, bulletin boards and so on, and regular courses for users are essential. It is also necessary to respond to requests for bug fixes and new features on an ongoing basis.

To date there is little open source software from Japan in the field of computational materials science. The main reasons for this are the trouble and cost involved in making software freely available. In order to lower the barriers to providing and maintaining open source programs, CMSI is working continuously to provide tools for creating sites for managing source code and providing programs and documentation, as well as improving courses for users and the website which explains the applications available (known as “AppliCafé”). At the same time, we are working to improve the skills of Division Researchers.

Conversely, what is the point of making software open source, and what are the benefits for developers? Releasing programs allows developers to receive feedback from lots of people, allowing them to make their programs more reliable. By accepting code from collaborators, it is also possible to enhance the software by adding new functions. In addition, communication with users frequently leads to the development of new algorithms, new joint research, and the creation of communities. Even if a superior algorithm is developed, there is almost no chance for that particular approach to be evaluated unless it is implemented in the form of software.

This trend has been particularly pronounced recently in the field of quantum chemistry calculation, but in future, it is likely to spread to the whole computational science in general. Ideally, code for new approaches to calculation will be made available as open source, and at the same time, the program will grow in the community as basic software for the implementation of new techniques. If this sort of “community code” can be fostered, it will greatly benefit not only the developers but also the whole community. Providing open source programs is certainly not just a service for other people, it is nothing short of leaving a record of your achievements (science) in the form of software.

In Japan, the K computer has just been made available for public use from the end of September 2012, but already feasibility studies have been started towards construction of next generation exa-scale supercomputers. We will provide application programs critical to the field of computational materials science that are tuned for massively parallel architecture, as well as work proactively with researchers in the computer science field to design the next generation of supercomputers accordingly. Without question, it will become increasingly important to pursue the consolidation of community code for computational materials science in order to establish a productive cycle.

(CMSI public relations subcommittee representative: Synge Todo, the Institute for Solid State Physics, the University of Tokyo)

Why is GAUSSIAN Used Worldwide?

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Establishment of a Global Standard

Today many programs for quantum chemistry calculation exist. But one has an overwhelming share worldwide. That program is GAUSSIAN. This program was developed by a group led by John A. Pople, co-winner of the Nobel Prize for Chemistry in 1998 for his development of computational methods in quantum chemistry. GAUSSIAN is currently provided by Gaussian, Inc. The program is so widely used — not only in academia but in industry as well, for education, academic research and developmental research — that it is said that a supercomputer will not sell unless it can run GAUSSIAN. It is in the background of this overwhelming share that GAUSSIAN has become the standard for quantum chemistry calculation. GAUSSIAN is a "standard" not only in the sense that it is used to verify whether or not the calculations of other programs are correct, but also because so many people use GAUSSIAN that the theory and calculation methods contained in GAUSSIAN are seen as being standard calculation methods. This is the result of researchers of the first rank developing state-of-the-art theory and calculation methods on an ongoing basis and then providing the code to GAUSSIAN.

Exceptional Ease of Use

The history of GAUSSIAN dates all the way back to the 1970 version (GAUSSIAN 70). But I first came in contact with the program in 1975. The shock of that initial encounter is still fresh in my mind today. As I recall, at the time it consisted of some 30,000 lines of Fortran (which made it an exceptionally large program for its time). I remember being amazed at the originality of the program's structure. At the time it was known as the overlay segment method. Each step of the calculations was almost completely independent of the others: a two-electron integral calculation section, an SCF calculation section and so on. For this reason, when new functions were added, it could be done with only the minimal amount of modification to relevant sections. This made GAUSSIAN an outstanding platform for verifying new theories and calculation methods. Another thing that had a profound impact on me was that fact that somewhere in the comments it said that GAUSSIAN was "a quantum chemistry calculation program designed for organic chemists." At the time, anywhere other than the United States, quantum chemists had just started to perform ab initio MO calculations. Looking back on it, it seems as if, even from the stage of initial development, GAUSSIAN had foreseen the situation today, in which it is used as a research tool not just for quantum chemistry but for chemistry in general. Beginning in the mid-1980s, the number of computational chemists increased, and experimental researchers themselves came to conduct quantum chemistry calculations on their own. As a result, the number of GAUSSIAN users increased dramatically. At the time, Hondo and a number of other ab initio MO calculation programs were popular, but among these GAUSSIAN distinguished itself from the others through its ease of use — particularly the ease with which input data could be created. It almost goes without saying that this was a necessary requirement for attaining widespread use. As the number of users increased, inevitably the amount of feedback on modifications and improvements increased as well, and responding to these needs caused the program to expand its advantages over similar programs even further.

A Rare Opportunity to Promote a Japanese Software Worldwide

For many years, people in Japan have been concerned at the total lack of an academic program developed in Japan that is popular worldwide. To avoid any misunderstanding, let me state that many Japanese researchers have provided code for GAUSSIAN and GAMESS and other quantum chemistry calculation programs that are used worldwide. These programs were "made in USA," but the code can be seen as a product of the international community. Each of them is an enormous program consisting of a million lines of Fortran. It would be unrealistic to expect a program that can compete with these to be developed overnight. If the chance for a reset challenge is to present itself, it will come only from inventing a new algorithm with a method that is completely different from existing methods (which would be desirable), or through innovations in computer architecture and programming language — something that turns existing programs into dinosaurs. If we think along these lines, then right now — when massively parallel computers with several orders of magnitude more CPUs and cores are beginning to come into widespread use — may be one of our few chances to develop a revolutionary parallel computing program that is designed for use by next-generation exaflop computers and promote it worldwide.

Current State of First-principles Simulation Programs in Japan and Issues to be Resolved

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Overview of First-principles Simulation Programs in Japan and Other Countries

As its name implies, first-principles electronic structure calculation is a method of calculating the state of electrons, which are almost the sole determinant of material's properties. The method calculates them within a graphic approximation by using density functional theory and so on. This property makes it an appropriate approach to elucidate the individual nature of materials. Although the method requires huge computational resources, there is no doubt that the K computer will greatly expand the range of possible applications for this method. For example, with it we will be able to perfectly handle statistical fluctuations and diversity in material structures, which has often inadequately handled up to now. Such novel scientific progresses are expected hereafter.

There are many programs both at home and abroad for first-principles calculations. However, the programs are becoming more complex as massively parallel computing becomes more and more necessary, and as the target physical quantities become more and more diverse. For this reason, determining the direction that first-principles calculation program development in Japan will take is an important issue to the relevant communities. To comprehend the current state of programs at home and abroad, the Japanese programs are surveyed and classified by the approximation for the electronic correlation and by basis functions to express electronic states (Table 1). First-principles calculations can be generally classified as either condensed matter physics calculations or molecular science calculations. This article will focus only on condensed matter physics calculations. On the other hand, the state of programs aboard is summarized well in the following web page: http://www.psi-k.org/codes.shtml. Among the programs listed on this web page, the ones whose names have been frequently seen or heard by the author are shown in Table 2. The author has also checked the functionality of the programs in the tables, but unfortunately there is not enough space in this article to include such information.

