CCS Report: PART II

Research Activities, Results, Collaborations and Plan

2004 - 2007

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Center for Computational Sciences

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1. Division of Particle Physics and Astrophysics: Computational Particle Physics Group

1.1 Research Activity

Computational Particle Physics group has performed researches in lattice QCD, using mainly massively parallel computer CP-PACS, constructed and operated at Research Center for Computational Physics, the precursor of our center. In addition to CP-PACS, other resources such as SR8000 at our center, VPP5000 at Academic Computing and Communications Center, University of Tsukuba, SR8000 at High Energy Accelerator Research Organization (KEK) and the Earth Simulator at The Erath Simulator Center have been employed for our researches.

Our research activities for the past 3 years are summarized below.

①. Calculation of hadron spectra and determination of fundamental parameter in QCD such as quark masses via numerical simulations in lattice QCD with dynamical quarks

②. Dynamical properties of hadorons such as the pion scattering in lattice QCD

③. Determination of hadornic matrix elements in lattice QCD, necessary to test the standard model and beyond

④. Lattice QCD at finite temperature and density

⑤. The nuclear force from lattice QCD

1.2 Research Results

Our research group has obtained many results in the areas of the above research activities. Main results for the past 3 years are given below item by item.

①. Calculations in lattice QCD with light dynamical up and down quarks have been performed by using CP-PACS and finished in 2003. We have found that a discrepancy of hadron masses from experimental values, which is about 10% in quenched QCD, is much reduced in 2 flavor QCD. We then have started the “complete QCD” (2+1 flavor QCD), which includes dynamical quark effects of a heavier strange quark as well as up and down quarks. Results obtained in the calculation are as follows.

(a) We have made a test of our simulation algorithm and a choice of the gauge action performing preliminary simulations in a small volume.

(b) In order to remove the lattice artifact liner in the lattice spacing a, we have determined the clover coefficient in 3 flavor QCD non-perturbatively.

(c) After preparations mentioned above、we have proceeded to a 2+1 flavor QCD

simulation in which we treat heavier strange quark dynamical in addition to light up and down quarks. Meson masses extrapolated to the continuum limit turn out to be consistent with experiment. All available computational resources such as CP-PACS, SR8000, VP5000 and the Earth Simulator have been devoted to this calculation. Although no clear effects of dynamical strange quarks are observed, determination of the meson spectrum for QCD without quenching approximation is an event of great significance in the history of lattice QCD simulations.

(d) In the 2+1 flavor simulation above, calculations have been made for up and down quark masses heavier than 70 MeV and results is extrapolated to the physical up and down quark masses of about 3 MeV. This long chiral extrapolation causes a possible systematic error. In order to overcome these difficulties, we have just started simulations with much lighter up and down quark masses down to 6 MeV on a large lattice of 3.2 fm. The simulation was carried out using the PACS-CS computer, a successor of CP-PACS, developed at our center. Fig. 1 shows results for the hadron spectrum, compared with those obtained for quenched and 2 flavor QCD. A consistency of all measured hadron masses with experiment is observed only for our new 2+1 flavor QCD results, though errors are still large and the results are obtained only at one lattice spacing.

(e) The masses of light quarks are fundamental parameters of QCD. It is known that quark masses in 2 flavor QCD are smaller those in quenched QCD by 20-30%. We have calculated quark masses in 2+1 flavor QCD and obtained a result that they are almost unchanged from those in 2 flavor QCD.

(f) Wilson chiral perturbation theory, which is a theoretical guideline of chiral extrapolation for the Wilson or clover quark action, has been extended to pseudo-scalar meson masses and vector meson masses in 2+1 flavor QCD.

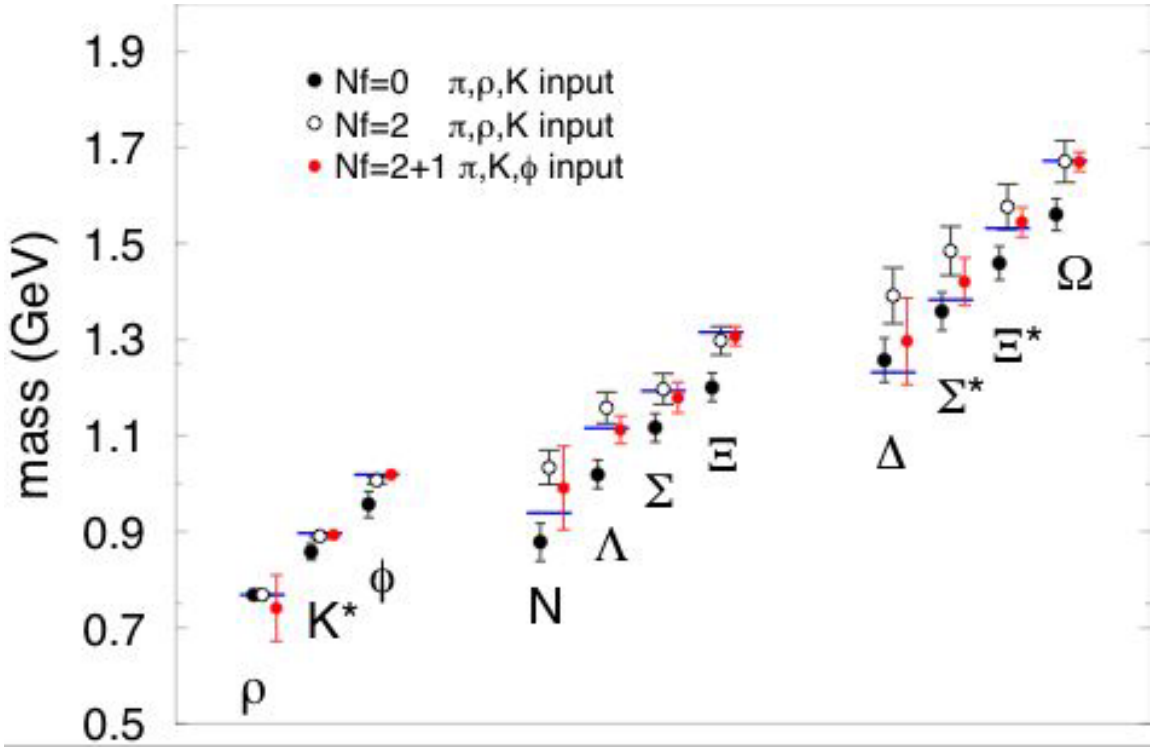

Fig.1: Hadron mass spectrum obtained from 2+1 flavor QCD simulations with very light up and down quark masses. Results for quenched QCD and 2 flavor QCD are overlaid. Horizontal bars represent experimental values.

②. Dynamical properties of hadrons.

(a) Calculation of scattering phase shift is an important step for expanding our understanding of strong interactions based on lattice QCD beyond the hadron mass spectrum. For scattering lengths, which are the threshold values of phase shifts, several studies have already been carried out. However there is none for the scattering phase shift. We calculated the I=2 S-wave two-pion scattering phase shift in the quenched QCD and the full QCD. We show that the results in the full QCD in the continuum limit are consistent with the experiments.

(b) The U(1) problem, which is to derive the flavor U(1) pseudo-scalar meson mass much heavier than the pion, is one of the longstanding issues in particle physics. We have carried out an 2+1 flavor QCD calculation, taking account of a mixing effect of U(1) and other mesons. So far, calculations are completed only at one lattice spacing and we obtain the U(1) meson mass roughly consistent with the experimental value.

③. Hadronic matrix elements

(a) We have calculated proton decay matrix element in lattice QCD with the quenched

approximation. Values obtained in the continuum limit is larger by about 3 times than the smallest prediction among various QCD models. This implies stronger constraints on models for the grand unified theories(GUTs).

(b) Matrix elements of hadrons which include heavy quarks are important to restrict parameters of the standard model. However it is difficult to put a heavy quark on the lattice. Therefore we have proposed a new formulation for a heavy quark on the lattice to overcome the difficulty. A quenched QCD simulation we have performed has shown that our formulation for a heavy quark works well.

④. Under usual conditions, quarks and gluons are confined within hadrons. However, at temperatures higher than about 10^{12} K, hadrons are expected to turn into the quark-gluon plasma phase. These unconventional states of matter are relevant to the early evolution of the Universe and maybe the structure of the central core of neutron stars. We have studied the quark number susceptibility and static quark free energy in 2 flavor QCD at zero chemical potential. From the static quark free energy in various color channels, we have found that the inter-quark force for quark-antiquark (quark-quark) pairs is attractive for color singlet (triplet) channels while it is repulsive for octet (sextet) channels. We are extending the study to finite chemical potentials.

⑤. It is one of the most important problems in nuclear physics to understand an interaction between nucleon (nuclear force). In particular, repulsion at short distance (repulsive core) necessary to explain stability of a nuclei has been theoretically less understood. We have proposed a new method to calculate a potential between hadrons, and applying it to nucleons we have calculated the nucleon potential in quenched QCD. Our result at one lattice spacing shows that not only repulsive core but also attraction at long and intermediate distances are reproduced.

1.3 Collaboration

Recognizing that gauge configurations generated in dynamical QCD simulations are valuable, we are now constructing ILDG (International Lattice Data Grid) in collaboration with Grid and Networks group in High Performance Computing Systems division, to share gauge configurations worldwide through internet. This year, supported by CSI (Cyber Science Infrastructure) project at National Institute of Informatics, we have constructed JLDG for domestic data sharing. We have also closely cooperated with System Architecture group in High Performance Computing Systems division, to develop and construct PACS-CS. We are currently collaborating with several peoples in High Performance Computing Systems division, for development and tuning of simulation codes on PACS-CS.

1.4 Future Plan

With the encouraging results in 2+1 flavor QCD at one lattice spacing, we plan to calculate the hadron spectrum at the physical up and down quark masses at the same spacing, so that no chiral extrapolation is necessary. We then will proceed to simulations for finer lattices, which will finally establish the QCD mass spectrum. Using gauge configurations generated in 2+1 flavor QCD simulations, we will investigate hadron interactions, hadronic matrix elements and nuclear force. In addition a lattice QCD study at finite density is also planed.

1.5 Publications

1.5.1 Journal Papers

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2. Division of Particle Physics and Astrophysics: Computational Astrophysics Group

2.1 Research Activity

In the computational astrophysics group, we have explored first generation objects in an early universe, formation and evolution of galaxies, large-scale structures in the universe, active galactic nuclei with the formation of supermassive black holes. In particular, we have concentrated on the coupling effects of radiation and matter. For the purpose, the methods of multi-dimensional radiative transfer and radiation hydrodynamics (RHD) have been developed. In addition, ultra-high resolution hydrodynamic simulations on the early evolution of galaxies through multiple supernovae, and the large-scale simulations of far-infrared or submillimeter galaxies have been performed, which can be compared with the future observations with ALMA.

To realize high-resolution RHD simulations, we have urged the *FIRST* project, and developed a new type of hybrid computer dedicated for astrophysical RHD, called *FIRST* simulator, in the collaboration with the Division of High Performance Computing Systems. This project is funded by a Specially Promoted Research in Grants-in-Aid for Scientific Research over four years (2004~2007) with the budget of JPY329.5 million (US$2.8 million), approved by The Ministry of Education, Culture, Sports, Science and Technology (MEXT) in Japan. With *FIRST* simulator, we have performed high-resolution simulations on the evolution of first generation objects, and obtained new results.

2.2 Research Results

2.2.1 Dedicated Computer and Numerical Methods

1) *First* Simulator

For the realization of 3D radiation hydrodynamics, we have built up a hybrid PC cluster, called *FIRST* (Fusional Integrator for Radiation-hydrodynamic Systems in Tsukuba University) simulator, where a newly-developed board for gravity calculations, called Blade-GRAPE, is embedded in each node. The Blade-GRAPE is composed of four GRAPE-6 chips and designed for PCI-X bus in a PC cluster. The theoretical peak performance of Blade-GRAPE is 136.8GFLOPS. Each board has 16MB memory and can calculate the self-gravity of 260,000 particles simultaneously at the maximum. The Blade-GRAPE is directly connected via PCI-X bus, and occupies the space of two PCI-X bus slots. The electric power supply is from the PCI-X bus (3.3V) as well as from the cluster server board, +12V (54W). Each server PC is equipped with multi-port Gigabit Ethernet NIC to be connected to a special interconnection network with commodity

FIGURE 1. Blade-GRAPE X64

FIGURE 2. *FIRST* simulator (256 node, 36.1TFLOPS)

Ethernet switches. Using Blade-GRAPEs, we have constructed a 256 node hybrid PC cluster system, that is, *FIRST* simulator. The host PC cluster node is a 2U-size of 19-inch rack mountable server PC (HP ProLiant DL380 G4) that has dual Xeon processors in SMP configuration. The peak performance of *FIRST* simulator is 36.1TFLOPS, where the host PC cluster is 3.1 TFLOPS and the Blade-GRAPEs are 33 TFLOPS. All nodes are connected uniformly with each other via multi-port Gbit ether interconnect switch. The total memory of *FIRST* simulator is 1.6TB. Also, the *Gfarm* Grid file system, which is the commodity-based distributed file system that federates local disk of each node (http://datafarm.apgrid.org/index.en.html), is installed. With *Gfarm*, the storage of 22TB is available as a seamless file server. In Figure 2, 256 node *FIRST* simulator is shown.

2) Numerical Methods for Astrophysical RHD

As for 3D radiative transfer, we have developed a grid-based scheme with CP-PACS （1992-2005）. Then, a SPH-based RHD (RSPH) scheme has been developed in "Development of Next Generation Massive Parallel Computer" Project (1997 - 2001), which is funded by the "Research for the Future Program" of Japan Society for the Promotion of Science. Also, in this project, HMCS (Heterogeneous Multi-Computer System) was constructed, where an RSPH scheme is installed. This RSPH scheme has been improved to optimize *FIRST* simulator.

3) Hydrodynamic Scheme with SSE

To utilize the potentiality of CPU to the maximum, an SPH scheme with SSE (Streaming SIMD extension), which is equipped in x86 architecture, has been developed. Also, we are planing to develop a radiative transfer scheme with SSE.

2.2.2 Large-Scale Numerical Simulations

1) RHD Simulations on First-Generation Objects

Using *FIRST* simulator, we have performed three-dimensional RHD simulations to scrutinize the feedback by a first star in first generation objects. It has been found that a nearby collapsing core is evaporated by a shock if an M-type I-front sweeps the core. But,

in higher density cores, the I-front changes to D-type and an H_2 shell forms ahead of the I-front, which effectively shields H_2 dissociating radiation from a source star. Then, the cores can collapse owing to H_2 cooling. The present numerical study has shown that almost all density peaks can collapse in first generation objects. Hence, the star formation

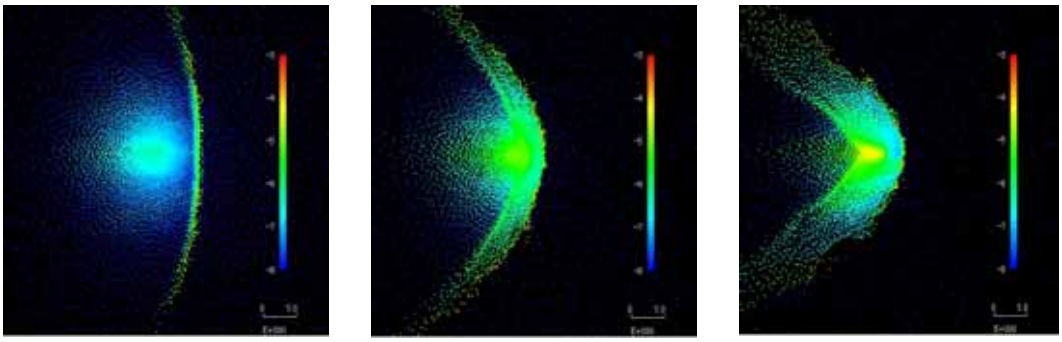

FIGURE 3. Time sequence of the propagation of I-front in a collapsing cloud. The colors of particles denote the H_2 fraction. The photodissociating radiation is shielded by an H_2 shell, which is produced by the propgation of ionizing radiation, and eventually the cloud can collapse.

efficiency in first generation objects is expected to be higher by an order of magnitude than argued so far.

FIGURE 4. Cover page of Nature (March 30, 2006).
Simulation by Mori and Umemura is presented.

2) Origin of Elliptical Galaxies

We have performed an ultra-high-resolution hydrodynamic simulation that follows evolution from the earliest stages of galaxy formation through the period of dynamical relaxation. The bubble structures produced by multiple supernovae at an early evolutionary stage ($< 3\times10^8$ years) resemble closely the high-redshift Lyman α emitters (LAEs). After 10^9 years these bodies are dominated by stellar continuum radiation and look like the Lyman break galaxies (LBGs) known as the high-redshift star-forming galaxies at which point the metallicity appears to be solar. After 1.3×10^{10} years, these galaxies resemble present-day elliptical galaxies.

3) Far Infrared and Submillimeter Galaxies

The large-scale structure of high redshift galaxies has been simulated, focusing on far infrared and submillimeter properties. The theoretical prediction can be tested by ALMA in near future.

