CCS Report: PART II

Research Activities, Results, Collaborations and Plan

2008 – 2013

February 2014

Center for Computational Sciences
University of Tsukuba

1 Division of Particle Physics: *Particle Physics Group*

1.1 Research Activity

Elementary particles have no internal structures. They are not composed of other particles. At present six flavors of quarks, six leptons and Higgs particle are known as the elementary particles in the universe. They interact via four fundamental interactions or forces: gravitation, electromagnetism, the weak interaction and the strong interaction. Among them the strong interaction, which acts only between the quarks through exchanges of the gluons, shows peculiar features depending on the energy scale. In the high energy region, where the quarks come close to each other, the interaction strength becomes getting weaker (asymptotic freedom) so that the quarks are allowed to move more freely. On the other hand, the quarks are "confined" in the hadrons at the low energy scale. They are never observed individually. Once the energy scale becomes even lower, the protons and the neutrons, which are members of the hadrons, constitute the nuclei in the atoms.

Particle physics group has performed researches with lattice QCD, whose purpose is to prove that QCD is the fundamental theory of the strong interaction and investigate its dynamics nonperturbatively based on the first principles. Our primary research subjects for the past six years are summarized as follows:

1) Precision measurement of hadron spectra and precise determination of fundamental parameters in QCD such as quark masses and strong coupling constant,
2) Dynamical properties of hadrons such as ρ - π π resonance,
3) Direct construction of nuclei from quarks,
4) Determination of effective potentials between baryons based on QCD,
5) Lattice QCD at finite temperature and density.

Main results are described in the next subsection.

Numerical simulations were performed on PACS-CS, HA-PACS and T2K-Tsukuba in our center. PACS-CS was a massively parallel cluster system with 2560 nodes developed in Division of High Performance Computing Systems. Its operation started in July 2006 and ended in September 2011. The successor to PACS-CS is a large scale GPU cluster HA-PACS consisting of 268 nodes, each of which is equipped with two sockets of CPUs and four GPUs. The machine is in operation from February 2012. T2K-Tsukuba is another large scale cluster machine, which was installed in June 2008 under the T2K Open Supercomputer

Alliance with the University of Tokyo and Kyoto University. This machine is about to be shut down at the end of February 2014.

1.2 Research Results

1) Precision measurement of hadron spectra and precise determination of fundamental parameters in QCD such as quark masses and strong coupling constant

After finishing the systematic studies in quenched and 2 flavor QCD in 2003, we performed a 2+1 flavor QCD simulation. While the quenching effects were successfully removed, we were left with a long chiral extrapolation: The lightest up-down quark mass reached with the plain hybrid Monte Carlo (HMC) algorithm was about 70 MeV, which was more than ten times larger than the physical value of up-down quark mass. The PACS-CS project aimed at calculations on the physical point to remove the ambiguity of chiral extrapolations. There are two types of difficulties in the physical point simulation. Firstly, we need to reduce the computational cost which rapidly increases as the up-down quark mass decreases. The second one is fine-tuning of the quark masses to the physical point after we reach around the physical point.

(a) The up-down quark mass is reduced from 70 MeV to 4 MeV incorporating various algorithmic improvements such as domain-decomposed HMC (DDHMC) and mixed precision linear equation solver. Corresponding pion mass range is

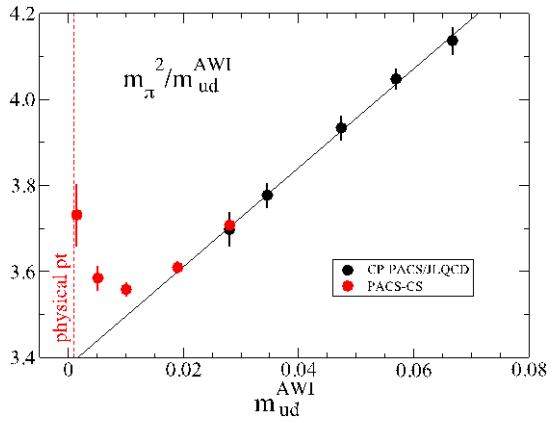

Fig.1. Chiral behavior of the pion mass squared divided by the up-down quark mass.