Please be aware that the information on programs in the tables may contain some errors, as the author is not familiar with transport calculations or augmenting methods. Also, the list of the developers in the tables may incomplete, although an effort has been made to survey those that have contributed significantly to the programs.

Although the survey may not be complete in some respects, a comparison of the domestic and overseas programs in the tables reveals that, taken together, the domestic programs cover almost all of the important functions provided by overseas programs. This is a testament to the efforts conducted by researchers of this area in Japan up to now.

Current Status of Programs based on Plane Wave Basis Sets

Among first-principles programs, those based on plane wave basis sets have long histories, and they are advanced in developing various functions and improving the user interfaces. In overseas, there are several famous programs in this category. In Japan as well, there are numerous programs, including one which the author has contributed to. Unfortunately, however, the domestic ones tend to be inferior in terms of diversity of functions and the quality of the user interface. This is probably because the majority of the users of programs in Japan are the developers and the related researchers, and they could not make serious effort to implement functions which are not important for their purposes.

Compared to other kind of programs, the programs based on plane wave basis sets have become popular not only among the developers and the related researchers but also among general users such as experimentalists. Internationally, VASP is a prominent example, and it is achieving popularity in Japan as well. VASP is a paid software, but it prepares good manuals and tutorials, and there is an established community that can answer questions and so on. The number of academic papers that declare the use of VASP is on the rise, and this has led to an increased comfort level for VASP.

Domestically, the programs that are making an energetic push to achieve general popularity include the suite of CMD® related programs by groups in Osaka University (STATE, MACHIKANEYAMA2002, Osaka2K, ES-opt and HiLAPW), OpenMX, Phase and DV-Xα. The DV-Xα uses a unique method which is good at calculating the energy spectrum of solids (including core levels in particular) at a low cost. My survey revealed that it has well written manual and tutorial and an active user community. The number of users seems to exceed that of the average plane wave basis set program in Japan.

Future Directions in First-principles Calculation

What direction should the development of the first-principles programs take from this point on?

It goes without saying that the adopted approximations are not always precise enough. Therefore we have to continue the development of new methods. In addition, to develop multi-physics, multi-scale and other kind of methods that need these calculations as their components, it is necessary to understand the details in them. These two points indicate the need to maintain a platform of the development of the simulation methods. On the other hand, increasingly diverse functions are required for such a platform to keep its competitiveness. Moreover, we have to develop the platforms to support the massively parallel computing and to be easy to use when we prepare input data (pre-processing) and when we visualize the results (post-processing). These make it difficult for a single developer to handle the entire process from the program development through its scientific application, so cooperation on the part of many people is needed.

From this perspective, we should unite the numerous domestic plane wave basis set programs. The need to do this has been discussed for a long time, but little progress has been made. The reason from the developer's standpoint is as follows: these programs were originally developed out of a need of developers themselves and the related researchers. Therefore naturally they are able to understand the details in them. Because the current programs consist of several tens of thousands of lines of code, or more than a hundred thousand, it takes considerable time to understand the details in the programs. This causes a tremendous resistance to switch to another program.

From a user's perspective, the first reason for the lack of progress is familiarity with input and output data formats. Another reason relates to the differences in the details of the programs which exist even if they use equivalent methods. Because of this difference, the results inevitably may include differences that arise from the subtle variations in the computation. This means that we have to calculate accumulated results again to confirm before migrating to another program.

As a result of these circumstances, the promotion for the unification of programs should proceed step by step, in order to persuade the community of users and developers of each program. A first step would be to make it possible to share and compare the input and output data for each program. Ensuring that the same results are obtained across multiple programs for an equivalent input is crucial in the sense of verifying programs and methods. It is also an indispensable requirement for comparing the performance between different programs.

It is also important to foster an environment that the migrating users and developers who do so as the result of the unification can join the community of the destination comfortably. For example, each program exhibits the developer's way of thinking. When programs with multiple ways of thinking are combined together, inevitably there will be some feeling of disunity. Unless this is accepted to some degree, it will not be possible for different developers to come together. Moreover, when encouraging migration from a certain program, it is essential for the candidate destination in Japan to be able to hold their own with those developed overseas, in terms of licensing, the manner of providing detailed information on the program codes and so on. If these things are not in place, the encouragement of migration will serve only to accelerate the "hollowing out" of Japanese software development in this area.

Table 1. Domestic first-principles simulation programs

name	developers	corr	basis
PHASE	Yamasaki (Fujitsu)	1	i
QMAS	Ishibashi (AIST)	1	i
STATE-Senri	Morikawa (Osaka)	1	i
CPVO	Oda (Kanazawa)	1	i
(x)TAPP	TAPP Consortium	1	i
FPSEID	Sugino (ISSP), Miyamoto (AIST)	2	i
unnamed	Oshiyama (Tokyo), Okada (Tsukuba)	1	i
ES-Opt	Kusakabe (Osaka), Ogitsu (Livermore), Tsuneyuki (Tokyo)	1	i
OSAKA2K	Shirai (Osaka)	1	i
TC++	Sakuma (Chiba), Tsuneyuki (Tokyo)	4	i
HiLAPW	Oguchi (Osaka)	1	iii
ABCAP	Hamada (SUT)	1	iii
Ecalj	Kino (NIMS), Kotani (Tottori)	1,3	iii
MACHIKANEYAMA	Akai, Ogura (Osaka)	1,4	iii
TOMBO	Ohno (Yokohama), Kawazoe (IMR)	1,3	iii
RS-DFT	Iwata,Oshiyama (Tokyo)	1	iv
FEMTECK	Tsuchida (AIST)	1	iv
RSPACE	Ono, Hirose (Osaka)	1	iv
ARTED	Yabana (Tsukuba)	2	iv
OpenMX	Ozaki (JAIST)	1	ii
ELSES	Hoshi (Tottori)	1	ii
DV-Xα	Adachi (Kyoto)	1	ii
Electron Transport Simulator	Kobayashi (Tsukuba) Hirose (NEC)	1	vi
unnamed	Watanabe (Tokyo)	1	vi
unnamed	Hu, Watanabe (SUT)	2	iv
ASCOT	Kondo (NIMS)	1	ii
CONQUEST	Miyazaki (NIMS), D. Bowler (UCL)	1	ii,v

Table 2. Overseas first-principles simulation programs

name	developers	corr	basis
VASP	J. Hafner (Austria)	1,2,3	i
abinit	X. Gonze (Belgium)	1,2,3	i
qbox	F.Gygi (US)	1	i
bigDFT	T. Deutsch, S.Goedecker (Germany)	1	vii
CASTEP	M.Payne (UK)	1	i
quantum espresso	DEMOCRITOS, SISSA (Italy)	1,2,3	i
Siesta	E. Artacho (Spain)	1	ii
octopus	A.Rubio (Spain)	1,2	iv
WIEN 2k	K. Schwarz (Austria)	1	iii
CP2K	J. Hutter	1,2	i,ii
CPMD	J.Hutter (US,Germany)	1,2	i
Ontep	P. Haynes (UK)	1	ii
LMTO	O. K. Andersen	1	iii

Approximation method for electronic correlations

1：density functional theory
2：time-dependent density functional theory
3：GW approximation
4：others

Basis set for the wave function

i: plane wave (Fourier transformation)
ii: localized basis set on atoms
iii: augmented basis (ex. augmented plane waves)
iv: real space mesh (structured grid)
v: finite element method (unstructured grid)
vi: 2D plane wave + 1D real space mesh
vii: wavelets

Open Source Software in the Field of Computational Materials Science

This section features publicly released software that has been developed primarily by CMSI researchers. Researchers can download the source code of each of these programs from the Internet and use it in their research. Up to now, few such programs have been released by researchers in Japan, but work is progressing on the construction of distinctive programs in the fields of condensed matter physics, molecular science and materials science in order to establish community codes.