2.3 Collaboration

In the collaboration with the Division of High Performance Computing Systems, HMCS (Heterogeneous Multi-Computer System) was constructed under "Development of Next Generation Massive Parallel Computer" Project (1997 - 2001), which is funded by the "Research for the Future Program" of Japan Society for the Promotion of Science. With this skill for hybrid computer systems, we have propelled the *FIRST* project (2004-2007), and developed the *FIRST* simulator. In this simulator, the *Gfarm* Grid file system, which has been developed in the Division of High Performance Computing Systems, was installed. As a result, the distributed storage has been integrated as a seamless file server.

2.4 Future Plan

We aim to develop a next-generation hybrid computer system that can extract the potentiality of special purpose processor, SSE, and new-generation graphic board to the maximum. Using such a next-generation hybrid computer, we would like to perform the 3D radiation hydrodynamics further. Then, a goal is to construct "Computational Observatory", which allows the direct comparison of simulation results to multi-wavelength observational data. Computational Observatory could be the third pillar in astronomy, with Astronomical Observatory and Virtual Observatory.

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2.5.2 Proceedings

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3. Division of Materials and Life Sciences: Computational Condensed Matter Science Group

3.1 Research Activity

In a group of Computational Condensed Matter Science, we try to clarify microscopic mechanisms for phenomena in condensed matters, predict new phenomena and then explore new materials with fascinating properties by theoretical and computational approaches. In particular, we clarify and predict properties of materials by computationally solving fundamental equations of quantum mechanics from the first principles since electrons and nuclei which constitute materials are described by quantum theory. We believe that this first-principle approach is valid for nano-materials and also for bio-materials. Hence Bio-materials are also our targets which are tackled by computational quantum-theoretical approaches.

Nano-crystal with 10 nm cube, for instance, contains about fifty thousands of atoms. A typical protein consists of ten thousands of atoms. One of our short-term research targets is thus to develop a method of total-energy electronic structure calculations that is capable of treating 10 thousands atoms from the first principles of quantum mechanics. By using the scheme, we aim to clarify mechanisms of appearance of functions in nano- and bio-materials where atom-scale reactions induce nano-scale shape variation and then cause particular functions. More specifically, we are developing real-space density functional theory (RSDFT) in which all the quantities are computed on lattice in real space. This scheme has several advantages in large-scale parallel computing.

To overcome multi-scale problems in time is another target. Usual chemical reactions take place in nano-, micro-, or milli-seconds. Electronic transitions described in quantum mechanics, on the other hand, take place in femto-seconds. We encounter intrinsic difficulty to describe phenomena with multi-scale in time. We now combine Car-Parrinello molecular dynamics method with meta-dynamics and tackle the multi- scale phenomena especially in biosystems.

We also focus on semiconductor materials that are basis of current technology and carbon nano-materials that may be boosters in the next-generation technology. A variety of total-energy electronic-structure calculations and DFT-based molecular-dynamics calculations are performed for those materials as well as bio-materials.

To develop a new scheme beyond local density approximation and generalized gradient approximation in DFT is another important task in our group.

Some members in our group are conducting several research projects supported from

government or other foundations. They include ``Construction of nano- architecture based on computational quantum-theoretical science" (JST-CREST; leader = A. Oshiyama), ``Quantum design of shapes and functions of nano- and bio-materials" (Grant-in-aid, MEXT, leader = A. Oshiyama), ``Prediction of properties of nano-scale silicon from first principles of quantum theory" (Grant-in-aid, MEXT, leader = K. Shiraishi), and ``Physical properties and material design of complex structures of carbon nanotubes" (Grant-in-aid, MEXT, leader = S. Okada).

3.2 Research Results

1) Developments and Applications of Large-scale Real-space Quantum Mechanical Methodology

We are developing a RSDFT method that is capable of describing phenomena in real materials with large number of atoms from the first principles of quantum theory. The RSDFT in which lattice is introduced in real space and all the quantities such as electron wave-functions are calculated on each lattice point has several advantages in the next-generation supercomputing: The advantages include that heavy all- to-all communications such as FFT are unnecessary and that flexible boundary conditions on wave-functions are able to be set at the boundaries of the computational cell, thereby expanding its applicability to various materials.

A newly developed code is now being tuned on PACS-CS, and a net performance of 10-20% to ideal peak performance has been achieved on 512-node computations. In particular, (a) the algorithm for Gram-Schmidt orthonormalization which is an order N cube part and becomes a bottleneck in large-scale computations has been changed so that it is reduced to the (matrix x matrix) form and the net performance becomes 60 % of the peak performance; (b) A Divide-and-Conquer method is introduced in the diagonalization of subspace and the net performance of 71 % has been achieved. Fig.1 shows calculated stable structure of the divacancy in Si. Calculations of ionization energies and electron affinities of 10,000-atom clusters are being processed with an aim to pave an unified approach for molecules, clusters and bulk materials.

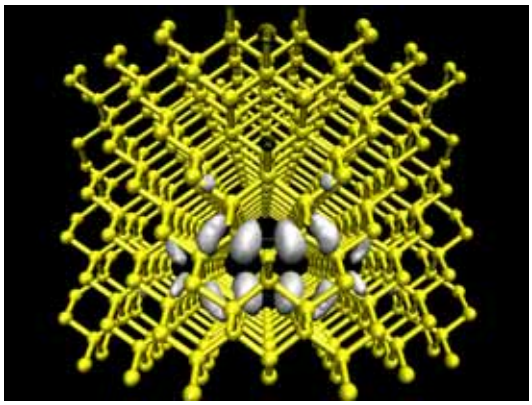

Fig. 1: Electron clouds around the divacancy in Si. When two Si atoms are missing in crystal (divacancy), a new electron states appear in the band-gap and thereby affects on electgronic and optical properies of Si. [Iwata, Shiraishi & Oshiyama: Physical Review B (2007) to appear]

2) Developments of Multi-scale Molecular Dynamics Technique and its Application to Biomaterials

We have been developing Car-Parrrinello molecular dynamics methods combined with meta-dynamics technique to tackle an important issue with multi scale in time where coupling between electron and ion degrees of freedom (femto seconds for electrons and micro seconds for ions) is important. In the meta-dynamics scheme, reaction coordinates are introduced in lagrangean and details of reaction processes and corresponding free energy barriers are obtained. Fig. 2 shows calculated free-energy barrier for the proton transfer process in cytochrome c oxidase in the relevant reaction coordinate space.

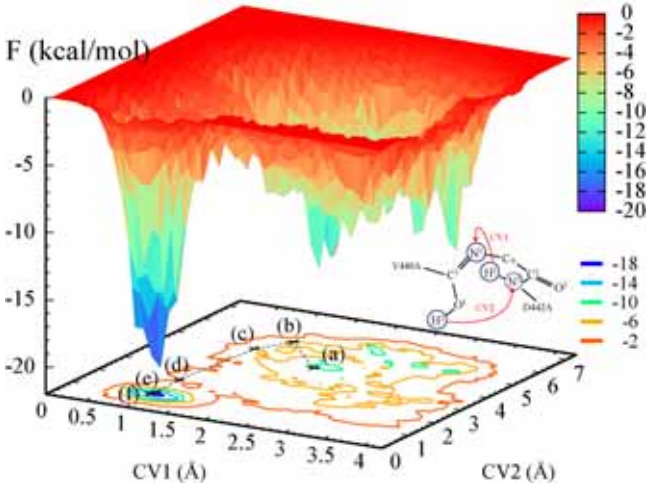

Fig.2: Cytochrome c oxidase is located in inner membrane of mytchondria and responsible for proton transfer which is a principal process in synthesizing ATP. Our calculations have clarified a new

mechanism of proton transfer through peptide bonds [Kamiya, Boero, Tateno, Shiraishi & Oshiyama: Journal of American Chemical Society (2007)]

Currently, a new code is being developed with real-space technique, considering efficient computations on the next-generation computers.

3) Atomic Structures and Electron States at Nanometer-scale Interfaces

It has been recognized that Schottky barriers at metal/semiconductor or metal/insulator interfaces are primarily determined by the workfunction of the metal and the electron affinity of the semiconductor (insulator), and they are modified by electric double layer generated at the interfaces. In recent experiments for metal/high-k insulator/semiconductor MOS structures, however, observed Schottky barriers are unable to be explained by the conventional concept above. We have shown that the observed barriers are beautifully explained by a new idea that electron states of the metal are hybridized selectively with particular atomic orbitals in the insulator. [Shiraishi et al: Thin Solid Films (2006)]

4) Properties of Carbon Nanotubes and their Hybrid Structures

One of the applications of Carbon Nanotubes (CNTs) may be electron devices in nano-electronics. From such viewpoints, clarification of electronic and physical properties of hybrid structures of CNTs and metal electrodes or semiconductor substrates becomes extremely important.

Fig. 3 shows calculated electron states of CNT adsorbed on surfaces of metal electrodes. Al and Ca are considered. It is found that CNT is bound to Ca loosely with the binding energy of 0.5 eV [Fig. 3(a)], whereas CNT on Al forms a covalent bonding with the binding energy of 3.2 eV [Fig. 3(b)]. It is also found that electrons of 5.2 x 106 cm-1 are injected from Ca to CNT, thereby inducing n-type conduction.

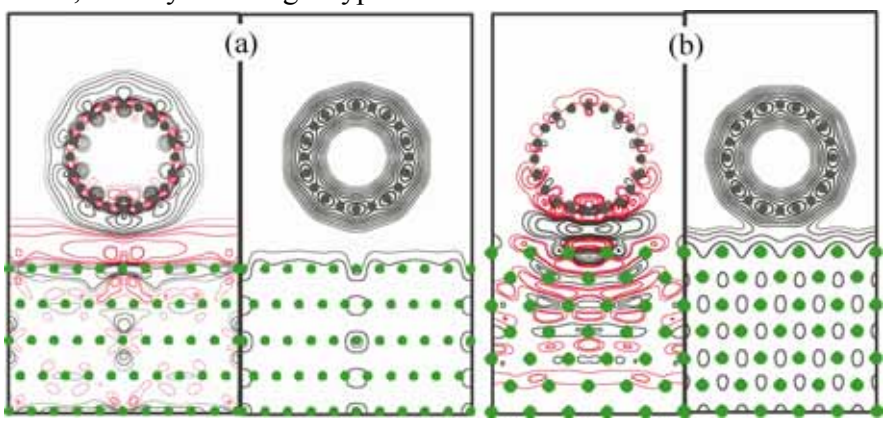

Fig. 3: Contour Plots of electron density of (10,0) CNT on (a) Ca(100) and (b) Al(100) surfaces. In (a) and (b), each left panel shows increase (black lines) and decrease (red lines) of electron density upon

adsorption. Each right panel shows total electron density [Okada & Oshiyama: Physical Review Letters (2005)].

We have also explored a possibility of placing CNTs regularly on semiconductor surfaces (Fig. 4). We considered Si(001) surface. For a thin (5,5) CNT, it has been found that the site on the terrace is most stable with the binding energy 2.77 eV and that the next most stable is the site along step edges with the binding energy 1.88 eV. The binding energies should depend on tube radii and thicker tubes favor step edges. In the Si(001) vicinal surfaces, double-layer step edges are known to align regularly. The present calculations show a possibility to align CNTs using step edges as templates.

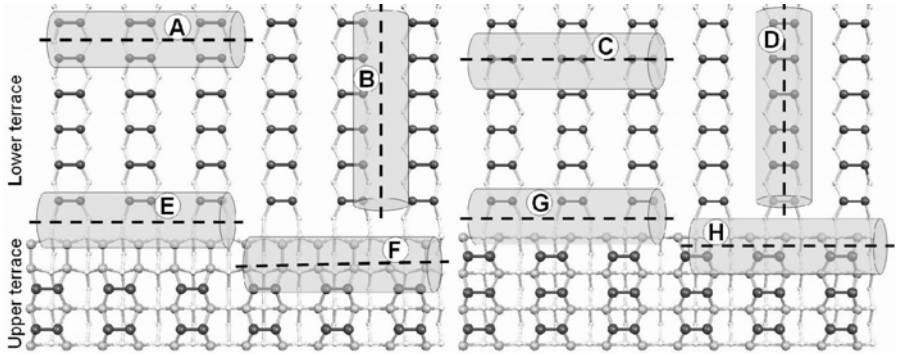

Fig 4: Various sites of CNTs adsorbed on Si(001) surface. A, B, C and D are the sites on terraces, whereas E, F, G and H are the sites near double-layer step edges (lower part of the figure is the upper terrace) [Berber & Oshiyama: Physical Review Letters (2007)].

CNT is expected to be used channels in next-generation transistors. In the case, quantitative determination of capacitance of tubular structures is imperative in device design. We have recently calculated capacitance of double-wall CNT which may be an ultimate cylindrical structure. It is found that quantum effects cause drastic variation of capacitance with changing bias voltage [Uchida, Okada, Shiraishi and Oshiyama: Physical Review B (2007)].

In application to medical engineering, waters or solutions in CNT may be important. Waters confined in nano-space have not been studied, however. We have recently calculated structures of ice in CNT and found that polygonal-shaped ice is stable in CNT. CNT works as templates for new polymorphs of materials [Kurita, Okada and Oshiyama: Physical Review B (2007)].

3.3 Collaboration

1) Alliance with Division of High Performance Computing System

Tuning of RSDFT code on PACS-CS has become possible in collaboration with people at division of High Performance Computing System. In addition to examination of algorithms as described above, detailed discussion on general aspects as well as particular coding has been done regularly and contributes a lot to promotion of research.

2) Collaboration with Computational Life Science Group

Our stance is to recognize common features in nano- and bio-materials, perform calculations based on quantum theory, and clarify and predict various phenomena in both materials. Collaboration with computational life science group is therefore essential. This is manifested as several publications which include the clarifications of microscopic mechanisms of (A) self-cleaving of ribozymes [Boero et al, Int J. of Theory and Computation (2005)] and (B) proton transfer in Cytochrome c Oxidase [Kamiya et al, JACS (2007)], using Car-Parrinelo Molecular Dynamics and Metadynamics.

3) Collaboration with Quantum Many Body Group

Time-dependent density functional theory is an important methodology in quantum many body group. The scheme has common aspects with our RSDFT code. Collaboration on efficient computations is now in progress.

3.4 Future Plan

In our research activity, there are several different phases: developments of new computational methodology, sophistication of current methodology , and the applications to real materials. It is important to make those different activities proceed interactively. By focusing all those phases, we try to contribute to materials science by computational approach and to the progress in theoretical physics and chemistry as well as computational science.

In the phases of developments and sophistication of methodologies, schemes which are capable of accurate and large-scale calculations are required. The DFT scheme is now capable of treating 10,000 atoms on 10-TFLOPS machine where 1,000 nodes (CPUs) at most are used. Yet to clarify stability and electronic properties of 10-nanometer-scale structures, including proteins, calculations for 100,000 atoms by using 10,000 or 100,000 nodes may be necessary. We are planning to optimize RSDFT scheme and introduce a hybrid QM/MM scheme to tackle this issue. The plat form we consider is the next-generation peta-flops supercomputers consisting of several hundred thousands nodes.

Improvement of accuracy is also important. That is a development of a new scheme which is capable of treating phenomena inaccessible by the current DFT. Our main target in this phase will be van der Waals forces which play important roles in carbon nanomaterials and biomaterials. It would be beneficial when a new scheme can be combined with large-scale DFT-based scheme.

In addition to total-energy electronic-structure calculations and molecular dynamics calculations, simulations or predictions of response functions of materials are important. We have already developed several computational schemes to calculate conductance and capacitance and applied them to real materials. We plan to continue those calculations for various materials and structures.

3.5 Publications

3.5.1 Journal Papers

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4. Division of Materials and Life Sciences: Computational Life Science Group

4.1 Research Activity

The Computational Life Science Group is one of the new research sections that planned and started at the beginning of the activities of the Center for Computational Sciences, just two years ago. In this respect, this is a relatively young group. As a general overview, the research activities assume, as a starting point, the 3D structures and functions of biological macromolecules such as protein, DNA, and RNA, and aims at the study of the reaction mechanisms and molecular system formation processes, as the basis of the living organisms. One of the ultimate goals is to address issues useful and of practical technological interest to the emerging field of nano-bio engineering.

Because of the complexity involved in these biological systems, various techniques in computational sciences, theoretical physics and chemistry, structural bioinformatics, and related fields are intensively used and integrated, thus allowing for the elucidation of the electronic, atomic, and molecular mechanisms involved in biological phenomena. Concretely, in order to apply molecular simulation techniques, such as molecular dynamics, first principles quantum-mechanics-based calculations, etc., to biological macromolecules with both high accuracy and high efficiency, fundamental algorithms are developed and implemented in computer codes. Specifically, the topics below have been tackled;

1) Development of quantum mechanics / molecular mechanics (QM/MM) hybrid schemes based on all-electron DFT calculations as a QM driver.

2) Development of an energy functional which accurately describes the electron correlation responsible for the stacking of aromatic rings in amino acid residues and bases in nucleotide residues.