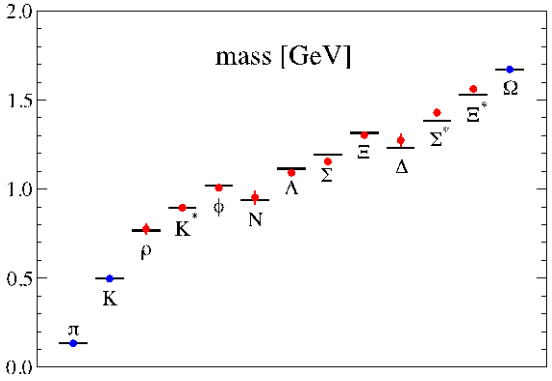

Fig.2. Light hadron spectrum in comparison with the experimental values.

sufficiently light to allow chiral analyses with the chiral perturbation theory (ChPT). Figure 1 plots the pion mass squared divided by the up-down quark mass. The PACS-CS results (red circles) show a clear curvature near the physical point, which confirms the characteristic features of the chiral logarithm predicted by ChPT. We find, however, that SU(3) ChPT up to the next-to-leading order does not describe data well due to bad convergence of the strange quark contributions. On the other hand, the SU(2) ChPT for up-down quark mass does seem to converge for the pion masses below m_π=300−400 MeV. Figure 2 compares our results for the

hadron spectrum with the experimental values. We find that most of them are consistent within the error bars, though some cases show 2–3% deviations at most.

(b) In lattice QCD, ChPT was often employed to reach the physical point from data obtained at up-down quark masses away from the physical point. This strategy, however, has several problems: (i) It is numerically difficult to precisely trace the logarithmic quark mass dependence predicted by ChPT. (ii) It may not be always possible to resort to ChPT as a good guiding principle for chiral extrapolation. (iii) The kinematics changes as the quark mass increases. A typical example is the $\rho \to \pi\,\pi$ decay which is not allowed for the increased up-down quark mass away from the physical value. (iv) Our final destination is to incorporate the different up and down quark masses. The isospin breaking effects are so tiny that reliable evaluation would be difficult by the chiral extrapolation method. In order to avoid these problems we have shown how the reweighting technique applied to the quark determinant allows us to adjust the up-down quark masses to the physical point.

(c) Now we have achieved the physical point simulation assuming artificial isospin symmetry with the degenerate up-down quark mass in 2+1 flavor QCD. In nature, however, the isospin symmetry is broken due to the up-down quark mass difference and their electric charge difference. Their effects are observed in mass splittings among isospin multiplets of light hadrons, e.g., K^0-$K^{\pm}$ and proton-neutron mass differences. The magnitude of splittings is tiny yet important since, e.g., it is this difference which guarantees the stability of proton. Thus, the next step should be 1+1+1 flavor QCD+QED simulation at the physical point including the isospin breaking effects. We employ the reweighting technique to incorporate the dynamical quark effects in QED and adjust the up and down quark masses to their physical values independently. Figure 3 shows the ratio of K^0 to K^+ propagators. The magnitude of the slope measures the K^0-K^+ mass difference. Our results (black symbol) are consistent with the expected slope from the experimental value of K^0-K^+ mass difference (red line) in large t region. By using the masses of π^+, K^0, K^+ and Ω^- as input, we have determined the physical values for the up, down and strange quark masses, individually.

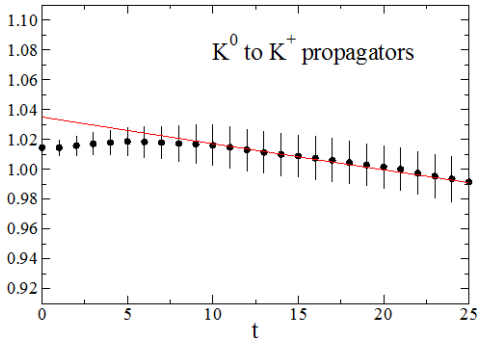

Fig.3. Time dependence of the ratio of K^0 to K^+ propagators.