ALPS

Code Name	ALPS
Method/Algorithm	Quantum Monte Carlo method, classical Monte Carlo method, exact diagonalization, DMRG, and DMFT
Overview	Open source software for simulating strongly-correlated quantum lattice models such as quantum spin systems, electron systems etc. The lattice structure, interactions etc. can be specified flexibly using XML. One can select the ideal algorithm (quantum Monte Carlo method, exact diagonalization, DMRG etc.) to match the target system and the physical quantities to be studied. Even researchers who are not specialists in computational physics can easily begin to simulate a variety of different models.
Target Materials	Quantum spin models, Bose-Hubbard models, Fermi-Hubbard models, and other generic quantum lattice models
Primary Developer	Mattias Troyer (ETH Zürich), Synge Todo (The University of Tokyo), etc.
URL	http://alps.comp-phys.org/

clupan

Code Name	clupan
Method/Algorithm	Thermodynamic calculations using the cluster expansion method
Overview	Clupan is software for modeling alloys through the use of the cluster expansion method etc. and evaluating the interaction between atoms by using first-principles calculation. If the effect of the atomic arrangement is estimated without affecting the precision of first-principles calculation, one can derive highly precise ground state structures, thermodynamic quantities, and equilibrium phase diagrams.
Target Materials	Solids containing two or more types of atomic species
Primary Developer	Atsuto Seko (Kyoto University)
URL	http://clupan.sourceforge.net/

DC

Code Name	DC
Method/Algorithm	HF, MP2, CC, and DFT calculations using the divide and conquer (DC) method
Overview	These days, fast quantum chemistry calculation methods attract attention around the world, and various approaches have been devised. The advantages of the DC method are that it can be applied to non-localized electron states and that it can also execute highly precise MP2 and CC calculations.
Target Materials	Nanomaterials and biological systems
Primary Developer	Hiromi Nakai, Masato Kobayashi (Waseda University)
URL	http://www.msg.chem.iastate.edu/gamess/

ermod

Code Name	ermod
Method/Algorithm	Free energy calculation and analysis for solution systems and nanoscale systems that represent inhomogeneous weak orders by using the energy representation method
Overview	This program calculates the coupling free energy of the target materials. From molecular simulations of the target solution and reference solvent, the distribution function for solution-solvent interaction energy is constructed, and free energy analysis can be performed quickly and accurately based on free-energy analysis of solutions in the method of energy representation.
Target Materials	Solutions (including nonaqueous systems and ionic liquids), lipid membranes, micelles, proteins, amorphous polymers, and QM/MM systems
Primary Developer	Nobuyuki Matsubayashi (Kyoto University), Shun Sakuraba (JAEA)
URL	http://ermod.sourceforge.net/

feram

Code Name	feram
Method/Algorithm	Molecular dynamics method
Overview	High-speed molecular dynamics simulator for ferroelectric thin films. The system is coarse-grained and modeled as a classical pseudo-spin system with dipole-dipole interaction (long-range force). FFT is used for quickly calculating the force in the reciprocal space.
Target Materials	Perovskite-type ferroelectrics
Primary Developer	Tsuyoshi Nishimatsu (Tohoku University)
URL	http://loto.sourceforge.net/feram/

GAMESS-FMO

Code Name	GAMESS-FMO
Method/Algorithm	Fragment Molecular Orbital (FMO) method
Overview	The entire system is divided into small fragments and ab initio MO calculations are performed for the fragment-fragment pairs. From these results, one can calculate the properties of the entire system. The calculation time is roughly proportional to the size of the system.
Target Materials	Biomolecules such as proteins, DNA/RNA, etc. and their complexes with organic compounds
Primary Developer	Kazuo Kitaura (Kobe University), Dmitri G. Fedorov (AIST)
URL	http://www.msg.chem.iastate.edu/gamess/

MACHIKANEYAMA2002

Code Name	MACHIKANEYAMA2002
Method/Algorithm	KKR-CPA method
Overview	A program package for first-principles electric structure calculations based on local density approximation (LDA) or generalized-gradient approximation (GGA). This includes coherent potential approximation (CPA), enabling it to be used for not only ordinary ordered crystals but also irregular systems such as impurity systems, disordered alloys, and mixed crystals.
Target Materials	Metals, semiconductors, oxides etc.
Primary Developer	Hisazumi Akai, Masako Akai
URL	http://kkr.phys.sci.osaka-u.ac.jp/

MDACP

Code Name	MDACP
Method/Algorithm	Molecular dynamics method
Overview	MDACP (Molecular Dynamics code for Avogadro Challenge Project) is a parallel MD code for simulating the Lennard-Jones particles developed in "Avogadro Challenge: Nanodynamics Study on Nonequilibrium Problems," a research project that was selected in the Kaust Global Research Partnership (GRP) Investigators competition. The program is written in C++ and parallelized by means of space division using MPI+OpenMP.
Target Materials	Phase transitions between general gases, liquids, and solids
Primary Developer	Hiroshi Watanabe (The University of Tokyo), Masaru Suzuki (Kyushu University), Nobuyasu Ito (The University of Tokyo)
URL	http://mdacp.sourceforge.net/

OpenMX

Code Name	OpenMX
Method/Algorithm	Density functional theory, localized numerical basis, pseudopotential method, Order N method, nonequilibrium Green's function method, effective screening medium method
Overview	OpenMX calculates electric structure in the ground state by using the localized numerical basis and pseudopotential methods based on density functional theory. This includes the order-N method based on the Krylov subspace method and is capable of large-scale molecular dynamics calculations in parallel computing environments. Also this has the capability to handle noncollinear magnetism with spin orbit interactions and electrical conductivity calculations based on the nonequilibrium Green's function method.
Target Materials	Carbon materials, metals, interface structures, transition metal oxides, liquids, etc.
Primary Developer	Taisuke Ozaki (JAIST)
URL	http://www.openmx-square.org/

phonopy

Code Name	phonopy
Method/Algorithm	Phonon dispersion calculations
Overview	Phonopy calculates phonon dispersion, density of state and various types of thermodynamic quantities based on the force calculated by first-principles calculation software such as VASP and Wien 2k. Phonopy is written mainly in Python.
Target Materials	Solids
Primary Developer	Atsushi Togo (Kyoto University)
URL	http://phonopy.sourceforge.net/