3) Development of a molecular docking calculation method for proteins and ligands including explicitly the solvent water molecules.

4) Development of a protein-protein docking calculation method based on hydrogen bond networks formed around the interface region.

The use of these computational systems is expected to lead to more accurate results than what can be achieved by conventional methodologies, thus allowing for a better elucidation of the basic functional mechanisms of living organisms. As far as the specific problems targeted by our group, we have focused on the following important topics:

1) Hydrolysis reaction mechanisms of RNA enzymes (ribozymes).
2) Energy conversion mechanisms by the electron transport system in mitochondria.

3) Charge localization and transport in synthetic Z-DNA and native DNA.
4) Reaction mechanisms of the ATP synthase (ATPase) in heat shock cognate proteins (Hsc70).
5) Molecular recognition and enzymatic reaction mechanisms in the protein biosynthesis system.
6) Gene expression mechanisms through interactions of transcriptional factors and DNA.
7) Dynamical mechanisms occurring in the formation process of three-dimensional structure of protein (folding).
8) Dynamical behavior of cellular reaction network systems for signal transduction.

In the next section, some research achievements are summarized from the topics listed above.

4.2 Research Results

1) Mechanisms of self-cleavage reaction of ribozymes

Enzymes include not only proteins, but also RNA; RNA enzymes were discovered in the 20th century latter halves, and the discoverers were awarded the Nobel Prize. An RNA enzyme is called ribozyme, and it led to a new hypothesis on the origin of life, i.e. the primordial organisms were originated from RNA (ribozyme), and such a phase in the evolution of organisms is called the "RNA world".

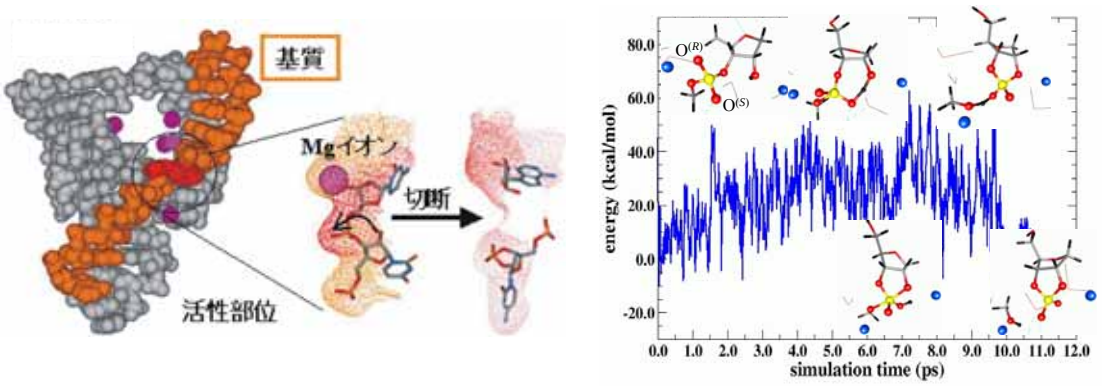

Fig. 1 (left) The crystal structure of the hammerhead ribozyme. [Boero, M., Tateno, M., Terakura, K., and Oshiyama, A., *J. Chem. Theo. and Comp.*, **1** (2005), 925-934] (right) The free energy profile and several conformations of the ribozyme obtained by performing CPMD coupled to metadynamics.

A ribozyme is able to cleave (hydrolyzes) its own phosphodiester bond or the one of

another RNA molecule. If one can tune this mechanism to specifically cleave the mRNA of oncogene, the ribozyme would work as an anticancer agent and/or can be used as a therapeutic agent in cancer gene therapy. This makes ribozyme an important research target in fundamental biology and medical sciences, and for this reason it has been the subject of intense studies by several research groups in the world since more than ten years. In our study, by using first-principles molecular dynamics simulations, the details of the mechanism of the ribozyme reaction have been elucidated at an atomic-scale level.

In the ribozyme reaction *in vitro*, it is well known that cations play the role of catalysts and help in enhancing the reaction rate. However, the number of the cation(s) involved in the catalytic activity was, and to a certain extent still is, one of the major open questions on the ribozyme reaction, i.e. some experimental results concluded that one single cation participates to the reaction, whereas other experiments claim that two cations are involved. We investigated this issue, performing first-principles molecular dynamics calculations for several models, both in the absence of cations and in the presence of one or two Mg^{2+} metal ions.

As a result, we found that the minimal activation barrier arises in the case in which two Mg^{2+} cooperate to the reaction. In contrast, if only one Mg^{2+} cation, or none, are present, the activation barrier increases remarkably, and thus, in those cases the reaction is not expected to occur. Furthermore, we found that the addition of an OH- hydroxyl anion, along with two Mg^{2+} decreases further the activation barrier. Moreover, we also elucidated the active role of each player, namely each Mg^{2+}, OH-, H_2O, in the reaction. Thus, we could address theoretically some of the basic issues about the ribozyme reaction and we provided a clear atomistic picture of the mechanisms.

2) Mechanisms of biological energy conversion in electron transport system

The role of the electron transport system in a cell (mitochondria) is to operate an energy conversion from carbohydrates into the chemical high energy bond of the ATP molecule, which is available at various sites in living organisms. One of the ultimate goals of our research is to clarify the entire picture of the mechanisms of the electron

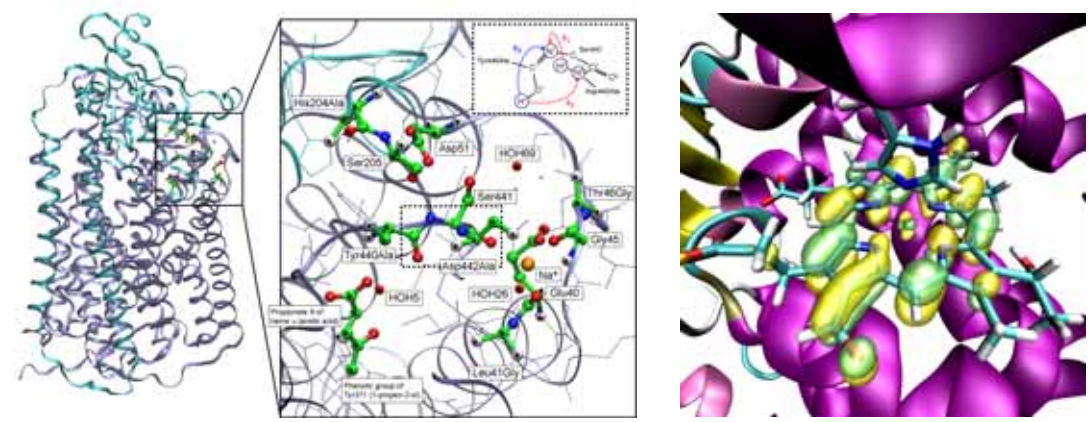

Fig. 2. (left) The functional subunits of cytochrome *c* oxidase (CcO) and the site analyzed by performing CPMD coupled to metadynamics are depicted. [Kamiya, K., Boero, M., Tateno, M., Shiraishi, K., and Oshiyama, A., *J. Ame. Chem. Soc.*, **129** (2007), 9663-9673] (right) Electronic structure calculated by the all-electron based QM/MM hybrid calculation.

transport system in organisms. In this respect, a molecular system that deserves special attention and that has been intensively studied is the cytochrome *c* oxidase (CcO), since it is one of the key factors in electron transport and cell respiration process. In particular, a Japanese research group (Tsukihara and Yoshikawa) has been able to determine, with high accuracy, the three-dimensional structure of the bovine CcO by X-ray crystallography; the result is certainly recognized as being worldwide unprecedented.

In our group, we have investigated the mechanisms of proton transfer, electron transfer, and catalytic reaction operated by CcO, performing electronic structure calculations based on the first principles molecular dynamics simulations and QM/MM hybrid calculations. As far as the proton transfer is concerned, in conventional propagation paths (K-path and D-path) proposed in the literature, it is expected to occur along hydrogen bond networks inside proteins. However, Tsukihara and Yoshikawa found an alternative pathway that includes a peptide group within hydrogen bond networks in CcO, which apparently interrupts the proton transfer. They suggested that the peptide group can transfer protons via an keto-enol isomerization, and therefore, that the hydrogen bond network would still result fully connected; this novel pathway is called H-path.

By using Car-Parrinello-based molecular dynamics simulations, coupled to the metadynamics method, we investigated the possibility that the proton transfer reaction can really occur through the covalent bond (peptide bond). As a result, protons of the amide groups of the two peptide groups (Y440-S441 and S441-D442), which are located close to

each other, could be transferred sequentially, leading to a continuous proton transfer reaction chain of the H-pathway. This could be a novel mechanism of proton transfer, if it is experimentally proven. However, for the calculation, crucial interactions of the peptide group and the side chain of the other amino acid residue could not be included in the model system, and this leaves still some open issues about the estimation of the actual activation barrier.

In order to overcome those difficulties, we pursued the investigation by performing QM/MM hybrid calculations for structures derived from the original X-ray data, where all of the functional subunits of CcO (i.e. subunits I, II, and III) and solvent water molecules are included explicitly. Moreover, since heme (which is a complex of a porphyrin ring and an iron) moieties play crucial roles in the enzymatic reaction, in proton/electron transfer reactions, in free energy transfer, etc., we investigate these relevant functional sites by QM/MM hybrid calculations. These projects on CcO are presently under execution.

4.3 Collaboration

For research projects on the ribozyme reaction and the proton transfer of CcO, we have collaborated with the Computational Condensed Matter Science Group. Furthermore, in order to improve the performance of CPMD code, in particular, on PACS-CS, we have collaborated with the High Performance Computing System Group. In particular, fruitful discussions, benchmarking, and testing of the CPMD code, both in the full quantum and in the hybrid QM/MM versions, done jointly with the High Performance Computing System Group, along with their suggestions, allowed to port and tune the code on the PACS-CS machine and provided a useful background in the development of CPMD.

Other development and functionalities of the code are now being implemented, such as the handling of different thermostats and thermostat chains for classical and quantum atoms, handling of ultrasoft pseudopotentials in the hybrid QM/MM code, new collective variables for the selection of the reaction coordinates in metadynamics and blue moon / umbrella sampling approaches, etc.

Furthermore, also for the QM/MM hybrid calculation system based on all-electron DFT calculations, similar collaborations with the High Performance Computing System Group are planned.

4.4 Future Plan

We have been developing and fundamentally improving several crucial calculation systems described in the above first section, since the former systems developed in this field turned out to be insufficient to several extents in analyzing functional mechanisms of

biological macromolecules. For the issues on the ribozyme reactions and the electron transport system, nearest future plans are briefly mentioned in the second section, as applications of those new systems. Also for the other issues described in the first and second sections, we are searching for a possible break-through of each of the fields summarized below.

1) Protein docking algorithm and its applications to the CcO-Cc complex

It is well known that the reaction of cytochrome *c* oxidase (CcO) requires the formation of the complex with cytochrome *c* (Cc), since electrons are transferred from the outside of CcO. However, despite intensive efforts by crystallographers, the crystal structure of the complex of CcO and Cc has not yet been experimentally determined. We have developed a novel protein docking simulation algorithm, based on theoretical identification of hydrogen bond networks at the interface of the two proteins.

This algorithm allows for the exploration and detection of specific interactions of proteins, which can decrease the large amount of both false positive and false negative candidate structures of the complex. The implementation of this algorithm enables us to perform the calculations necessary to obtain an accurate docking model of the CcO-Cc complex. This theoretical model makes now possible to investigate in detail the mechanisms of the electron transfer and enzymatic reaction of CcO.

2) Development of an energy functional able to describe the electron correlation effects responsible for the stacking of aromatic side chains in protein and nucleic acids.

It is well known that the stacking of aromatic side chains (the parallel- and T-types) is crucial for the stabilization of proteins and nucleic acids. However, this stabilization cannot be obtained by any of the present-day DFT-level approaches and one has to rely on computationally more demanding methods, such as MP2 and CCSD.

We have developed an effective energy functional for describing those interactions of aromatic side chains, allowing for accurate calculations at a small computational cost, which is available not only in the case of static calculations, but also in the case in which classical molecular dynamics simulations are performed. We are now applying this scheme to the protein folding problem, to explore the free energy surface at a level of accuracy not yet reached.

3) QM/MM hybrid calculation system

Using the all electron-based QM/MM hybrid simulation program, large scale calculations are scheduled in our group through collaboration with the High Performance

Computing System Group. For CcO and the CcO-Cc complex, the catalytic center, which amounts to about 1000-atom, is treated as the QM subsystem, whereas the rest is described by classical force fields.

These QM/MM calculations would make possible a close inspection of the changes in the electronic structure occurring in the catalytic reactions involved in the various processes. Also for aminoacyl-tRNA synthetases, which are crucial for the protein biosynthesis inside the cell, simulations including 1000 QM-atom, are planned, in order to elucidate the entire mechanisms of the enzymatic reaction indispensable to convert genetic information into amino acid sequences.

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4.5.1 Journal Papers

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4.5.2 Proceedings

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5. Division of Materials and Life Sciences: Quantum Many-Body Systems Group

5.1 Research Activity

The members of the research group of quantum many-body systems are Kazuhiro Yabana, Yukio Hashimoto, Takashi Nakatsukasa, who belong to Institute of Physics, and Ken-ichi Hino, Hiroyasu Koizumi, Xiao-Min Tong, who belong to Institute of Material Sciences. Most of the members joined the Center for Computational Sciences when the Center has started in 2004. Xiao-Min Tong joined this group in October, 2005. Ken-ichi Hino moved to a position outside the Center in the Univ. of Tsukuba in April of 2007. Takashi Nakatsukasa moved to RIKEN as Associate Chief Scientist in August, 2007. Applications of candidates for the position after Ken-ichi Hino are being accepted.

We study a variety of matters in the physical world such as atomic nuclei, atoms, molecules, and solids. In the world of quantum physics, all the constituent particles of matters behave as waves. We are developing methods of calculating time evolution of the wave function based on quantum theory to describe individual motion of particles – protons and neutrons in nuclei, electrons and nuclei in materials – and to investigate a variety of quantum phenomena taking place in nature. The researches in our group include (1) interaction between laser-light and materials [Hino, Tong; Yabana, Nakatsukasa], (2) quantum dynamics of few-body reaction [Hino, Tong; Yabana, Nakatsukasa], (3) transport phenomena of strongly-correlated systems [Koizumi], and (4) quantum dynamics of excitations, responses, and reactions of atomic nuclei [Yabana, Hashimoto, Nakatsukasa].

○ Interaction between laser and material

Laser sciences are rapidly developing as an interdisciplinary field of various scientific areas. One of the frontiers in laser sciences is the interaction of ultra-short and intense laser pulse with matter. In this field, there have been observed a variety of electron dynamics which originates from nonlinear interaction between the laser and matter in a time scale as short as femto- or even atto-second. Such processes are expected to be useful to control the properties of materials quantum mechanically. We are developing computational approaches to understand elementary processes of laser-matter interaction, to predict new phenomena, and to assess and/or propose possible ways of quantum control with laser.

Atoms and molecules in the intense laser field are ionized through multiphoton and tunneling mechanisms. Emitted electrons in the ionization are accelerated by the laser field and re-scattered by the parent core. This re-scattering is a characteristic process in intense laser field, causing such nonlinear processes as high-order harmonic generation and

non-sequential multiple ionization. The ionized molecules are then fragmented by dissociation or by Coulomb explosion. To understand these processes, we are developing approaches solving the time-dependent Schroedinger or Kohn-Sham equations in real-time.

In the optical interaction between laser and low-dimensional semiconductors, there has been observed a variety of electronic states reflecting the nanostructure in low-dimension. Such laser-material interactions are expected to be useful for quantum control of low-dimensional structure. We are developing a new computational method for them, extending a frameworks developed in atomic and molecular physics.

For the interaction of intense laser pulse with electrons in bulk crystal, we have developed a new framework describing electron dynamics in infinite periodic systems. This framework has opened a new field, a simulation of nonlinear electron dynamics in bulk material, and has been applied to investigate such phenomena as optical breakdown and coherent phonon in dielectrics.

○ Quantum dynamics of few-body reaction

Accelerated particles are the basic probes to investigate microscopic structure of matters through scatterings and reactions. Recently, the accelerated particles have come to be used to synthesize new matters through reaction processes. These studies are now under progress as big-science projects in several fields of fundamental sciences. We are developing computational approaches for quantum few-body reactions relevant to new matter syntheses such as an anti-proton helium which is produced by a collision of anti-proton and matter, and reactions of exotic atomic nucleus produced in the RIBF (Radioactive Ion Beam Factory project) in RIKEN.

In traditional scattering theory, one solves the time-independent Schroedinger equation for a fixed energy to obtain scattering wave function. We have developed a new computational method solving the time-dependent Schroedinger equation for the scattering process. This approach is especially useful for scattering processes involving more than three-particles.

○ Transport phenomena in strongly correlated systems

Compounds containing transition metals are known to show a variety of functions depending on the transition-metal atom in them and ligands surrounding it. They are susceptible to interaction between contacted molecules or external fields such as light, heat, pressure, electric and magnetic fields. We have been studying anomalous electronic transport phenomena and superconductivity for these systems of transition metal complex with strong electronic correlations and strong electron-lattice interactions. In particular,

elucidations of the mechanism of huge magnetoresistance in manganese-oxide and the elucidation of high-temperature superconductivity in copper-oxide have been studied with high priority.

○ Quantum dynamics of excitation, responses, and reactions in atomic nuclei

In the history of quantum many-particle theory, electronic many-body systems composed of electrons and atomic nuclei, and nuclear many-body systems (atomic nuclei) composed of protons and neutrons are the two major matters where the quantum many-body theory has been developed. In recent development of computational quantum sciences, common methods have also been successful in both systems such as the density-functional theory. We are developing a time-dependent density-functional approach for excitation and responses of atomic nuclei. Yabana and Nakatsukasa take part in the project UNEDF (Universal Nuclear Energy Density Functional) organized as a SciDAC project in USA.

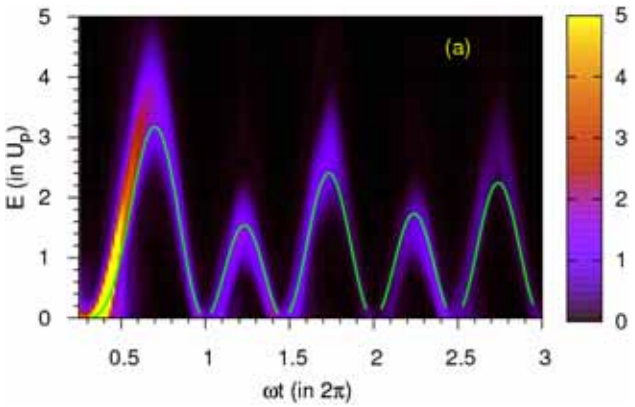
The number of published papers in this group is as follows:

2004 : 28 (refereed journal 20 + conference paper 8)
2005 : 40 (refereed journal 24 + conference paper 16)
2006 : 25 (refereed journal 17 + conference paper 8)
2007 : 19 (refereed journal 12 + conference paper 7)

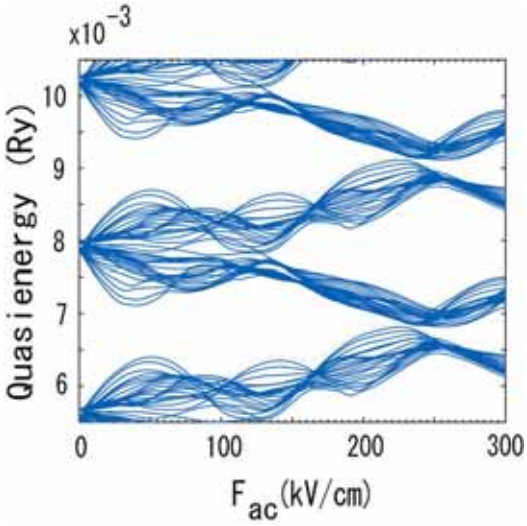
There are 6 grants from MEXT (4 for Kiban (C), and 2 for Priority Area) for which a member of this group is a representative researcher.

5.2 Research Results

○ To describe and understand physical phenomena relevant to a few-body systems with Coulomb interaction, we have developed a numerical method solving the time-dependent Schroedinger equation with high accuracy. The method has been applied to phenomena such as a tunnel ionization of atoms under ultra-short intense pulse laser, a synthesis and decay dynamics of an anomalously long-lived anti-proton helium system, and reactions of exotic nuclei with halo structure. These calculations have been useful to describe measured data accurately and to obtain deep insight of their physical mechanisms. The figure shows the time evolution of the electron energy distribution re-scattered in the field of intense laser. [Hino, Tong; Yabana, Nakatsukasa]

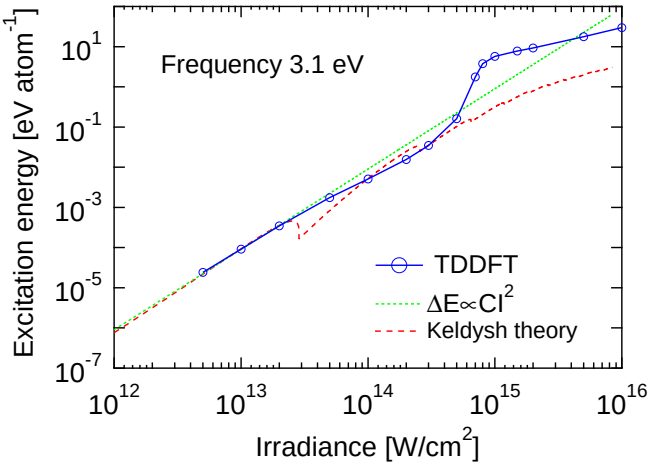


○ We have made a large-scale calculation for the quasi-energy structure of Floquet state (dynamical Wannier-Stark ladder state) which shows a strong coupling between the semiconductor Wannier-Stark ladder and the laser field. The right figure shows the band structure of quasi-energy band of Floquet state by monochromatic laser. Our work clarified the exciton effects, Zener effects, and the acceleration effect by periodic pulses. In particular, we have found a new approach of quantum control erasing both static and dynamics Zener effect coherently by periodic pulse sequence and a curious behavior in the density of states of Floquet states. [Hino, Tong]

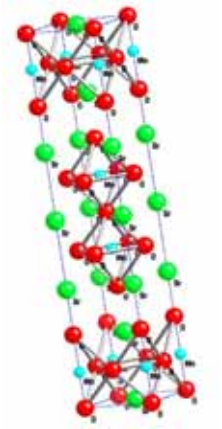


○We have succeeded the first-principles calculation of the electron dynamics for laser induced dielectric breakdown of dielectrics. When an ultra-intense laser field is irradiated to the dielectrics, a great number of electron-hole pairs are excited even for a visible light which should be transparent in large-gap dielectrics. These excitations make the response of the dielectrics metallic, and are employed for the purpose of laser machining and surgeries. We have shown, for the first time, that this process of optical dielectric breakdown can be

naturally described by solving the time-dependent Kohn-Sham equation. The figure shows the energy transfer from the laser pulse to the electrons in diamond as a function of the maximum intensity of the laser pulse. Around 10^{15} W/cm^2, a substantial increase of the energy transfer is seen where the dielectric breakdown occurs. A part of this calculation is achieved by PACS-CS. [Yabana, Nakatsukasa]



○We have achieved cluster calculations employing molecular-orbital method for manganese-oxides and copper-oxides, and have obtained new insights on local electronic structure and electron-phonon interactions. In the both systems, electron-phonon interaction is so strong that the doped carriers become small polarons. We have also obtained a new mechanism for electronic current generation in which a fictitious magnetic field that is induced by spin vortex excitations gives rise to electric current. [Koizumi]



○ We have developed a computational code of many-electron dynamics with real-time and real-space method appropriate for massively parallel computers. To describe electron dynamics based on the time-dependent density-functional theory, one need to calculate time

evolution of the orbital functions,$\varphi_i(x,y,z,t)$. We have developed two computational codes, one is parallel in orbitals or k-points, and the other is the code parallel in spatial division, and we have evaluated the efficiency of the codes in PACS-CS. The k-point parallel code is used in the calculations of optical breakdown at PACS-CS. The parallelization with space division is expected to show good scalability for massively parallel computation. Further developments to achieve better communication costs and better computational efficiency are now under progress. [Yabana, Nakatsukasa, Hashimoto]

5.3 Collaboration

The members in the Institute of Physics who have experiences in nuclear physics (Yabana, Hashimoto, Nakatsukasa) and the members in the Institute of Material Sciences who have experiences in atomic and molecular physics (Hino, Tong) have common interests in laser sciences and quantum dynamics, and employ similar computational methods. We are now considering to promote a close cooperation on large-scale computation in quantum dynamics.

The real-time, real-space DFT code as well as the real-space DFT code which runs efficiently in massive parallel machines have been developed under close cooperation with the group of computational material sciences and the group of computer system. A regular monthly meeting has been organized for this purpose. A considerable part of the source code of the real-time calculation is common with a real-space density-functional code which has been developed in the group of computational material sciences.

Besides present cooperation described above, we hope to initiate the followings in future. Since the electronic excitation and dynamics are important to understand functions of biological molecules, real-time DFT calculation may be useful. We hope to cooperate with computational biology group on this subject. In the group of computational elementary particles, the lattice QCD calculations of nuclear force and nuclear matter have been rapidly developing. They may bring a breakthrough and may open a new frontier for the studies of nuclear structure. Cooperation with them on nuclear DFT study will be expected.

Since the group members have their own offices in two different areas in the campus outside the Center, there is a problem of insufficient daily interchange among members in the group and with members in other groups.

5.4 Future Plan

We consider the time-dependent computational approach for quantum dynamics is a promising field. We plan to further develop methods of solving time-dependent Schroedinger and Kohn-Sham equations and to explore quantum dynamics in a variety of

fields, especially in optical sciences. To extend the areas of application and to investigate quantitatively for large systems and/or correlated systems, computational codes which work efficiently in massive parallel computers need to be developed.

In the fields of laser-matter interaction and few-body quantum dynamics calculations, we plan to proceed with the following researches:

1. To explore electron dynamics in atto-second scale, multipole ionization process of atoms will be explored taking account of the effect of electronic correlations.
2. The interaction of laser with biological molecules is a promising fields. We will develop first-principle calculations of electron dynamics, taking into account future experiments in XFEL (X-ray free electron laser).
3. The optical breakdown and the coherent phonon are typical examples reflecting nonlinear interaction between intense laser and solid. We explore their basic mechanism with the first-principle calculation.
4. A new real-time computational method will be explored for the electronic states dressed with light (Floquet state).
5. A new method of quantum control will be investigated making use of the coupling between laser and materials.

In the cluster calculations for strongly correlated systems, a large-size cluster calculation with the molecular orbital method is planned. It will be compared with the band calculation in the density functional theory. In the future, we plan to design biosensing materials by using molecules with strong correlation and electron-lattice interaction; their unique transport phenomena and high susceptibility to external fields are expected to be suitable for detecting molecular environments. This part of the work will be conducted by collaboration with Prof. Satoko of Nihon University.

In nuclear physics, we proceed with a study of unstable atomic nuclei which are now rapidly developing in the RIBF (Radioactive Ion Beam Factory) project. One of the ultimate goals is a construction of computational nuclear data for both stable and unstable nuclei, by developing the density-functional approach for nuclei. We expect simultaneous research on both systems of Coulombic and strong interactions will be beneficial to promote computational sciences of quantum dynamics with wide scope.

5.5 Publications

5.5.1 Journal Papers

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6. Division of Global Environment and Biological Sciences: Global Environmental Science Group

6.1 Research Activity

In the Group of the Global Environmental Science of the Division of Global Environment and Biological Sciences, there are two fulltime staffs of Prof. Hiroshi L. Tanaka and Asst. Prof. Hiroyuki Kusaka (Dept. of Life and Geoenvironmental Science) and one collaborative staff of Prof. Fujio Kimura (Dept. of Life and Geoenvironmental Science) and one affiliated staff of Prof. Akio Kitoh (Meteorological Research Institute, Japan Meteorological Agency).

6.1.1 Activity in 2005

The main research activity of the group in 2005 was to establish a new collaboration with the groups of High Performance Computing System and Computational Informatics because it was the first year for our group as the newly founded division in the Center for Computational Sciences (CCS). As the first attempt of our group, we started to archive the daily numerical weather prediction data called grid point values (GPV) provided by the Japan Meteorological Agency (JMA). This activity of archiving initial data and ensemble prediction data was organized by the world-wild project called THORPEX: The Observing System Research and Predictability Experiment. The THORPEX project has started in 2003 and will continue to 2012 under the leadership of the WMO: World Meteorological Organization, with a special emphasis of improving the deterministic weather predictability and developing the advanced observational system.

The aim of the THORPEX is to improve the prediction skill especially for the extreme events for the range of one day to two weeks by combining the advanced observational technology and the sophisticated high-performance prediction models based on the recent technology of the ensemble prediction, four-dimensional data assimilation, targeted optimal observation, high-tech satellite imageries, etc. Under the THORPEX project, our university held a research contract with the JMA and started to archive the ensemble prediction data provided by the JMA. The project is called GPV/JMA project that attempts to establish a large meteorological database within the CCS facility.

The Group of Global Environmental Science started the collaboration with the High Performance Computing System and Computational Informatics in CCS, assembling periodically once a month. First, we bought a data server named gpvjma to archive the various kinds of GPV/JMA data, assisted by the Computational Informatics group for the

maintenance and by the High Performance Computing System group for the technical support. The data archive and release to the public began in January 2005. The GPV data are not only archived but also analyzed to present many kinds of weather maps and animations of the maps to present for the public.

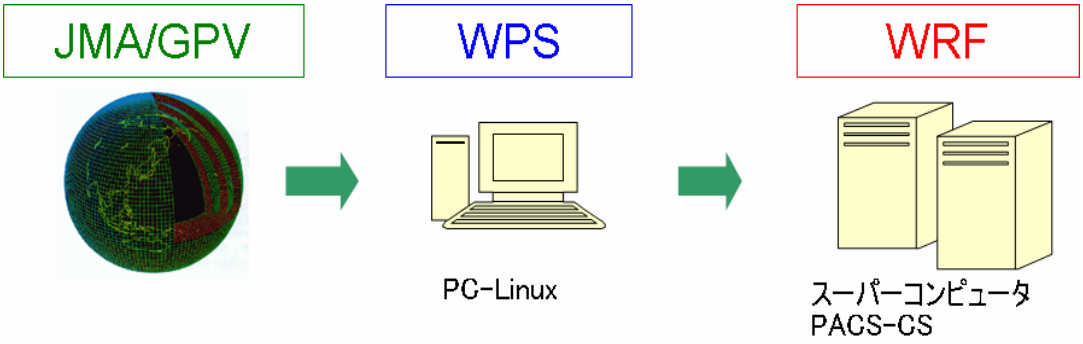

Figure 1. Weather data called GPV (grid point value) provided by JMA (Japan Meteorological Agency) and the data flow to CCS.

Under the research contract between the University of Tsukuba and JMA, we sent one graduate student in the doctoral degree program for the project of the Advanced Ensemble Prediction Technology. We imported the operational weather forecasting model of the JMA called Global Spectral Model (GSM T63L40) in order to conduct ensemble prediction by installing the model to the PACS-CS under the construction at CCS. The test run was performed under the PC cluster system.

Since the GPV/JMA project of archiving real-time weather data became an operational phase with steady increase of the users, a new plan of archiving and releasing the Japan Reanalysis Data for 25 years (JRA-25) is proposed. The JRA-25 data are provided by the collaborative work by the JMA and the Central Research Institute for Power Industry (CRIPI), although the plan was still pending by the restrictions and regulations announced by the JMA.

As the application studies of the global environment and atmospheric science, Prof. Tanaka obtained a research fund from the National Science Foundation (NSF) by way of the collaboration with International Arctic Research Center (IARC) of the University of Alaska Fairbanks in USA for the study of the global warming in connection to the Arctic climate. With this fund the 6th International Conference on Global Change: Connection to the Arctic (GCCA-6) was held in December 2005 at the Miraikan in Tokyo Japan. The former GCCA-5 was held at the University of Tsukuba in 2004.

At this time, the fulltime staff in the group was only Prof. Tanaka. An employment of

additional young staff was the urgent problem to enhance the group activities. As the future plan of the group, an expert in the regional weather prediction modeling was proposed to compensate the research activity in the global ensemble predictions with the general circulation model.

6.1.2 Activity in 2006

In 2006, the main activity of our group was devoted to the study of the Arctic Oscillation, which causes the global scale abnormal weather. The increased occurrence of the abnormal weather in recent years is accompanied by the geographical distribution characterized by the Arctic Oscillation which may have a close relation to the global warming.

For example, an extreme heavy snow along the west side of Japan Island was broken out in the winter of 2005/06, which was named as Heisei 18 Heavy Snow Event. The subsequent winter of 2006/07 was, on the contrary, abnormally warm with the extremely late first snow fall in Tokyo recorded on 16 March 2006. These abnormal winters were explained by the manifestation of the Arctic Oscillation phenomenon.

Figure 2. Arctic Oscillation and the abnormal weather in the Northern Hemisphere.

Assisted by the sever weather in recent years, the Grant In Aid research proposal of Category A to the JSP by Prof. Tanaka was granted. The research title is The dynamical understanding of the Arctic Oscillation and the low-frequency variability. Additional research fund has arrived from the IARC/UAF in the USA and from Asahi Brewery Foundation for the study of the Arctic Oscillation and its prediction. In February 2007, the 7th International Conference on the Global Change: Connection to the Arctic (GCCA-7) was held in Fairbanks Alaska, USA. University of Tsukuba is one of the organizing

members.