RSPACE

Code Name	RSPACE
Method/Algorithm	Electron state calculations using the real space finite difference method and transport properties calculations using the overbridging boundary-matching method
Overview	RSPACE calculates nanostructure electron states and transport properties with the real space finite difference method. By using PAW pseudopotential, one can precisely calculate electron states for models that include transition metals and models in which orbit interactions play a crucial role. RSPACE can calculate not only electron states but also transport characteristics for nanostructures with using semi-infinite boundary conditions.
Target Materials	Molecules, clusters, semiconductor surfaces, and interfaces
Primary Developer	Tomoya Ono, Marcus Heide (Osaka University), Shigeru Tsukamoto (FZJ), Yoshiyuki Egami (Hokkaido University)
URL	http://cmdcm.phys.sci.osaka-u.ac.jp/

STATE

Code Name	STATE
Method/Algorithm	First-principles molecular dynamics method with plane wave basis set
Overview	STATE is a first-principles molecular dynamics simulation program based on the density functional approach. This calculates GGA, ultrasoft pseudopotential, and Van der Waals force. STATE not only analyzes the energy of materials but also determines reaction paths and activation barriers at interfaces and in liquids by using the ESM method, NEB method, and BM method.
Target Materials	Analysis of electron state of bulk and surface of solids, simulation of reactions in liquids and at solid-gas and solid-liquid interface
Primary Developer	Yoshitada Morikawa, Koji Inagaki, Hidetoshi Kizaki (Osaka University), Osamu Sugino (ISSP), Ikutaro Hamada (Tohoku University), Minoru Otani (AIST)
URL	http://cmdcm.phys.sci.osaka-u.ac.jp/

CONQUEST Aims for Global Domination

Interview with David Bowler and Tsuyoshi Miyazaki, developers of CONQUEST

CONQUEST is an application designed to predict the functions and structures of materials that contain on the order of one million atoms or more, such as next-generation semiconductor devices and DNA. Dr. David Bowler of University College London (UCL) and Dr. Tsuyoshi Miyazaki of the National Institute for Materials Science (NIMS) are two researchers who are on the front lines of application development. Taking advantage of the fact that their application is currently being run on the K computer, they plan to begin full-fledged efforts to promote the use of CONQUEST in Japan.

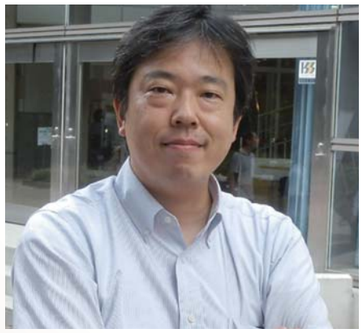
In front of the flower of cherry trees at UCL
David Bowler (University College London)

Bowler's motivation: "Wanted to reproduce experimental results"

"At Oxford University, I started my Ph.D project on silicon gas-source growth by conducting experiments at the same time as performing calculations, though I quickly found it was better to concentrate on calculations and to collaborate closely with colleagues conducting experiments," says Dr. Bowler. He has had experience as an experimental researcher, and continues to collaborate extensively with experimental groups. “But there were limitations to the number of atoms that could be handled in first-principles calculations that faithfully calculate the behavior of atoms, and this helped to form the direction for my future research.” Dr. Bowler soon focused on the "order-*N* method" in his career. In 1997, he joined the research group of Professor Michael J. Gillan at Keele University, the developer of an application called "CONQUEST" that had incorporated this new technique. In 1998, he and Professor Gillan transferred to UCL, and together they began building the center for CONQUEST development.

Miyazaki's motivation: "Wanted to do large-scale computing"

"Many of the participating members of the Joint Research Center for Atom Technology (JRCAT) constitute the driving force behind present-day computational materials science research in Japan," says Dr. Miyazaki. In 1993, he became a participant in the JRCAT project, a national project conducted with the cooperation of industry, government and academia. For this project, many rival researchers developed programs that used first-principles calculations, and they used these programs to provide the world with important findings in the area of semiconductors and the like. Subsequently, Dr. Miyazaki transferred to the National Institute for Materials Science. "I decided that, in order to stay one step ahead in the field of material science, it was essential to increase the number of atoms for calculation," he says. So he began studying references on the development of the order-*N* method, and in the course of his research he discovered a paper on CONQUEST by Professor Gillan. As soon as he began looking through it, he thought, "Eureka!" In no time, he had acquired credentials as an expatriate researcher, and he joined the CONQUEST group at University College London in 1999, soon after its establishment. "For the first year, I was immersed in program development," Dr. Miyazaki said. This period formed the backbone for Dr. Miyazaki's work of popularizing the application after he returned to Japan.



At the meeting of the Physical Society of Japan
Tsuyoshi Miyazaki (the National Institute for Materials Science)

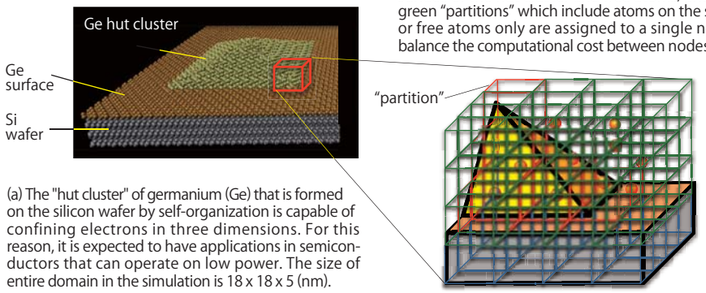
Program development from a user's perspective

Dr. Bowler says that he and Dr. Miyazaki share a common vision that "developed applications only have value if people use them." They continued the policy that the creator of CONQUEST, Professor Gillan, had established, of maintaining a user's perspective. By 2007, CONQUEST had matured into an application that used the state-of-the-art order-*N* method. But further development of the technique was needed to enable it to be used for applied computing. Accordingly, they issued a public invitation for joint researchers, and selected five topics and released a limited beta version of the source code. "As a result of this joint research, the application was used on supercomputers with different architectures in a wide range of fields — nanotechnology, biotechnology, etc. — in various countries such as the United States, Germany and France," says Dr. Bowler. "So we were able to discover common issues for the achievement of a high degree of precision and massively parallel computing, and to use these to develop a program that is highly versatile." Subsequently, they continued to issue invitations for joint researchers. As of September 2012, 10 groups have become users of the program, and they are working to expand the applications for CONQUEST to catalysts and other areas.

One step ahead through massively parallel computing and calculation accuracy

In the conventional first-principles calculation for material properties, the numerical cost increases in proportional to N^3 or faster, where N is the number of atoms. For this reason, even on the K computer, the material for which calculations can be performed is limited to approximately 100,000 atoms. Yet there are many examples of electronic devices, biomolecules and so on whose functions are only manifested when a million atoms are gathered together. There is a strong need to increase the number of atoms that can be calculated. The “order-*N* method,” in which the calculation cost is directly proportional to the number of atoms, was developed for this purpose. There are several different variations of the order-*N* method; CONQUEST uses a method in which the electron state is expressed in the form of an $N \times N$ density matrix. The electrons in a certain location are assumed to be only slightly affected by electrons far away, so to minimize the cost of calculations, only the elements near the diagonal of the matrix are preserved and the other values are set to zero. The result is the order-*N* method that can be used to determine electron state and total energy. Dr. Miyazaki says that the major characteristics of CONQUEST are that it enables massively parallel computers to be used effectively, and that the calculated results are highly precise. The name "CONQUEST" stands for "Concurrent Order-*N* Quantum Electronic Simulation Technique," and the word "concurrent" is used in the sense of being premised on parallel computing. The program divides the entire domain to be calculated into small localized calculation units called "partitions." The cost of calculations differs depending on the state of the atoms making up each partition. For this reason, if the calculations for each partition are assigned using the same proportion as that of the nodes that are the calculation units in the supercomputer, some nodes will be busy and others will not be busy, and this will prevent calculations from being performed efficiently. To resolve this problem, a method was developed in which the number of partitions assigned to each node is optimized to equalize the burden on all nodes (Fig.1).

Fig.1 Results of simulation of a "hut cluster" of germanium (Ge) on a silicon wafer and explanation of "partition"



(a) The "hut cluster" of germanium (Ge) that is formed on the silicon wafer by self-organization is capable of confining electrons in three dimensions. For this reason, it is expected to have applications in semiconductors that can operate on low power. The size of entire domain in the simulation is 18 x 18 x 5 (nm).

(b) Example of assignment of “partitions” to computation nodes. One blue “partition” which is filled with atoms and thus has the larger computation cost, two red “partitions” which contain the atoms near the surface of the hut cluster and free atoms, and three green “partitions” which include atoms on the surface or free atoms only are assigned to a single node to balance the computational cost between nodes.

"Even if a computer becomes enormous in scale, it will be able to respond quickly if the assignment of partitions to nodes is optimized, and that will enable it to handle a larger number of atoms" says Dr. Miyazaki. In recognition of the strengths of massively parallel computing, CONQUEST was selected to be a critical application software in the HPCI Strategic Program, and they started trial use of the K computer in April 2011. CONQUEST has already reproduced the experimental results in the simulation of hut clusters of germanium (Ge) atoms on a silicon wafer — a technique that is expected to produce the next generation of semiconductor devices — and its high calculation precision has been demonstrated on the K computer as well. "Thanks to the order-*N* method, CONQUEST is one step ahead in terms of massively parallel computing and calculation accuracy," Dr. Miyazaki says with pride.

Training researchers with a broad perspective

Dr. Bowler is also putting effort into training. "One of my strengths is that I know the appeal of both experimental research and simulation research," he says. "I want to communicate my experience to students and help them develop into well-balanced researchers." Dr. Bowler is also conducting joint research with students who have graduated and started on the path of experimental research.
As a visiting professor at Tokyo University of Science, Dr. Miyazaki also accepts students. He is also conducting biomolecule simulations that are outside his area of specialty, working to expand the areas of use for CONQUEST. In order to continue to develop the application software and expand the community of users, it is essential to train young researchers who have a broad perspective.

Popularization in Japan: Bowler and Miyazaki's strategies for activities

Dr. Bowler and Dr. Miyazaki are using the opportunity afforded by CONQUEST running on the K computer as a springboard to activities to popularize the application in Japan.
"Japan should to continue to cooperate with other countries in the field of nanoscience and provide more opportunities to promote person-to-person interchange among students and postdoctoral researchers," says Dr. Bowler. In the course of such research, the program would be shared and spread throughout the world. Although CONQUEST has developed into a global program, there is no Japanese manual, and dissemination of the program in Japan has lagged. "We plan to actively hold training sessions in Japan on the use of the application and so on, and also to make the official version of the source code public," says Dr. Miyazaki. The opportunity appears to be ripe for activities designed to popularize CONQUEST.

Clare Gryce, Head of Research Computing and Facilitating Services within UCL’s Information Services Division (which has a supercomputer), hopes that this research will give rise to further collaborative opportunities for UCL researchers. "I hope the joint research between Great Britain and Japan being conducted by Dr. Bowler and Dr. Miyazaki leads to many more such fruitful collaborations." CONQUEST appears to have the potential to promote collaborative activities that go beyond the boundaries that separate different disciplines and different countries. We plan to keep an eye on the global CONQUEST of Dr. Bowler and Dr. Miyazaki.
Reporter: Hikaru Kouta (CMSI Project Manager)

Application SPEC Sheet [CONQUEST]	
Code Name	CONQUEST
Method & Algorithm	Order-N method first-principles calculations by means of density matrix optimization
Description of Code	Order-N method first-principles calculations are used to achieve structural optimization and molecular dynamics. The order-N method — in which the calculation cost (amount of memory, number of computations) is proportional to the number of atoms (N) included in the system being calculated — makes it possible to use first-principles calculations for ultra-large scale systems that include hundreds of thousands of atoms or more. This method, which can also be used for ordinary calculations, offers extremely high parallelization efficiency.
Target materials for simulation	nanostructure materials (semiconductor surfaces, oxide surfaces), biomaterials
Developers	David Bowler (University College London), Tsuyoshi Miyazaki (NIMS), et al

2 Visiting Our Graduates

Kazuyoshi Yoshimi

Social Infrastructure Systems Department, Kozo Keikaku Engineering Inc.

After receiving his Master's degree for research into organic conductors and his doctorate for theoretical research into fluctuations in charge order phenomena, both at the Institute for Solid State Physics of the University of Tokyo, Dr.Yoshimi worked as a researcher at the Tokyo Medical and Dental University and the National Institute of Advanced Industrial Science and Technology (AIST). After that, he joined Kozo Keikaku Engineering Inc., where he is presently employed.

From the Fields of Research to Systems Engineer for Social Infrastructure

For the second in our series "Visiting Our Graduates," in which we talk to computational materials science graduates who are currently employed in the industry, we spoke to Kazuyoshi Yoshimi of Kozo Keikaku Engineering Inc. He joined the company six months ago and is currently working on the analysis of radio wave propagation of cellular telephones and other mechanical devices. We asked him about his graduate research, what led him to choose this type of work, and the type of work he would like to do in the future.

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

Work Environment Infused with a "Work Plus Something Extra" Attitude

Konishi : I imagine that "Social Infrastructure Systems Department" means pretty much what it says, but would you explain in detail what kind of work you do?

Yoshimi : It's mainly analysis relating to radio wave propagation and signal communication. For example, Kozo Keikaku Engineering developed a radio wave propagation analysis package called RapLab (Radio Propagation Laboratory). It's a software program for analyzing the signals from cell phones, radio, TV and so on. Its distinguishing feature is that it is marketed as a program that incorporates new research achievements so it can meet market needs. I'm working on the algorithms that are used in the package and finding ways to improve them.

Konishi : Do you work with research institutions, universities, and so on when you look for ways to improve the algorithms?