The operational global spectral model in JMA was update from GSM T63L40 to GSM TL159/319 due to the replacement of the new computing system in JMA. We need to re-install the GSM every time whenever updated. Since the operational spectral model will not fit in the PC cluster scalar machine, using GSM of JMA for the PACS-CS must be reconsidered for the future plan.

In parallel with global weather forecasting model, we wish to install a regional weather forecasting model for the future plan. Dr. Hiroyuki Kusaka was hired as a new Assistant Professor in our group who is an expert of the WAR regional model, especially for the urban climate model development nested in the regional and global weather forecasting model. Combined with the real-time GPV/JMA data and the JRA-25 analysis data, the regional model experiments of heavy shower and heavy snow events in Japan had started in our group. Currently, the latest WAR model is version 2.2 released on 23 December 2006 by the National Center for Atmospheric Research (NCAR), where the urban model originally developed by Dr. Kusaka is installed in the official WRF module.

6.1.3 Activity in 2007

In 2007, the operation of the PACS-CS has started. In association with the PACS-CS project, we established a new research contract with the Center for Climate System Research (CCSR) of the University of Tokyo in order to collaborate for the development of the next generation cloud resolving non-hydrostatic icosahedral general circulation model (NICAM), which was developed by the group in CCSR and the Frontier Research Center for Global Change (FRCGC) in JAMSTEC. The NICAM of CCSR/FRCGC is superior to the GSM of JMA in that the dynamical core of the model is formulated specifically for the massively parallel processing using MPI which fits perfectly with the PACS-CS. The traditional spectral model like the GSM needs all to all data transfer. Therefore, the spectral dynamical core would reach to the dead end in the future development.

In contrast, the NICAM can extend the model resolution to 3.5 km global mesh with cloud resolving physical process. The testing phase with an aqua planet model (no topography) has completed successfully, and full terrain has just installed in the model. Using the latest version of the NICAM with topography, a near real-time prediction experiments are conducted attached with the realtime GPV/JMA data archive under the PACS-CS facility.

The GPV/JMA data is free to the public. Yet, the data resolution released to the public is quite coarse and not sufficient for the accurate weather prediction as the initial data. The JMA and the Meteorological Society of Japan (MSJ) established a comprehensive research

contract in July 2007 as the Weather Research Consortium. Prof. Tanaka is elected as one of the first board member of the consortium. Under this contract, the accurate initial data with full resolution of the operational weather forecasting model by JMA are released to the member of the consortium. Our group in CCS is expected to serve as the data mirror site of the consortium data. We purchased 8.25TB raid server and started to archive the consortium data in addition to the GPV/JMA data.

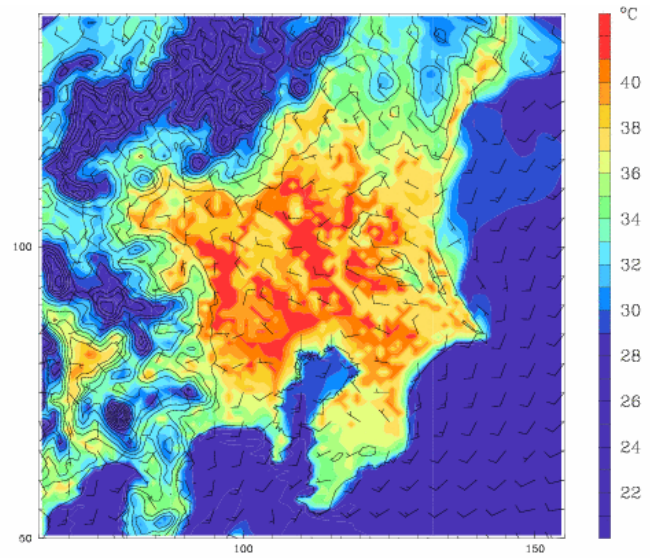

Figure 3. Simulation of surface temperature by the regional model called WRF. A record high temperature of 40.9 deg C was observed on this day.

The WRF regional model was progressively developed under the PACS-CS project. Coupled with the real-time GPV/JMA data, the real-time regional weather prediction system was constructed experimentally. A test run was demonstrated for the explosive cyclogenesis event occurred on 7 January 2007 to confirm that the system is useful for educational purpose as well as research. Since the real-time weather prediction is restricted to release for the public without the permission by the JMA, the prediction is used only internally within the group.

As the product of the collaboration with the Computational Informatics group, a research project of the advanced utility of weather information based on the weather ontology leaded by Prof. Kitagawa was promoted to show a real time weather maps superimposed on the Google Earth. Various weather maps of GSM (global spectral model), RSM (regional spectral model), and MSM (meso-scale non-hydrostatic model) are combined with Google Earth in terms of the KML files. The product was released to the

public in conjunction with the GPV/JMA products by the effort of Asst. Prof. Amagasa. The real time monitoring is displayed at the entrance of the CCS using large screen TV since the Opening Ceremony of the PACS-CS System in September 2007.

6.2 Research Contributions

Contributions by Dr. Hiroshi L. Tanaka for 2005-2007

(1) Articles, Papers and Reports: total of 38 papers
Books: 3, Papers with peer review 19, other 16
(2) Arctic Oscillation in connection to the global warming
(3) Arctic Oscillation and abnormal weather
(4) Singular eigenmode theory of the Arctic Oscillation
(5) Changes in tropical circulations under the global warming
(6) Theory of energy saturation by Rossby wave breaking
(7) Energy spectrum of E=mc^2 observed in general circulation

Contributions by Dr. Hiroyuki Kusaka for 2005-2007

(1) Articles and papers reviews for regional and urban model
(2) Review paper on meso model in Japan Wind Engineering
(3) Review paper on urban model in Tenki MSJ
(4) Review paper on urban climate in Regional Geography Japan
(5) Research fund by Japan Weather Association (PI)
(6) Research fund by Weather Engineering Institute (PI)
(7) Research fund by Ministry of the Environment (Co-PI)
(8) Forecast experiment for the record hot on 16 August
(9) Educational application of the forecasting system

6.3 Collaboration

Our Group of Global Environmental Science has a close collaboration with High Performance Computing System and Computational Informatics under the common subject of constructing the large database of real time weather data, named GPV/JMA project. This project is to archive real time weather data of the global spectral model (GSM), regional spectral model (RSM), meso scale non-hydrostatic model (MSM) provided by the JMA. In addition to those model data, weekly ensemble forecast data and monthly ensemble forecast data are also archived, and released to the public using the CCS homepage. The archive started in January 2005 and stably maintained up to now:

September 2007. Those data are useful for the study of developing ensemble Kalman filter, which is the state-of the-art four dimensional assimilation system. The knowledge of the staff in Computational Informatics is helpful to construct the safe distribution of the data to the public. The technical support by High Performance Computing System was essential to install and maintain the system. The weather map presented on the Google Earth is the product by the staff in Computational Informatics.

A unique general circulation model, called barotropic S-model, has been developed by our group in the university of Tsukuba, which predict the vertical average status of the atmosphere. The model is useful to predict the low-frequency variability such as blocking phenomenon and the Arctic Oscillation. An ensemble prediction system has been developed using the barotropic S-model on the platform of the PACS-CS. Although it is EP application of a number of simple predictions, we can extend the ensemble size up to 256 members. This ensemble prediction is applied to construct the four dimensional assimilation by means of the ensemble Kalman filter. Since the solution by the true Kalman filter is possible to compare with the approximation of the ensemble Kalman filter for this model, the research subject is important for the study of the four dimensional assimilation. The research is supported by the knowledge of the High Performance Computing System.

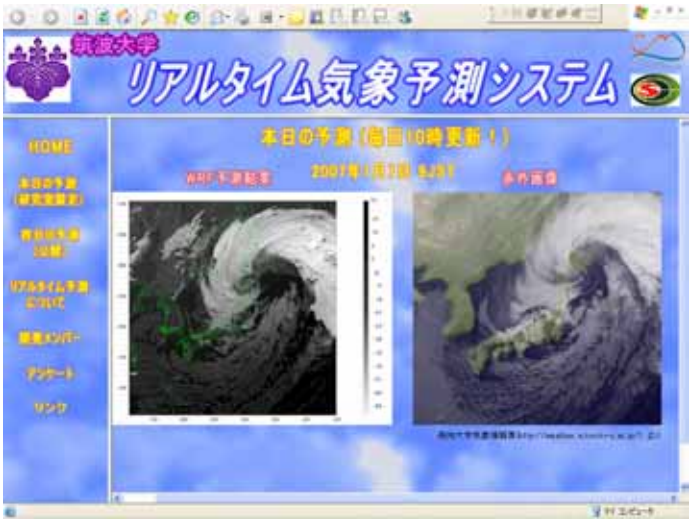

Figure 4. Real time weather prediction system by the regional model WRF.

6.4 Future Plan

The most important subject of the future plan in CCS is how to collaborate with other groups of computer science and other application sciences in astrophysics, particle physics,

materials and life sciences, biology, etc; without it the success in the research by CCS would be questioned. We expect further support by those groups in CCS. Following is the list of the future research subjects:

(1) Prediction model for the Arctic Oscillation
(2) Ensemble Kalman filter using the barotropic S-model
(3) Numerical experiments with the next generation model NICAM
(4) Urban climate simulation with the regional model WRF.
(5) Organize a regular session in Earth and Planet Conventions
(6) Organize a special session in Meteorological Society of Japan
(7) Organize an International Symposium on the Arctic Regions
(8) Collaboration with IARC/UAF USA
(9) Organize the Meteorological Research Consortium
(10) Collaboration with National Institutes: NIRP, JAMSTEC, MRI, NIES
(11) Collaboration with Commercial Industries: JWA, JAL, TEPCO

6.5 Publications

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- Tsunematsu, N., F. Kimura, T. Sato, K. Kai, Y. Kurosaki, T. Nagai, H. Zhou, and H. Mikami (2006) Extensive dust outbreaks following the morning inversion breakup in the Taklamakan Desert. J. Geophys. Research. 110, D2120720.1029/2005JD005994.
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7. Division of Global Environment and Biological Sciences: Biological Science Group

7.1 Research Activity.

All organisms on earth are classified into three "domains," such as eubacteria, archaebacteria, and eukaryotes. Recent progress in evolutionary biology suggests that eukaryotes are comprised of 6 "supergroups" below (Fig. 1).

1) **Opisthokonta**; includes multicellular animals, fungi, and their closely related unicellular cells.
2) **Planta**; photosynthetic cells with the "primary" plastids that are direct descendents of an endosymbiotic cyanobacterium.
3) **Chromalveolata**; unicellular eukaryotes presumably evolved from photosynthetic ancestral cells that captured their "secondary" plastids from an endosymbiotic red alga. This group includes non-photosynthetic lineages that probably experienced secondary losses of plastids.
4) **Rhizaria**; comprised of Cercozoa, Foraminifera, and Radiolaria.
5) **Excavata**; diverged unicellular eukaryotes commonly possess a set of unique morphological/ultrastructural features. Many amitochondriate eukaryotes are included in this supergroup.
6) **Amoebozoa**; an assemblage of amoeboid-like eukaryotes.

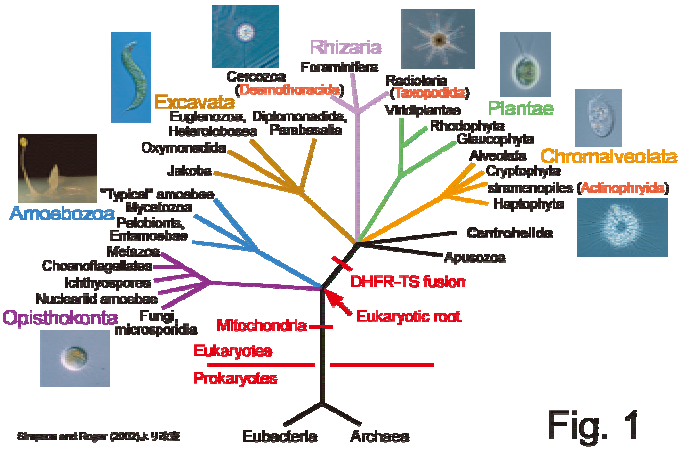

Fig. 1

Among the six supergroups, only monophyly of Opisthokonta has been concreted by molecular phylogenetic analyses, it remains controversial whether the rest of the five supergroups are natural groups. Furthermore, there are several eukaryotes that bear no clear evolutionary affinity to any of the 6 supergroups. By using molecular phylogenetic analyses, we aim (i) to resolve global relationships amongst the major eukaryotic groups, and (ii) to investigate the origin and evolution of organelles in eukaryotic cells (mitochondria and plastids).

To investigate global eukaryotic phylogeny, it is essential to assemble large scale sequence data from phylogenetically diverged lineages. Although genome sequencing projects have

rapidly progressed, the currently available sequence data are not sufficient for robust global phylogeny of eukaryotes for the reasons below: The lineages that are beneficial/pathogenic to human have been mainly subjected to genome-scale analyses, while few sequence data are available for the lineages of which evolutionary affinities are uncertain. Furthermore, it is almost certain that massive number of eukaryotes that can hold the keys to understand eukaryotic evolution remain unidentified in natural environments. Considering the bias in taxonomic sampling for sequence data, we firstly need to grow the key organisms and sequence multiple marker genes to achieve our research goals for eukaryotic evolution. By combining our original sequence data and those in public genome databases, we can assess global relationship among major eukaryotic groups by large-scale phylogenetic analyses (Fig. 2).

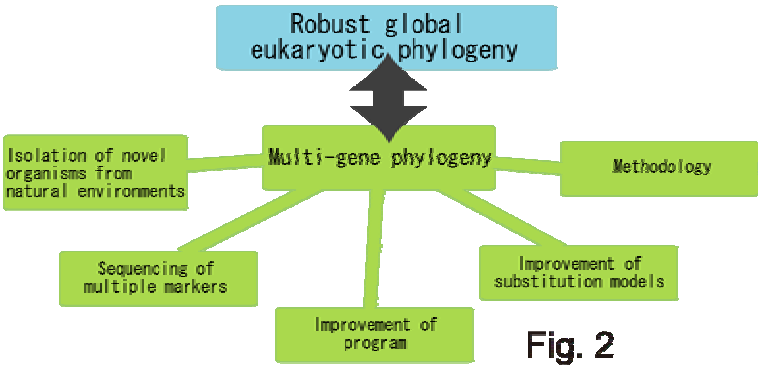

Fig. 2

Phylogenetic analyses based on single-gene data sets (single-gene analyses) have been extensively conducted to date, while we just recently start analyzing multiple genes (multi-gene analyses). Thus, we need to accumulate the knowledge regarding multi-gene analyses. So far, multi-gene data sets have been assessed mainly by maximum-likelihood (ML) and/or Bayesian analyses under the “concatenate” (or “linked”) model, in which a single set of parameters was enforced on the genes that are potentially evolving under different substitution patterns in a multi-gene data set. Under such model conditions, the actual sequence evolution in the multi-gene data may not be sufficiently described, since the concatenate model ignores the heterogeneity of substitution processes across genes. Importantly, studies of both empirical and simulation data indicate that such “model misspecification” can introduce significant artifacts in tree reconstruction. On the other hand, the model misspecification in concatenate analyses can be overcome by the analyses under the “separate” model: Under this model, the heterogeneity of sequence evolution across genes can be taken into account. Thus, the multi-gene estimates under the separate model may be much less biased than that under the concatenate model.

ML analyses under the separate model are indispensable to achieve robust phylogenetic estimates from multi-gene data sets. Nevertheless, separate analyses are computationally much more intensive than concatenate analyses in general, and no phylogenetic program allows estimation of ML trees from multi-gene data using efficient heuristic tree search procedures. Under the separate model conditions, ML trees are now exhaustively searched

for, but the number of test trees quickly becomes very large. For instance, log-likelihood (lnL) scores of more than 2.0 x 10^6 trees are required to select the ML tree from a data set including only 10 sequences/groups. In order to facilitate large calculation of lnL scores, we modified sequential lnL calculation in a widely used phylogenetic program Tree-Puzzle into parallel with MPI.

7.2 Research Results

We analyzed the following multi-gene data sets.

7.2.1 Testing the monophyly of red algae and green plants

We prepared a multi-gene data set comprised of 26 nucleus-encoded genes to assess the evolutionary relationship between red algae and green plants. Translation elongation factor 2 (EF2) phylogenies strongly support the monophyly of red algae and green plants. The sisterhood between red algae and green plants recovered by EF2 analyses has been widely accepted since this tree topology agreed with the single origin of the primary plastids in red algae and green plants. However, the robust sisterhood between red algae and green plants recovered in EF2 phylogenies has been suspected as a gene-specific artifact, since the estimates from a multi-gene data set with EF2 and that without EF2 were sometimes conflict with one another regarding the relationship between red algae and green plants. We separately investigated and compared phylogenetic signals in the 26 genes, and found that EF2 and α-tubulin signals are largely different from the signals in the rest of the genes. Importantly, the monophyly between red algae and green plants was successfully recovered by the analyses excluding EF2, suggesting that the particular tree topology is also supported by other genes. The multi-gene analyses under the separate model conditions described above were conducted by using the MPI version of Tree-Puzzle ("MPI-Puzzle").

7.2.2 Monophyly between cryptophytes and haptophytes

Cryptophytes acquired their plastids by the secondary endosymbiotic uptake of a red alga. Several other algal lineages acquired plastids through such an event, but cryptophytes are distinguished by the retention of a relic red algal nucleus, the nucleomorph. The nucleomorph (and its absence in other lineages) can reveal a great deal about the process and history of endosymbiosis, but only if we know the relationship between cryptophytes and other algae, and this has been controversial. Several recent analyses have suggested a relationship between plastids of cryptophytes and some or all other red alga-containing lineages, but we must also know whether host nuclear genes mirror this relationship to determine the number of endosymbiotic events, and this has not been demonstrated. We

have carried out an expressed sequence tag (EST) survey of the cryptophyte *Guillardia theta*. Phylogenetic analyses of 102 orthologous nucleus-encoded proteins (18,425 amino acid alignment positions) show a robust sisterhood between cryptophytes and haptophytes (*Pavlova lutheri* and *Isochrysis galbana*) which also have a red alga-derived plastid. This relationship demonstrates that loss of nucleomorphs must have taken place in haptophytes independently of any other red alga-containing lineages and that the ancestor of both already contained a red algal endosymbiont.

7.2.3 Phylogenetic position of Centrohelida

Centrohelida, one of major heliozoan groups, are eukaryotes of which evolutionary affinity remains uncertain. In this study, we newly determined the genes encoding EF2, cytosolic heat shock protein 70 (HSP70), and cytosolic heat shock protein 90 (HSP90) from the centroheliozoan *Raphidiophrys contractilis*. The three Raphidiophrys genes were then combined with previously determined actin, α-tubulin, β-tubulin, and SSU rRNA sequences to phylogenetically analyze the position of Centrohelida in global eukaryotic phylogeny. Although the multi-gene data sets examined in this study are the largest ones including the centroheliozoan sequences, the relationships between Centrohelida and the eukaryotic groups considered were unresolved. Our careful investigation revealed that the phylogenetic estimates were highly sensitive to genes included in the multi-gene alignment. The signal of SSU rRNA and that of α-tubulin appeared to conflict with one another: the former strongly prefers a monophyly of diplomonads (e.g., *Giardia*), parabasalids (e.g., *Trichomonas*), heteroloboseans (e.g., *Naegleria*), and euglenozoans (e.g., *Trypanosoma*), while the latter unites diplomonads, parabasalids, metazoans, and fungi. In addition, EF2 robustly unites red algae and green plants, while the remaining genes considered in this study do not positively support the particular relationship. Thus, it is difficult to identify the phylogenetic relatives of Centrohelida in the present study, since strong (and some are conflicting) gene-specific "signals" are predominant in the current multi-gene data. We concluded that larger scale multi-gene phylogenies are necessary to elucidate the origin and evolution of Centrohelida. We constructed a cDNA library of *R. contractilis* and recently started the expressed sequence tag (EST) analysis.

7.2.4 Origin of chlorophyll-*c* containing plastids

Recent multi-gene phylogenetic analyses of plastid-encoded genes have recovered a robust monophyly of chlorophyll-*c* containing plastids (Chl-*c* palstids) in cryptophytes, haptophytes, photosynthetic stramenopiles, and dinoflagellates. However, all the plastid multi-gene phylogenies published to date utilized the concatenate model, which ignores the

heterogeneity of sequence evolution across genes in alignments. Both empirical and simulation studies show that, compared to the concatenate model, the separate model, which accounts for gene-specific evolution, can greatly improve multi-gene estimations. Here we newly sequenced 46 genes of Chl-*c* plastids, and examined the Chl-*c* plastid evolution by multi-gene analyses under the separate model. Unexpectedly, Chl-*c* plastid monophyly received only low to medium support in our analyses based on multi-gene data sets including up to 4829 alignment positions. Although we systematically surveyed and excluded the genes that could mislead estimation, the (inconclusive) support for Chl-*c* plastid monophyly was not significantly altered. We conclude that the estimates from the current plastid-encoded gene data are insufficient to resolve Chl-*c* plastid evolution with confidence, and are highly affected by genes subjected to the analyses, and methods for tree reconstruction applied.

7.2.5 Sisterhood between Cercozoa and Foraminifera

Recently, there has been increasing molecular evidence of phylogenetic affinity between Cercozoa and Foraminifera in the eukaryotic lineage. We performed phylogenetic analyses based on the combined (concatenated) amino acid sequence data of actin, α-tubulin, and β-tubulin from a wide variety of eukaryotes, including the foraminifers *Planoglabratella opercularis* and *Reticulomyxa filosa*, as well as cercomonad and chlorarachniophyte members of Cercozoa. A monophyletic lineage composed of two foraminiferan species branched with the centroheliozoan species *Raphidiophrys contractilis* was reconstructed in both Bayesian and maximum-likelihood (ML) analyses under concatenate models, enforcing a single set of the parameters (the parameters for among-site rate variation and branch lengths) on the entire combined alignment. Considering the extremely divergent nature of Foraminifera and *Raphidiophyrs* tubulins, the union of these lineages recovered is most probably a long-branch attraction artifact due to ignoring gene-specific evolutionary processes. On the other hand, the foraminiferan lineage was within the radiation of Cercozoa in Bayesian analyses under the separate model conditions, accommodating differences in evolutionary processes across the three genes in the combined alignment. The Foraminifera + Cercozoa affinity recovered in the latter multi-gene analyses is most likely genuine, and thus our data presented here provide further support for the close relationship between these two protist lineages.

7.2.6 New excavate flagellates

In addition to the multi-gene analyses described above, we isolated and analyze previously undescribed eukaryotes. *Dysnectes brevis* n. gen., n. sp., a

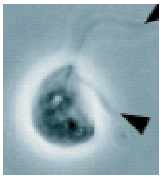

Fig 3. *Dysnectis brevis*

free-living heterotrophic excavate flagellate was isolated from microaerophilic sediment (Fig. 3). Our detailed microscopic observations revealed that *D. brevis* possesses all the key ultrastructural characters considered typical of Excavata. Among the 10 excavate groups previously recognized, *D. brevis* displays an evolutionary affinity to members of the Fornicata (i.e. *Carpediemonas*, retortamonads, and diplomonads), while the internal branching pattern of the *D. brevis*–Fornicata clade was not resolved with confidence.

We also isolated another excavate flagellate NY176 from oxygen-depleted sediment from a deep-sea methane cold seep of Sagami Bay, Japan (Fig. 4). The morphological characteristics of this flagellate appeared to be similar to those of *D. brevis* and *Carpediemonas*. In a SSU rRNA phylogeny, the flagellate NY176 grouped with the members of the Fornicata, but did not show strong affinity to any member of the Fornicata previously described. We constructed a cDNA library of the flagellate NY176 and randomly sequenced 3,000 clones. Based on those sequence information, we plan a multi-gene phylogenetic analysis to resolve the internal relationship amongst the member of the Fornicata.

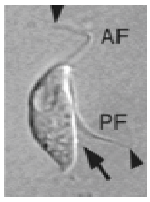

Fig 4. *Dysnectis sagami*

7.3 Collaboration

The MPI version of Tree-Puzzle was developed in co-operation with Dr. M. Sato in the HPC group. As described in section 2.1 this program has been utilized for multi-gene analyses under the separate model conditions.

7.4 Future Plan

We will utilize the MPI version of Tree-Puzzle (MPI-Puzzle) for various multi-gene data sets. As described in 2.3 and 2.6, we are currently conducting the EST analyses on the centrohelid *R. contractilis* and the excavate flagellate NY176. The sequence data generated from these analyses will be subjected to multi-gene analyses using the MPI-Puzzle. In addition, we are now investigating the impact of a heuristic tree search method on ML bootstrap analyses. In this study, it is critical to compare the trees heuristically searched for with the exact ML tree. We will prepare 100 bootstrap replicates including 9 sequences (the possible trees for 9 sequences are 135,135). By using MPI-Puzzle, the exact ML trees will be exhaustively selected from all the possible trees, and subsequently compare with the trees that are heuristically searched for. We will also start exploring the possibility for a heuristic tree search method under the separate model conditions.

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8. Division of High Performance Computing Systems

8.1 Research Activity

In this division, high performance computing systems as the basic technology for computational sciences and grid computing technologies on wide area network are studied.

The primary research facility in our center is a massively parallel cluster system PACS-CS with 2560 nodes which has been developed in this research division. PACS-CS started its operation from July 2006 and we have been supporting the development of various application programs with researchers in these fields as well as the basic performance evaluation of the system. The division also contributed to develop the FIRST cluster system, a large scale hybrid PC cluster by Astrophysics Research Department.

For the research on next generation computing system, all the members of the division joined to a project of "Mega-scale Computing" (leaded by Prof. Hiroshi Nakashima, Kyoto University) as a JST-CREST program. In the project, Prof. Sato and Prof. Boku contributed to the low-power computing technology for high-performance parallel computing and high-reliability and high-performance communication, respectively. This research project was on fundamental technologies for next generation large scale parallel processing system for high performance computing. The project finished successfully on November 2006, and the research theme was continued to another JST-CREST project of "Low-Power and Dependable Parallel Processing Platform with Embedded Technology" leaded by Prof. Sato, which started from October 2006 for five years. In this project we will develop a new low-power and highly reliable embedded system for next generation parallel processing.

The division also proceeds a research of "Low-Power and High-Speed Device, Circuit and Logic for Next Generation Supercomputer Systems" as a collaborative research with Hitachi Ltd. and University of Tokyo. The research group of University of Tsukuba and Hitachi is contributing the subtheme "Research and Development on Fundamental Logic on Processor Architecture and Memory Hierarchy". In the division, we have been studying the on-chip memory architecture and computing acceleration mechanism for low-power and high-performance systems. Besides this activity, we have also proposed our original solution for "Next Generation Supercomputer System Development" project managed by the supercomputer development division of RIKEN. After the proposal, the research contract on the next generation supercomputer between University of Tsukuba and RIKEN was established, and currently Prof. Ukawa, Sato and Boku joined to the abstract designing team of RIKEN as visiting researchers.

As a research on development of high-performance numerical library, we studied "Fast

Fourier Transform Algorithm on Heterogeneous Environment" for cluster systems.

For the practical grid research, we have been studying ILDG (International Lattice Data Grid) with the research group on particle physics for data sharing of computational results by them. We also developed the JLDG (Japan Lattice Data Grid) system to share the Lattice QCD computational results with nation wide researchers, under support of CSI (Cyber Science Infrastructure) by NII (National Informatics Institute).

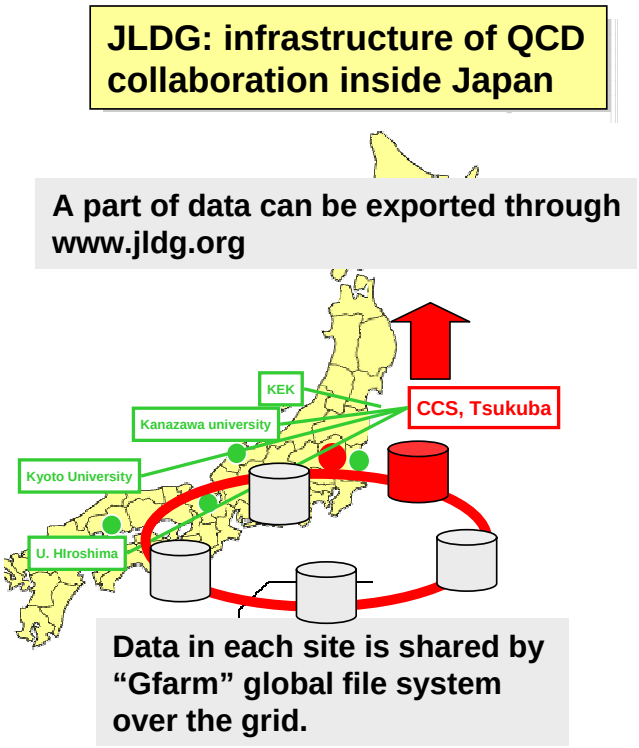
As the grid environment research, we have been developing the OmniRPC grid programming system as well as "the Research on Scalable P2P Grid Environment for Large Scale Distributed Computing" supported by Grant-in-Aid of MEXT for future grid and distributed environment. On these research themes, we have also performed the Japanese-French collaborative research with INRIA on P2P grid environment.

From April 2006, Prof. Tatebe from AIST (Advanced Institute on Science and Technology) joined as an Associate Professor to the division, and new projects based on his developed system Gfarm, a file system on distributed environment.

8.2 Research Results

- We have completed a massively cluster system PACS-CS with 2560 nodes.
- We joined to JST-CREST project "Mega-Scale Computing" (leaded by Prof. Hiroshi Nakashima, Kyoto University) and Prof. Sato and Prof. Boku contributed a low-power high-performance parallel processing technology and high-performance highly-reliable interconnection network, respectively. Especially in the research exhibition on SC06, we demonstrated the prototype system "MegaProto" and fault-tolerant interconnection network system and they are highly evaluated.
- We have been constructing the ILDG (International Lattice Data Grid) environment for data sharing among world-wide particle physics researchers, and developed the JLDG (Japan Lattice Data Grid) environment for nation-wide data sharing in this year.
- We performed a collaborative research with KEK (High Energy Accelerator Research Organization) on Gfarm distributed file system, and got the prize of the winner in Large System division on HPC Storage Challenge at SC06.

Low-Power and High-Performance Cluster Unit “MegaProto”



JLDG (Japan Lattice Data Grid) to share nation-wide data sharing of Lattice QCD computational results

8.3 Collaboration

- On the PACS-CS system, we developed the high-performance Gram-Shmidt

Orthogonalization Algorithm for accelerating the computation of RS-DFT (Real Space Density Function Theory) with Nano-Bio research group. We are also developing the high-speed communication library for the nearest neighboring communication especially required for Lattice QCD simulation.

- On the Molecular Evolution Tree Program in Biological Science research group, we are supporting the parallelization and speed-up of the program.
- We have been supporting the development of a large scale hybrid PC cluster FIRST for Computational Astrophysics research group. In this year, we supported the deployment of Gfarm system on FIRST cluster for convenience for users.
- We are collaborating with Particle Physics research group for construction of ILDG and JLDG environments for data sharing among international and nation-wide particle physics researchers.
- In the research project of Next Generation Supercomputer System by RIKEN, Lattice QCD and RS-DFT applications were listed as the most important large scale target applications, and our division and other related divisions will develop the practical codes for them.

8.4 Future Plan

The most important issue is to enhance the performance of PACS-CS on real applications in the center with supporting research groups to improve the parallelization and effectiveness of the codes. In addition, the University of Tsukuba will introduce the next supercomputer system, and the center will operate it from 2008. It is an important mission of us to support the operation not only within the university but also among other universities and institutes based on grid technology. The basic system architecture and specification are shared by three universities; University of Tsukuba, University of Tokyo and Kyoto University, and they will introduce their own systems based on the same architecture at the same time. We are considering to apply our grid technology currently under development on the collaborative operation of these supercomputer systems. Another project to develop new system software and compiler is also under going.

The national project on the development of Next Generation Supercomputer is now on the stage of detailed designing, and our division will contribute not only to the designing of the system but also to the evaluation and performance improvement of real target application codes. We consider that such a contribution becomes possible by the unique center like ours where the researchers of computer science and computational science are collaborating as daily works.

There are two important issues on the future high performance computing systems;

low-power technology and effective accelerating mechanism for high-performance computation. For the former research topic, we will proceed based on current JST-CREST research project. For the latter one, there are several ways including the starting of follow-up project of FIRST.

Grid technology is now on the practical stage, and it is required to apply to the real applications and systems as well as the study on highly scalable systems reaching to the exa-scale data sharing.

8.5 Publications

8.5.1 Journal Papers

- **岡田真幸，櫻井鉄也，寺西慶太：近似係数行列に対する疎行列用直接解法を用いた前処理，日本応用数理学会論文誌**, Vol. 17, No. 3, pp. 319--329,(2007).
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9. Division of Computational Informatics: Computational Intelligence Group

9.1 Research Activity

In the field of computational sciences, management and utilization of massive data are extremely important issues. The computational intelligence group in the computational informatics division is in charge of research and development in the field of data engineering. In particular, we have been engaging in the following research topics: infrastructure for integrating heterogeneous databases and various information sources, data mining and knowledge discovery technologies to discover knowledge and rules from massive data, XML-related technologies to deal with various data uniformly in the Internet environment. Additionally, we also have engaged in application studies, such as development and maintenance of meteorological databases and knowledge discovery from the database, in cooperation with Global Environment and Biological Sciences division.