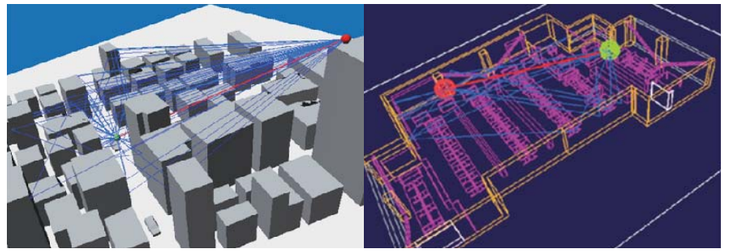
Yoshimi : Yes. I search for algorithms in conference presentations, academic papers and so on, and if I think we can use those algorithms, I actively try to incorporate them. If issues that are unclear pop up in the process of doing so, I contact the researcher directly, and in most cases ultimately I'm the one who takes it all the way to implementation in the package. In that sense, coordination with academia is crucial.

Konishi : What is it that you find appealing about the work you do now? How is it different from academic work, and is anything about it the same?

Yoshimi : I guess the major difference is that I do a lot of different things that have a close connection to society. In the academic world, you're doing things by yourself, or interacting with natural phenomena. But in my work now, the best solution desired by the customer is often not what I had in mind. I think finding a way to skillfully coordinate those differences is very interesting in the sense of being involved with society.

Also, the workplace itself is very appealing. The awareness that we are always trying to start something new is very high. People try to expand their perspective in all directions. They're always looking, even in fields that appear to be unrelated, to see if they can find any ideas that will enable them to skillfully use our technology in those fields. And everyone in the department thinks about it, and we all discuss it together. There are many opportunities to do this type of thing, and that makes it a stimulating environment.

I think what's similar to an academic environment are the technical aspects, in terms of basically being able to know how radio waves are handled. Even saying that, I don't have any knowledge or technical expertise in cell phone signal analysis and so on, so I'm still at the stage of trying to absorb a lot of things.



Sample image of a tool for analysis of radio wave propagation in use, in a downtown area (left) and indoors (right). Tracking the radio waves that are emitted from the transmission point and arrive at the reception point makes it possible to simulate and calculate the propagation distance, reflection status, reception level and so on. When there are many buildings, the number of reflections increases and the path becomes complex. In an actual urban setting, extremely large-scale calculations are required.

Konishi : I get the impression that it's closer to electrical engineering than physics. Does your work include putting together and implementing projects?

Yoshimi : Yes. The Social Infrastructure Systems Department has a staff of around 30, and each project team consists of between five and 10 members. Once we launch a project, we figure out how much work it will involve, estimate how many people and work days it will require, and prepare a Gantt chart with the project schedule. Then, as we proceed with the project, we check for any discrepancies with the work schedule. That's different from academic work. Also, a lot of people use the same code within that project, so we make sure to do the coding in a way that will make it easy for others to read.

Research Activities that Teach the Importance of Self-Supervision

Konishi : What kind of research did you do in graduate school?

Yoshimi : I studied organic conductors in Professor Hatsumi Mori's laboratory in the Institute for Solid State Physics at the University of Tokyo for my master's course. At the time, organic transistors and so on were in the news a great deal, and being interested in that was the reason that I decided to do research in that area. However, originally I was theory-oriented, and in the process of going from the master's course to the Ph.D. course, I changed to Professor Takeo Kato's laboratory within the Institute for Solid State Physics. That's when I began to study superconductors and magnetic susceptibility.

Konishi : So you got your doctorate at Professor Kato's laboratory and afterward became a researcher.

Yoshimi : That's right. For the first year after I'd gotten my Ph.D., I was an assistant teacher in the laboratory of Professor Kazuki Koshino at Tokyo Medical and Dental University, where I conducted research into quantum optics. After that, I spent two years as a postdoctoral fellow under Dr. Shoji Ishibashi at the National Institute of Advanced Industrial Science and Technology (AIST), where I returned to the study of organic conductors.

Konishi : What did you learn from each of these professors?

Yoshimi : From Professor Mori, I learned that if you have an idea, you should feel free to take up the challenge. From Professor Kato, I learned the importance of not only freedom but self-supervision. And from Professor Koshino and Dr. Ishibashi, I learned the importance of producing output.

Konishi : How was your involvement with numerical calculations?

Yoshimi : In my master's degree program, I was one of those who used a numerical calculation package. In the Ph.D. program, I learned how to put together my own code for research purposes. Then, at Tokyo Medical and Dental University, the calculations were mainly analytical calculations, so I went back to using a program. I used Mathematica to check the results of calculation. At AIST, my involvement in numerical calculations was to use a first-principles program (QMAS) for modeling and then conduct analysis using an exact diagonalization program.

Goal : Building a System for Industry-Academic Collaboration that will Develop Spontaneously and in a Concerted Manner

Konishi : After that, you joined your current company. What prompted your decision to do that?

Yoshimi : I'd been wanting to work in a company since my time in the Ph.D. program. But I also wanted to do something similar to working at a research institute. One day, I got the opportunity to talk with a friend who worked at Kozo Keikaku Engineering Inc. I think that was a bit of a catalyst, although a minor one. At the time, I just made a mental note of it, but later I actually checked out the website of the company. And that was the major catalyst. Their corporate philosophy was something you don't normally see companies come right out and say: "A general engineering company that forms a bridge between universities/research institutes and industry." I was very impressed that they'd come right out and say that. Almost before I realized it, I'd sent in an application.

Konishi : And it's been six months since you entered the company. What kind of challenges do you want to tackle from this point on?

Yoshimi : First, I'd like to gain a thorough understanding of the market for social infrastructure work and become able to skillfully match what I'm looking for and what the customer is looking for. I'm also interested in applications of big data.

Konishi : Do you mean how to gather and use data?

Yoshimi : It's already possible to gather data. I think the problem is how to interpret the information and how to use it. First you establish generally where the end point is and then you select data from the wide variety of perspectives that exist. Personally, I think it would be really interesting to include education, for example e-learning, that is based on smart technologies.

I also want to take on the challenge of something new in addition to my current work. When I did so, I'd adopt a perspective that's closer to that of a research institute as opposed to the normal company perspective. I'd also like to enhance the corporate philosophy of the company, and simultaneously conduct academic development and return the knowledge to the company. I'd like to be involved in putting together a system that produces this kind of industry-academic collaboration spontaneously and in a concerted manner. I think that would be a win-win.

(September 11, 2012 at the Kozo Keikaku Engineering Inc. head office)

CMSI Research Group 1 "Basic Science of Novel Quantum States and New Materials" Summer School Report

Akiko Masaki
CMSI Priority Area Researcher
Institute for Solid State Physics,
The University of Tokyo

The CMSI Research Group 1 "Basic Science of Novel Quantum States and New Materials" Summer School was held for six days, August 20 - 25, 2012. It was attended by approximately 40 persons, mostly graduate students and postdoctoral researchers and other young people but including veteran researchers as well. The Summer School did not only feature presentations but also included ample time for discussion, affording the kind of opportunities for deep-level interchange that only a training camp style program can provide.