9.1.1 Infrastructure for Information Integration

(Research funds: Grant-in-Aid for Scientific Research (A), Grant-in-Aid for Scientific Research on Priority Areas, Grant-in-Aid for Young Scientists (B), JST CREST)

(1-1) System for Information Integration

We have been investigating infrastructures, systems, and applications which enable us to integrate heterogeneous and distributed databases and information sources. In particular, we have been developing StreamSpinner, which allows us to integrate not only conventional data sources, such as relational databases and Web data, but also stream data, such as sensor data and location information. The model of StreamSpinner is based on the relational model, and StreamSpinner has a basic functionality for information integration based on the model. However, it can also deal with continuous media, such as video and audio, due to its extensible features. Specifically, it allows us to plug-in programs for specific applications as external functions, and it can then integrate diverse information by invoking external functions. Examples are similarity search on time-series data and analysis of video data streams captured by severance cameras.

Moreover, we have been addressing the problem of stream processing in distributed environments where StreamSpinners are distributed on multiple nodes. We also have been studying the sustainable stream processing system, which is dependable even when some nodes fail.

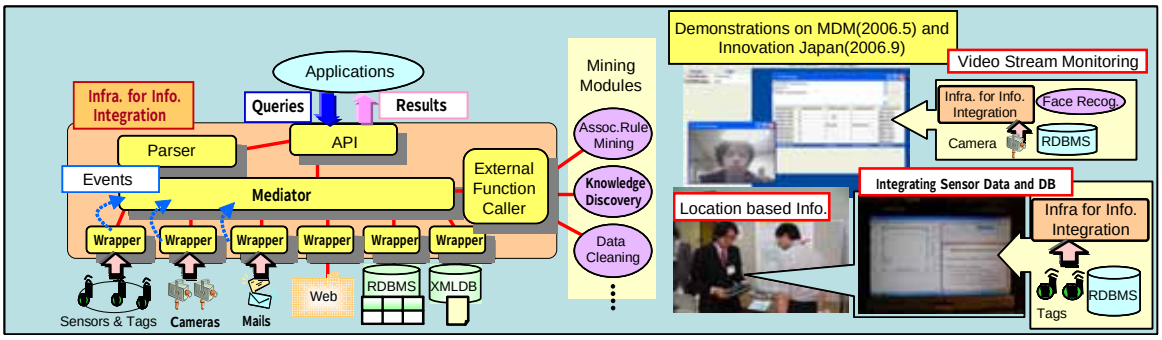

Fig. 1 StreamSpinner and its applications.

(1-2) Sensing Database Infrastructure

Demands on DBMS for time-series data obtained by real-world monitoring are increasing. To cope with it, a DBMS should have super fast data insertion function, data analysis function, and continual query function. We have developed a sensing database infrastructure KRAFT to realize such functions. The features of KRAFT are: fast data insertion utilizing UPS attached memories, similar sequence retrieval functions, and signal processing functions.

9.1.2 Data Mining and Knowledge Discovery

(Research funds: Grant-in-Aid for Scientific Research on Priority Areas, Grant-in-Aid for Scientific Research (A), Grant-in-Aid for Young Scientists (B), JST CREST)

We have been studying various data mining and knowledge discovery techniques, such as outlier detection, ratio-rule mining, information extraction from documents, time-series document clustering, document topic analysis, topic-structure mining, and mobility histogram construction for mobile objects. In the following, we explain some topics out of the above main activities.

(2-1) Outlier Detection

Outliers are data objects that are greatly different from other objects, and they are useful for detecting malfunctions and discovering interesting data objects.

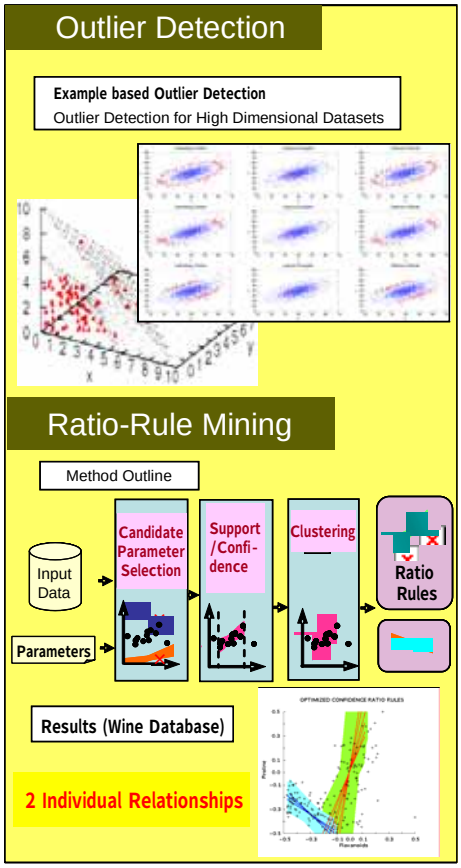

Fig. 2 Outlier detection and ratio-rule mining.

Distance-based and density-based methods are the major outlier detection methods today. When applying those methods, it has been pointed out that there are several problems. That is, it is difficult to find an appropriate set of parameters for a given dataset, and it is difficult to characterize objects in high-dimensional data spaces.

To tackle these problems, we have studied several approaches in which user-provided examples are used to find outliers. Also, we attempt to find low-dimensional subspaces which characterize sample outliers the most, instead of dealing with all dimensions.

In the meantime, so far, few papers have addressed the problem of outlier detection for discrete values, whereas most conventional methods mainly deal with numerical data. For this reason, we attempt to apply association-rule mining to the problem of outlier detection in data records and/or transaction data which are mainly consisting of discrete values.

(2-2) Ratio-Rule Mining

Extraction of ratio rules from numerical dataset is an important research issue due to the fact that ratio rules can be used for interpolation, prediction, and outlier detection. However, the principle component analysis (PCA), which is a basic technique to extract ratio rules, is not able to detect individual linear relationships when multiple linear relationships are mixed. It is not able to deal with such linear relationships that hold for limited ranges of axes, either.

In our novel method, we define the concept of support and confidence of ratio rules in a similar spirit of association-rule mining, and extract ratio-rules by following the definition. The technique enables us to obtain ratio rules which reflect users' intentions.

(2-3) Information Extraction from Documents

Although massive information is available on the Web, we have not yet been able to make the best use of it because of the heterogeneity of information resources. So far, many researchers have devoted their efforts to extracting useful information from the Web and/or documents, and noticed that it is quite important to choose appropriate information sources out of numerous information sources. In this research, we have developed a system for extracting information from document databases, in which user specified records (seeds) are used to retrieve related records. Our idea is to select document sources by evaluating quality of extracted records, which improves accuracy as well as efficiency in terms of the number of extracted records.

(2-4) Time-Series Document Clustering

Currently, a large number of documents are circulated in the Internet, and it is therefore important to be able to summarize their information outline. This research focuses on clustering time-series documents, each of which is assigned temporal information like the issue date of a news article. Specifically, we investigate clustering techniques which takes

into account of novelty of documents. For news articles, articles with fresh information usually have more values compared to those with older information, and old articles will be forgotten in time. Our algorithm takes into account such real-life features, and achieves efficient clustering over temporal documents.

9.1.3 XML and Web Programming

(Research funds: Grant-in-Aid for Scientific Research on Priority Areas, Grant-in-Aid for Young Scientists (B), JST CREST)

XML is a meta-language for data representation, and has been widely used as a standardized data format for data interoperability in network environments. As a consequence, the amount of data generated and/or stored in the form of XML is explosively increasing, and this seems to be the trend for the foreseeable future. For this reason, we have been addressing diverse issues, as described in the following, aiming at developing efficient and effective means for the management of massive XML resources.

(3-1) OLAP for XML Data

In general, searching is one of the most common ways to find out necessary information from XML data. However, more complicated ways to make analysis of XML data, which allow us to discover valuable information out of large XML data collections, are becoming important due to the recent diffusion of XML. In this work we attempt to develop XML-OLAP (Online Analytical Processing), which enables us to perform analytical processing of XML data.

In OLAP systems, the target data being analyzed is regarded as a multidimensional cube consisting of several attributes, and we make analysis of the cube by applying operations dedicated to OLAP analysis. However, when dealing with XML data, it is not a trivial task to apply (existing) OLAP techniques to them due to the nature of XML, in which XML data is modeled as trees, and the data model is flexible enough to accommodate structurally heterogeneous instances. This gives rise to the need of novel (formal) definitions of XML data cube and related operators, efficient algorithms and indexing structures dedicated to the model and operators to achieve interactive analysis of large XML datasets. We have been addressing these problems, and developing a system based on the scheme.

(3-2) Parallel XML Data Processing

The diversification of XML use-cases causes the emergence of large-scale XML data ranging from Giga-bytes to Tera-bytes. As a consequence, it is important for us to be able to deal with such large-scale XML data efficiently. However, the fact that XML data have tree-structures makes it difficult to query large XML data efficiently. To cope with this problem, we have been trying to incorporate parallel processing in querying XML data

using PC-cluster systems. The technical challenges are partitioning XML data for subsequent distribution to cluster nodes, optimal load-aware distribution of XML data, parallel query processing algorithm, etc. In this research, we attempt to make the best use of the techniques of relational XML databases, which have been well-studied for the past several years.

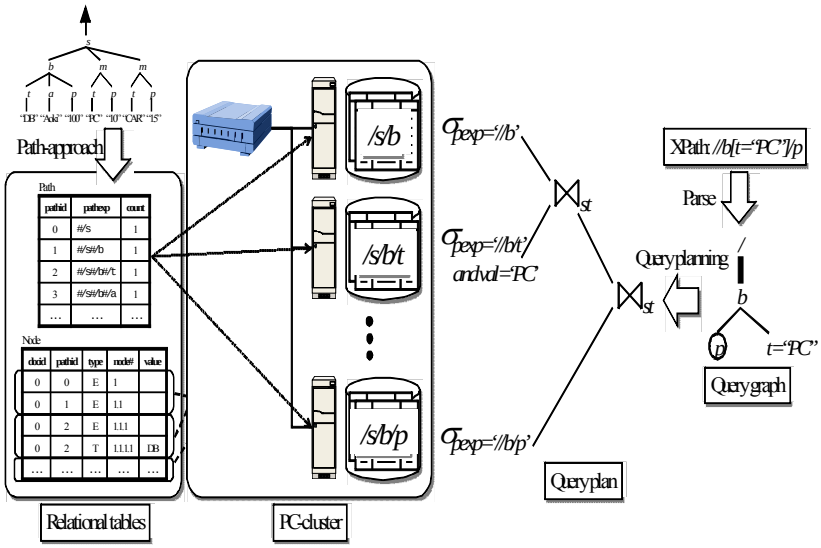

Fig. 3. Parallel XML data processing.

(3-3) Searching XML Data in P2P Networks

The recent dissemination of the Internet is making the global data interoperability come true. In the meantime, there is a growing demand for constructing networks over the Internet exclusively dedicated for particular groups or organizations. This is due to the recent trends in which security preserved efficient information distribution has attracted much public attentions. Peer-to-peer networks, which allow us to construct such networks that are dedicated for specific applications, have been widely used as the bases of overlay networks, and there have been several research projects which aim at sharing scientific data using overlay networks. In such applications, XML is used as a standardized data format. From these observations, we have been studying a scheme for storing and querying XML data using P2P networks.

9.1.4 Meteolorogical Databases

(Research funds: Grant-in-Aid for Exploratory Research)

(4-1) GPV/JMA Archive

As a collaborative work with the global environmental science group in CCS, we have been developing, maintaining, and managing GPV/JMA Archive

(http://gpvjma.ccs.hpcc.jp). Its objective is to store meteorological data provided by the Japan Meteorological Agency (JMA), and make the stored data publicly available to external users. The archive stores 6 kinds of JMA/GPV data, i.e., global spectral model data (GSM), regional spectral model data (RSM), meso-scale non-hydrostatic model data (MSM), weekly ensemble forecast data, monthly ensemble forecast data, and seasonal ensemble forecast data. In addition, it provides weather maps rendered from the grid data and KML (Keyhole Markup Language) data, which allow users to view the weather maps by GoogleEarth.

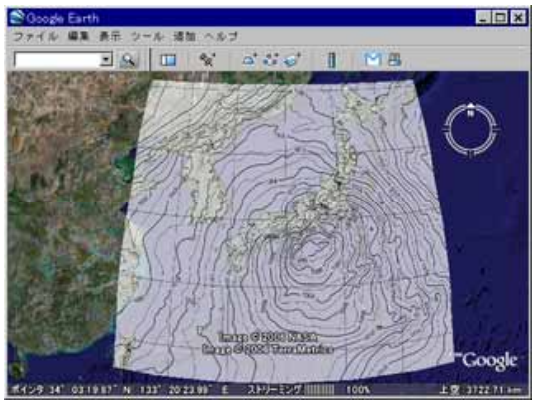

Fig. 4. Viewing a weather map by GoogleEarth.

(4-2) Information Integration using Web Services

At this moment, GPV/JMA Archive only provides simple form-based query interfaces to search for stored data. We have been developing a Web service system for GPV/JMA Archive for aiming at improving the usability, as well as promoting interoperation of meteorological data across related databases in other countries. Specifically, we attempt to implement major functionalities concerning meteorological data, such as metadata extraction, query retrieval, format conversion, and rendering, as Web services. We also provide BPEL-based workflow engines for allowing users to combine those functionalities to support their research activities.

9.2 Research Results

1) Infrastructure for Information Integration

- We have developed a stream-processing engine, StreamSpinner, and have constructed various demonstration systems for empirical study. We demonstrated them in many exhibitions, such as Innovation Japan 2005, 2006, and 2007.
- We have developed a stream database system, KRAFT, and released it as OSS.

2）Data Mining and Knowledge Discovery

- We have developed several example-based methods for outlier detection in high dimensional spaces, and confirmed its effectiveness by experiments. Furthermore, we have developed basic algorithms for detecting outliers in discrete data, and investigated some approaches to make the processing more efficient.
- We have developed a basic method for mining ratio-rules, and confirmed its effectiveness by experimental data. In addition, we made related software as a package for data analysis.
- We have developed a basic method for extracting information from document collections and several variations as extensions. We confirmed its feasibility by experiments using a news article archive.
- We have developed a clustering method for time-series documents as an extension of k-means algorithm, and realized incremental update of clusters.

3) XML and Web Programming

- We gave a formal definition of multidimensional datacube of XML data based on XPath expressions. Based on the definitions, we have developed a prototype system using relational databases, and evaluated its performance.
- We have developed a basic approach for parallel XML query processing, and confirmed its feasibility by a prototype system.
- We have developed a prototype system for storage and retrieval of XML data in P2P networks based on DHT (Distributed Hash Table), and tested its performance by experimental evaluations.

4) Meteorological Databases

- We have constructed GPV/JMA Archive, which stores GPV data provided by JMA, and it works in a stable manner. As of the end of August, 2007, the amount of stored data is 700GB and there are 174 registered users. We have implemented several Web services on top of the archive, and confirmed its feasibility using the prototype.

5) Numbers of Refereed Papers

2004: 17 (Journal papers 10, Refereed conference papers 7)
2005: 14 (Journal papers 7, Refereed conference papers 7)
2006: 18 (Journal papers 7, Refereed conference papers 11)
2007: 20 (Journal papers 9, Refereed conference papers 11)
(As of August, 2007)

6) Relating to the above research activities, we have received two paper awards, one award for young researchers, and two fellowships from domestic academic societies. In addition, students in our laboratory have received 15 awards in total.

9.3 Collaboration

We are having regular meetings with the computational media group for discussing computational informatics in the real-world. In addition, we have been developing, maintaining, and managing GPV/JMA Archive in cooperation with the global environmental science group. Recently, we have started a new project in which we apply data mining techniques to meteorological data.

9.4 Future Plan

1）Research and Development of Technologies for Data Engineering Infrastructure

Owing to the recognition that information integration, data mining, knowledge discovery, XML and Web programming are all important as technologies for data engineering infrastructure, we continue to intensively perform research and development in those areas. We also attempt to make our research activities practical as much as possible in cooperation with other groups in CCS. As for the topic of infrastructure for information integration, we attempt to integrate functionalities such as data mining and knowledge processing methods, and also attempt to make further development on the topics of distributed query processing and sustainable processing. As for data mining and knowledge processing techniques, we try to speed up the processing and apply it to large-scale real datasets. We also plan to address novel information sources, such as Blogs and SNSs. As for techniques related to XML and Web programming, we plan to make further development on the current methods. From the viewpoint of trust, we plan to address the problem of data traceability.

2) Scientific Databases

We continue to develop and maintain GPV/JMA Archive in cooperation with the global environmental science group. In addition, we plan to construct a new database for JRA-25 (Japanese Re-Analysis 25 years). As for Web service systems, we continue the development, and try to improve the usability of the system. Another topic is related to gfdnavi, which is a tool for analyzing geophysical fluid data, and we try to cooperate with its developers. We do not limit the research domain to meteorology, and try to address data engineering problems in other scientific domains.

3) Reinforcement of Cooperation with Other Divisions and Challenge of New Research Issues

We will further strengthen collaboration with the computational media group, and jointly develop the infrastructure of sensing, data processing, high performance computation as a framework of real-world computational informatics.

We also promote research on data mining applications for meteorological data (with Global Environment and Biological Sciences division), data infrastructure and knowledge discovery technology (with High Performance Computing Systems division and AIST), and database processing over grid file systems (with High Performance Computing Systems division).