The venue was the Takamiya Village Hotel Jurin, one of the hotels with a long history that are located in the ski resort of Zao, Yamagata Prefecture. Despite being held at the height of summer, at night it was cool enough that people had no problems sleeping. With fresh mountain air and a beautiful natural setting, it was the ideal environment to enable the attendees to forget the heat of the lowlands and focus on their research.

Quantum Chemistry Topic: Why is Gold Gold?

The backgrounds of the attendees can be generally divided into two types: quantum chemistry and condensed matter physics. However, they were identical in terms of studying materials science dealing with strongly-correlated quantum many-body systems. There are no clear boundary lines, but if one looks closely at each area of specialty, the differences become apparent. So naturally there were rich variations in knowledge, approach and the methods used for calculation.
The theme of the Summer School program was "Non-equilibrium and Strong Correlation." The content of the presentation was extremely robust, ranging from the basics about which all attendees could share knowledge to the results of the latest cutting-edge research. Moreover, like many CMSI conferences, the aim was not only to provide knowledge of physics and chemistry but also to make an effort to disclose the details of calculation methods that go across disciplinary boundaries. That aspect made it a very appealing program.

In general, the program started each morning at 9:30 with presentations by invited speaker. These continued throughout the day until evening, with rest periods interspersed. Beginning at 8:00p.m., there were "short talks," research presentations by young researchers, followed by a free discussion period. The schedule was undoubtedly a very healthy one for young researchers who tend to keep irregular hours.
The first half of the training camp style program focused on topics in quantum chemistry. Personally, I was very intrigued by the presentation entitled "Relativity effect in quantum chemistry calculations" by Dr. Takahito Nakajima of the RIKEN Advanced Institute for Computational Science (AICS). The question "Why is gold colored gold?" arises from the relativity effect. For someone like me, who is new to the field of quantum chemistry, the fact that the relativity effect and spin-orbit coupling play a major role in the inner shell electrons of heavy atom molecules was genuinely fascinating.

Increasing Interest in Tensor Networks

The latter half of the program focused on condensed matter physics. The presentation entitled "Renormalization of Tensor Network States" by Professor Tao Xiang, who came all the way from Peking University, has a close relationship to the research topic of our group. I myself had previously studied Time-Evolving Block Decimation (TEBD), so I had been looking forward to this presentation.
As a priority area researcher in the Kawashima-Todo Group, I am in charge of developing new parallelizable world-line Quantum Monte Carlo method (QMC) algorithms. QMC has the advantage of being able to easily calculate large-scale high-dimensional systems at finite temperatures exactly besides statistical errors. However, its weakness is that it has not yet resolved the notorious negative sign problem in frustrated spin systems and Fermi systems. The tensor network method, derived and developed from the numerical renormalization group method, has attracted a great deal of attention in recent years as a quasi-rigorous, large-scale calculation method that does not suffer from the negative sign problem. The method can also track dynamics, something that is still difficult by the QMC, through the projection of time evolution operators.
There are several variations of the tensor network method. Professor Xiang Tao uses PEPS. PEPS is basically the same as the DMRG and TEBD, apart from differences in the method of creating tensor products. However, I learned that, unlike those methods, PEPS can easily be applied to two dimensions and above. Attending this presentation made me even more interested in tensor networks, and I definitely want to try my hand at writing code. Professor Kenji Harada of Kyoto University also covered Fermi system tensor networks in his Short Talk, and that was extremely enlightening as well.

Training and Encouraging Interchange Between Young Researchers through an Overnight Seminar Program

I myself am in the field of condensed matter physics, using QMC to conduct research on statistical physical properties at equilibrium and quantum states for lattice bosons and quantum spin system. It is comparatively far removed from the field of quantum chemistry. However, through the overall presentations, I was able to learn about the research of other people (which I had not fully understood before) starting from the basics, and I think my understanding of the technical aspects was also enhanced.
There were long rest periods between the lecture presentations at the Summer School, so we were able to take brief walks through the hot springs town, which has a long history for about 1900 years, and the highlands. As we walked, we recalled and casually discussed what we had learned in the presentation. Therefore it was a training camp style summer school that also provided a refreshing break from the hustle and bustle of the city (although I'm speaking not of Tokyo but of Kashiwa). I would definitely like to attend this type of training camp style seminar program again. I hope such programs continue, and that they promote even more in-depth young researcher training and technical cooperation across disciplines.

CMSI Research Group 1 Summer School Program

August 20 (Monday)

1:00 - 1:10 p.m.	Greeting (Seiichiro Tenno, Kobe University)
1:10 - 2:10 p.m.	Lecture: Foundations of electron correlation theory for molecular systems and multi-reference perturbation theory (1) (Haruyuki Nakano, Kyushu University)
3:30 - 4:30 p.m.	Lecture: Foundations of electron correlation theory for molecular systems and multi-reference perturbation theory (2) (Haruyuki Nakano, Kyushu University)
5:00 - 6:00 p.m.	Lecture: Electron and proton dynamics (1) (Koji Ando, Kyoto University)

August 21 (Tuesday)

9:30 - 10:30 a.m.	Lecture: Electron and proton dynamics (2) (Koji Ando, Kyoto University)
11:00 a.m. - noon	Lecture: Relativity effect in quantum chemistry calculations (1) (Takahito Nakajima, RIKEN)
3:00 - 4:00 p.m.	Discussion Comparison of quantum chemistry calculation methods and future prospects
8:00 - 9:00 p.m.	Short Talks (quantum chemistry calculations / excitation states) Development of highly precise quantum chemistry methods (Yuya Ohnishi, Kobe University) Quantum chemistry calculations for charge transfer states (Ryota Jono, The University of Tokyo)

August 22 (Wednesday)

9:30 - 10:30 a.m.	Lecture: Relativity effect in quantum chemistry calculations (2) (Takahito Nakajima, RIKEN)
11:00 a.m. - noon	Lecture: Nonequilibrium phase transition of strongly-correlated electron systems and nonequilibrium dynamical mean field theory (1) (Takashi Oka, The University of Tokyo)
2:00 - 5:00 p.m.	Free discussion
8:00 - 9:00 p.m.	Short Talks (nonequilibrium / strongly-correlated electron systems) Nonequilibrium transport, quantum measurement theory and the relaxation process (Yasuhiro Yamada, The University of Tokyo) High-temperature cuprate superconductors (Kazutaka Nishiguchi, The University of Tokyo)

August 23 (Thursday)

9:30 - 10:30 a.m.	Lecture: Nonequilibrium phase transition of strongly-correlated electron systems and nonequilibrium dynamical mean field theory (2) (Takashi Oka, The University of Tokyo)
11:00 a.m. - noon	Lecture: Renormalization of Tensor Network States(1) (Tao Xiang, Peking University)
3:00 - 4:00 p.m.	Lecture: Renormalization of Tensor Network States(2) (Tao Xiang, Peking University)
8:00 - 9:00 p.m.	Short Talks (numerical calculation methods for the issue of quantum many-body systems) Variational methods with Tensor Network States (Kenji Harada, Kyoto University) Variational Monte Carlo method (Satoshi Morita, The University of Tokyo)

August 24 (Friday)