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10. Division of Computational Informatics: Computational Media Group

10.1 Research Activity

The Computational Informatics Research Division is a young division founded in 2004. The medium-term/long-term mission of this division is to investigate novel methods at the frontier of computational sciences. We are now conducting researches to establish a new framework of computational science whose target is the human society and its environment.

The new computational science should handle a system including human as a core element. This means that the timescale of computational process cannot be changed arbitrarily depending on the power of computer. A real-time processing is essential. The new computational science handles enormous amount of sensing data which come from the real world. It visualizes the data and merges with related simulation results and presents the output to human eyes in easily understandable manner. We call this new framework as "Real-World Computational Informatics."

The backbone of real-world computational informatics is a fusion of technologies on sensing, database, grid computing, and computer network. Researches on cutting-edge core technologies and development of needs-oriented application systems are conducted in parallel.

The achievements have been published to flagship international journals in the areas of computer vision or virtual reality. We exhibit our booth at Innovation Japan (Tokyo International Forum) every year since 2005 for public relations. In 2007, our exhibition titled "Visual Assistance Technologies Using Mixed Reality" received a Microsoft Innovation Award as the best technology in IT division.

Outline of research activities in the Computational Media Group conducted by major research funds are listed below.

1) Live 3D video (3D-TV): Multiple audiences can arbitrarily select their viewing positions of sports events such as soccer games. Our technology enables live transfer of 3D-TV via network. (Supported by Strategic Information and Communication R&D Promotion Programme, Ministry of Internal Affairs and Communications).
2) Visual augmentation for pedestrians using surveillance cameras (See-Through Vision): Citizens can effectively utilize the video data obtained by many surveillance cameras in town. A novel framework is proposed and fundamental technologies are developed. (Supported by Grant-in-Aid for Scientific Research (A), Japan Society for the Promotion of Science).

3) Visual augmentation for drivers in ITS (NaviView): Drivers can see the blind spots by an augmenting visual support utilizing the videos obtained by road surveillance cameras. (Supported by Special Coordination Funds for Promoting Science and Technology, Japan Science and Technology Agency).
4) Autonomous Cooperation of Multimedia Sensor Arrays (Massive Sensing): The goal is to establish a novel method in computer vision that can automatically extract a set of meaningful images expressing what is going on in daily scene. (Supported by Grant-in-Aid for Young Scientists (A), Japan Society for the Promotion of Science).
5) Privacy Protecting Video Surveillance System: The goal is to develop an advanced video surveillance system by combining mobile and fixed cameras, and video media capable to handle privacy information included in the videos. (Supported by Grant-in-Aid for Young Scientists (A), Japan Society for the Promotion of Science).

10.2 Research Results

10.2.1 Network Transmission and Interactive Display of Live 3D Video

For 2004-2006, we have conducted a research project "Network Transmission and Interactive Display of Live 3D Video" with Japan Institute of Sports Science (JISS). It was supported by Strategic Information and Communication R&D Promotion Programme (SCOPE), Ministry of Internal Affairs and Communications. The project leader is Yuichi Ohta.

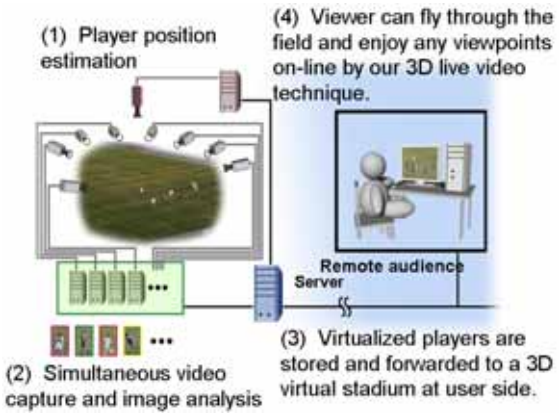
The project aims to realize a 3D free-viewpoint video system that multiple audiences can watch a live sports event played in a distant large-scale space such as a soccer stadium with freely moving their viewpoints as they like. The other purpose is to create an advanced contents technology by developing an interactive method for 3D video display which enables an ordinary person, without any special knowledge about video capturing and editing, to enjoy the 3D video.

We have developed the world first live 3D free-viewpoint video system in which all the following processes are executed in real time; capturing multiple videos, constructing 3D models, transmitting data via network, and rendering 3D video. The key technology to realize the system is a novel 3D modeling method "Player Billboard" that represents a person by a single plane (polygon) and the dynamic texture mapped on the plane.

In order to realize a 3D video system which works in practical environments such as soccer stadiums rather than laboratory rooms or camera studios, we concentrated our effort on the R&D to improve the reliability, versatility, and robustness of the 3D video system by conducting more than 20 experiments in Tokyo National Olympic Stadium and Yoyogi National Gymnasium. As the result, an unexemplified system for live 3D video in a

large-scale space has been successfully developed.

A paper describing the technology of the live 3D video system has been accepted and published by International Journal of Computer Vision (IJCV), the flagship journal in computer vision. The system has been awarded "2006 Image Electronics Technology Award" from The Institute of Image Electronics Engineering of Japan.



Outline of live 3D video system.

Experiments in Tokyo National Olympic Stadium.

A snapshot of 3D Video.

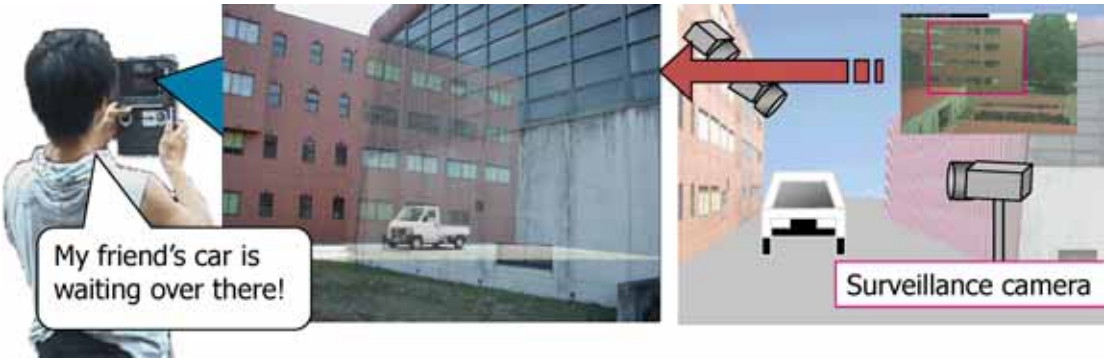
10.2.2 Visual augmentation for pedestrians using surveillance cameras

For 2006-2009, we are conducting a research project whose title is "See-Through Vision: Visual Augmentation for Pedestrians Using Surveillance Cameras." It is supported by the Grant-in-Aid for Scientific Research (A), Japan Society for the Promotion of Science. The project leader is Yuichi Ohta.

The aim of this research is to create a novel framework for the application of surveillance cameras under the inevitable tendency toward to increase the number of cameras in public space. Usually the surveillance cameras provide an invisible service "safety" to citizens. The use of images obtained by surveillance cameras, however, is closed to the owners of the cameras. In the framework, each pedestrian can enjoy a

visible service provided by utilizing the images from surveillance cameras; “See-Through Vision” is an example. A pedestrian can see-through a blind area occluded by a building, etc. simply by holding up his PDA toward the blind area. The images of a surveillance camera looking at the blind area are converted by computer-vision technology and presented on the display of PDA. As the result, he can see-through occluding objects as if he were the superman.

The research includes highly original elemental technologies; geometric registration based on outdoor natural landmarks observed from surveillance cameras, overlaying methods of see-through image to real scene, visual navigation between multiple images from distant viewing positions, image treatment for protecting the privacy of people in the images, etc.



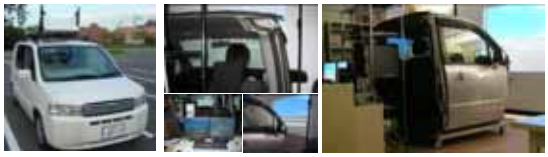
See-Through Vision: Visual augmentation for pedestrians.

10.2.3 Visual Augmentation of Drivers by Dynamic Sensing of Environment

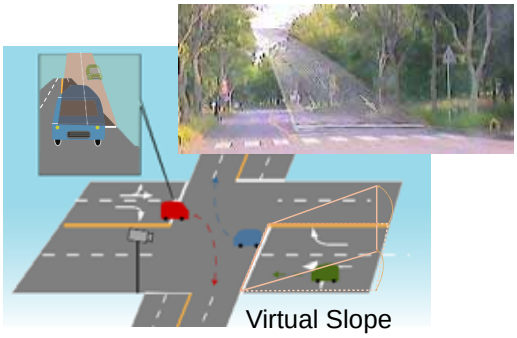
For 2004-2006, we have conducted a research project named “Visual Augmentation by Dynamic Sensing of Environment (Project Leader: Yuichi Ohta)” in “Risk Discovery and Avoidance based on Scene and Intention Recognition (General Manager: Toshiyuki Inagaki)” supported by Special Coordination Funds for Promoting Science and Technology, Japan Science and Technology Agency.

Our goal is to realize a novel vision augmentation technology that can show hazardous areas, which drivers cannot see normally in intersections. This technology is useful to diminish the possibility of accidents.

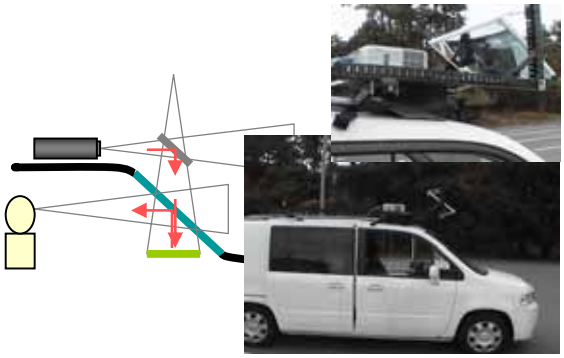
As all the proposed methods are based on Mixed Reality technology, we first have developed a prototype Wind Shield Display (WSD) on which drivers can see various visual keys through a wind shield on driving.



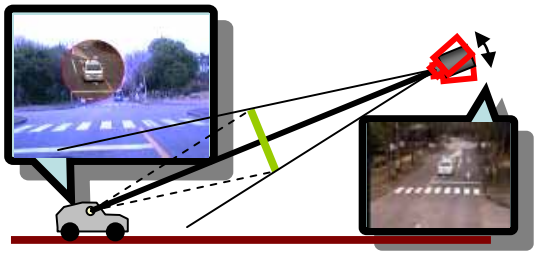
Vehicle and Simulator



Virtual Slope



Wind Shield Display



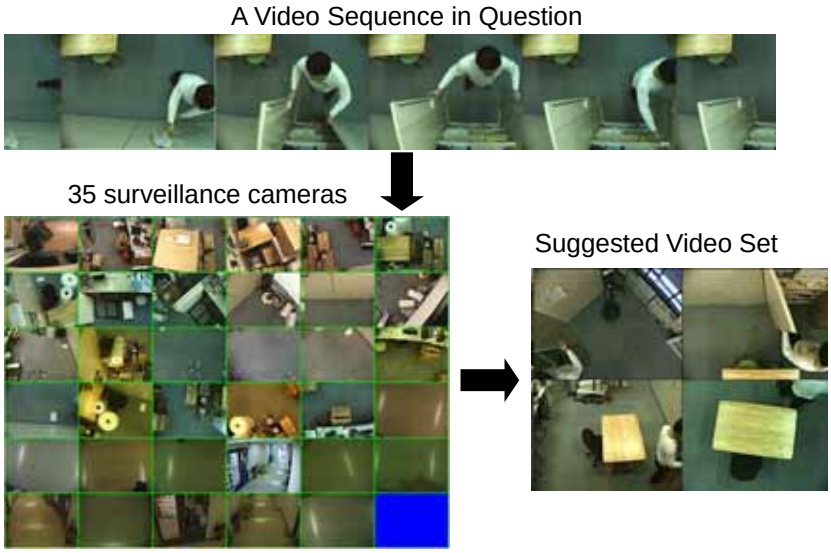
Floating Virtual Mirror

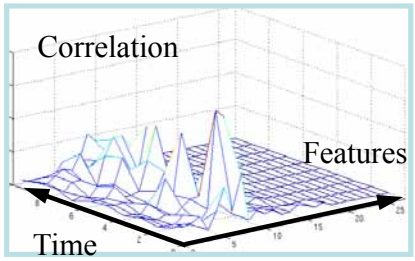
Then, we have proposed and evaluated a number of visualization methods including virtual slope, virtual corner mirror, floating virtual mirror, etc. For example, "Virtual Slope" is designed for drivers who are going to make a turn over opposite lanes. If some cars are also waiting to make a turn on the opposite lane, they cannot see the vehicles approaching to the intersection at opposite lanes. Virtual Slope can show all the coming vehicles as if they were coming down a virtual slope.

10.2.4 Autonomous Cooperation of Multimedia Sensor Arrays Tightly Connected over Network (Massive Sensing)

For 2004-2006, we have conducted a research project named "Autonomous Cooperation of Multimedia Sensor Arrays Tightly Connected over Network (Project Leader: Yoshinari Kameda)" supported by Grant-in-Aid for Young Scientists (A), Japan Society for the Promotion of Science (JSPS).

Our goal in the project is to establish a novel computer vision method that can automatically extract a set of meaningful images that expresses what is going on in daily scenes. The challenge is that all the locations of a number of cameras and microphones (sensors) are not measured in advance; hence the method needs to estimate the spatial relationship among sensors on the fry. Based on our proposed methods, our preliminary system that holds 35 cameras and 8 microphones can suggest the best set of video clips that is closely related with a video sequence that is given by a user.





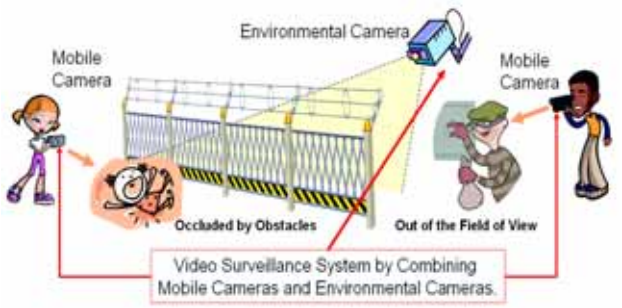
By mixing data from microphones with video data from a number of cameras, our system can estimate a set of video/audio data that expresses an action and browse it visually and acoustically. We exploit correlation matrix to segment the video/audio data

10.2.5 Privacy Considering Video Surveillance System by Combining the Advantages of Mobile and Environmental Cameras

Since 2006, we are conducting a research project "Privacy Considering Video Surveillance System by Combining the Advantages of Mobile and Environmental Cameras (Project Leader: Itaru Kitahara)" for three years. This project is supported by Grant-in-Aid for Young Scientists (A), Japan Society for the Promotion of Science (JSPS).

This project aims to research/develop an advanced video surveillance system by combining the advantages of mobile and environmental cameras, and video media which can appropriately capture, record and display the video information with considering about the privacy information in the videos. We are developing a mobile camera calibration method by using visual information captured by mobile and multiple environment cameras, and a video surveillance system which expands field of view of environment cameras by merging mobile videos. We are going to implement a video surveillance system with

privacy protecting capability on these developed platforms.



Video surveillance system by combining mobile and environmental cameras.

Mixed reality display demonstrating our camera calibration method.

10.3 Collaboration

We organized and continually held "Computational Informatics Seminar" in order to share the awareness of the problems involved in the frontier field, Computational Informatics. The seminar member includes all the faculties of Computational Informatics Division and active researchers in related fields invited from other departments of the university and from the National Institute of Advanced Industrial Science and Technology (AIST).

The Computational Media Group and the Grid Research Group of High Performance Computing Division have jointly planned a research proposal with other research groups from Kyoto University, etc. The theme of the proposal is "Sensing Grid," and is originally targeted to the Grant-in-Aid for Scientific Research on Priority Areas. This activity opened a door of new project "Sensing Web" for 2007-2009 supported by the Special Coordination Funds for Promoting Science and Technology.

10.4 Future Plan

Mixed Reality is a cutting-edge technology to present a novel visual world to our eyes, and is regarded as a promising next-generation human-interface technology. It seamlessly merges the visual data obtained from the real world and the visualized data generated in the computer. The Computational Media Group will continue the researches on the state-of-the-art technologies; technology for acquisition/analysis/recognition of massive visual data, computer vision technology for recovery of 3D world from 2D images, real-time sensing technology of human pose and eye expression, computer graphics technology for processing/generating visual images, and the Mixed Reality as the technology fusion of these elemental ones.

The Computational Media Group is an outstanding research group in the area of Mixed Reality. We are one of a few groups which continually present high-level papers in oral sessions of ISMAR every year; the ISMAR, International Symposium on Mixed and Augmented Reality, is the flagship symposium in Mixed Reality. We intend to develop novel methods to apply this technology to the framework of Computational Science Researches, and to create a new framework of Computational Science, which should be called “Real-World Computational Informatics.”

10.5 Publications

10.5.1 Journal Papers

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