9:30 - 10:30 a.m.	Lecture: Foundations and applications for first-principles molecular dynamics (1) (Yoshitada Morikawa, Osaka University)
11:00 a.m. - noon	Lecture: Foundations and applications for first-principles molecular dynamics (2) (Yoshitada Morikawa, Osaka University)
2:00 - 3:00 p.m.	Discussion The science of nonequilibrium calculation: methods, frontline applications and future prospects
8:00 - 9:00 p.m.	Short Talks (nonequilibrium and strongly-correlated electron systems) Optical response of low dimensional strongly-correlated electron systems (Shigetoshi Sota, RIKEN) Strongly-correlated many-electron systems (Yohei Yamaji, The University of Tokyo)

August 25 (Saturday)

9:30 - 10:30 a.m.	Lecture: Quantum fluctuation of electrons and lattices observed using the resonating Hartree-Fock approach (1) (Norikazu Tomita, Yamagata University)
11:00 a.m. - noon	Lecture: Quantum fluctuation of electrons and latticesobserved using the resonating Hartree-Fock approach (2) (Norikazu Tomita, Yamagata University)
1:00 - 2:00 p.m.	Discussion New methodology for strongly-correlated electron systems
	Closing Address (Masatoshi Imada, The University of Tokyo)

CMSI Calendar

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

●SC12
Date : November 10 - 16, 2012
Venue : Salt Lake City, Utah, USA

●2nd TCCI Symposium on Experimental Chemistry Collaboration
Date : November 16 - 17, 2012
Venue : Fukui Institute for Fundamental Chemistry, Kyoto University

●7th ACCMS-VO International Conference
Date : November 23 - 25, 2012
Venue : Sendai, Miyajima (Miyagi Prefecture)

●3rd CMSI Workshop
Date : December 3 - 5, 2012
Venue : Okazaki Conference Center, National Institutes of Natural Sciences (NINS)

●TCCI Winter College (Molecular Simulation)
Date : December 11 - 14, 2012
Venue : Okazaki Conference Center, National Institutes of Natural Sciences (NINS)

●TCCI Winter College (Quantum Chemistry)
Date : December 17 - 18, 2012
Venue : Okazaki Conference Center, National Institutes of Natural Sciences (NINS)

●Materials Science MPI Workshop
Date : December 2012
Venue : Not yet decided

●Elements Strategy Symposium (Structural Materials Division)
Date : January 7 - 9, 2013
Venue : Kyoto University

●Elements Strategy Theory Symposium
Date : January 9 - 11, 2013
Venue : Institute for Solid State Physics, University of Tokyo

●2nd CMRI Workshop
Date : January 21 - 22, 2013
Venue : Institute for Materials Research, Tohoku University

●2nd TCCI Symposium on Industry-Government-Academia Cooperation
Date : January 24, 2013
Venue : Nakanoshima Center, Osaka University

●2nd International Workshop on Massively Parallel Technology
Date : January 28, 2013
Venue : Waseda University

●7th CMSI Young Researcher Technical Workshop
Date : Mid-February, 2013
Venue : Kanazawa

●CMD® Workshop
Date : March 7 - 8, 2013
Venue : Nichii Gakkan (Kobe)

"K" News

The K computer has been made available for general use from September 28, 2012.

The K computer, the supercomputer that RIKEN has been constructing since FY 2006, was made available for general use beginning September 28 of this year. In addition to projects in the 5 fields of High Performance Computing Infrastructure (HPCI) Strategic Program (SPIRE), comprising seven priority projects and 24 general projects, 62 projects within the general use category have also been selected (29 general use projects, 8 young researcher training projects and 25 industry-related projects) for the period up to the end of FY 2013). These issues within the general use category were reviewed from a neutral and fair perspective by the Research Organization for Information Science & Technology (RIST), the Registered Institution for Facilities Use Promotion. RIST will also accept applications for industry-related trial use in the general use category as the need arises.

What are Applications?

CMSI members every day work on development of applications. But what exactly is an application?

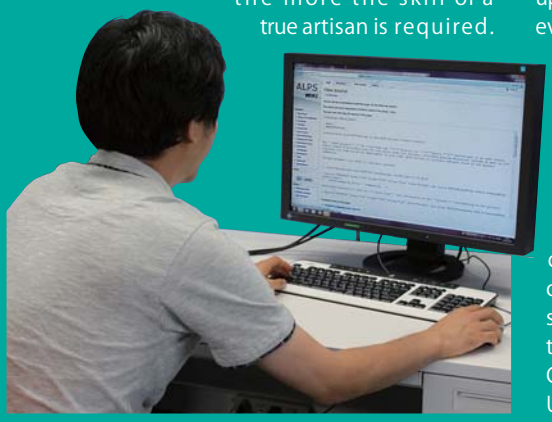
Software and Hardware

Hardware is the corporeal, nuts-and-bolts part of your PC. Software is the non-corporeal information that is loaded into the hardware. Software may be basic software or application software — "applications" for short. The Windows and Macintosh operating systems (OS) are examples of basic software. Applications include the software you use to check your email, Internet web browsers, and other software that runs on the OS and is used by the users themselves.

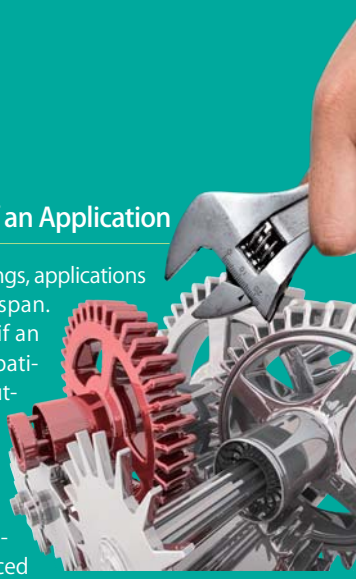
In the field of computational science, applications are developed for purposes such as predicting the properties of materials and analyzing complex chemical reactions.

Programs

Programs are the blueprints for software. Every day, CMSI members write programs to create and modify applications. Bringing out the best possible performance from state-of-the-art computers requires parallelization technologies that coordinate the operation of many machines, and advanced optimization technologies that are only achieved by programmers with a thorough understanding of the internal mechanisms of computers. The more powerful the computers, for example the K computer, become, the more the skill of a true artisan is required.



The Life Span of an Application



Just like human beings, applications have a limited life span. For example, even if an application is compatible with the computers of the past, it may not run on modern computers, or it may not be able to take full advantage of their advanced calculation capabilities. If the application is not updated, soon no one will be able to use it, and eventually its existence will be forgotten. For an application to live on, someone must continue to maintain the program. But this is difficult for a single person to do. If the developer makes the program public, others may continue to develop it. But programs are filled with all of the expertise of the developer, which many developers are reluctant to give away. Whether or not to make the program public and, if so, how to license it, are difficult decisions that must be made by each developer.

Cooperation: Hiroshi Watanabe (The University of Tokyo)

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Cover :
As for the colored leaves, it is said that the more the temperature difference of the night and day is intense, the brighter the color becomes. Also in researches, the more failure, success, and friendly competitions are repeated, the more colorful they will be.

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