(d) The values of the strong coupling constant and the quark masses are fundamental constants of nature. Since they both vary under scale change, we need to understand their renormalization, and specify the scale μ and the scheme to quote their values. We employ the Schrödinger functional (SF) scheme, where a unique renormalization scale is introduced through the box size L in the chiral limit and the scheme is mass independent. It has an advantage that systematic errors can be easily controlled. We have presented the values of the strong coupling constant and the up, down and strange quark masses in the MS-bar scheme, which is one of the most popular scheme, with the use of the perturbative conversion from the SF scheme at the renormalization scale much higher than the QCD scale.

2) Dynamical properties of hadrons such as ρ - π π resonance

Recent progress of simulation algorithms, supported by the development of computer power, has made it possible to study hadron physics at the physical quark mass by lattice QCD. The studies are mostly concentrated on stable hadrons, however. Masses of resonances such as ρ, K* and Δ cannot be correctly extracted from the exponential decay of the two-point functions. Instead one can use the finite size formula relating the energies of two-particle states on a finite box with the elastic phase shift, from which one can extract the pole position and the resonance width. Among the resonances, the ρ meson is a primary case for the lattice calculations, because the final state of the decay is the two-pion state which can be treated on the lattice precisely. The first study using the finites size formula was carried out by our group using 2 flavor QCD configurations in 2007. We have extended these studies to 2+1 flavor QCD at two up-down quark masses corresponding to 410 MeV and 300 MeV for the pion masses. The ρ resonance mass and the decay width were successfully obtained with small statistical errors.

3) Direct construction of nuclei from quarks

The strong interaction dynamically generates a hierarchical structure: Three quarks are bound to form a nucleon with an energy of 1 GeV, and nucleons are bound to form atomic nuclei with a binding energy of about 10 MeV per nucleon. Since all nuclei are ultimately made of quarks and gluons, lattice QCD should help us quantitatively understand the structure and property of known nuclei based on its first principles. This direct approach will be more important and indispensable if we are to extract reliable predictions for experimentally unknown nuclei in the neutron rich regions of the nuclear chart. In 2010 we carried out a first successful attempt to measure the binding energies of the ^{4}He and ^{3}He nuclei in quenched QCD with a rather heavy quark mass corresponding to 0.80 GeV for the pion mass, thereby avoiding a high computational cost. We followed this work with a renewed investigation of the bound state for the two-nucleon channel in quenched QCD at the same quark mass, which found that not only the deuteron in the $^3S_1$ channel but also the dineutron in the $^1S_0$ channel is bound. In the latest work we have investigated the dynamical quark effects on the binding energies of the helium nuclei, the deuteron and the dineutron performing 2+1 flavor lattice QCD simulation with the degenerate up-down quark mass corresponding to 0.51 GeV for the pion mass. Figure 4 show the spatial volume dependence of $\Delta E_{L,}$ which is the energy shift between the ground state of the multinucleon system and the free nucleons on an L^3 box, in GeV units for the ^{4}He, ^{3}He, deuteron and dineutron channels, respectively. The systematic change of the spatial volume is a key ingredient to distinguish a bound state from an attractive scattering state. While the binding energy for the ^{4}He nucleus is comparable with the experimental value, those for the ^{3}He nucleus and the deuteron are much larger than the experimental ones. Furthermore, we detect the bound state in the $^1S_0$ channel as in the previous study with quenched QCD, which is not observed in nature. Although the two-nucleon system which includes deuteron is the simplest nucleus, dynamics for this system is quite subtle: The binding in the spin triplet deuteron channel is very shallow and the spin singlet state is marginally unbound. A possible scenario

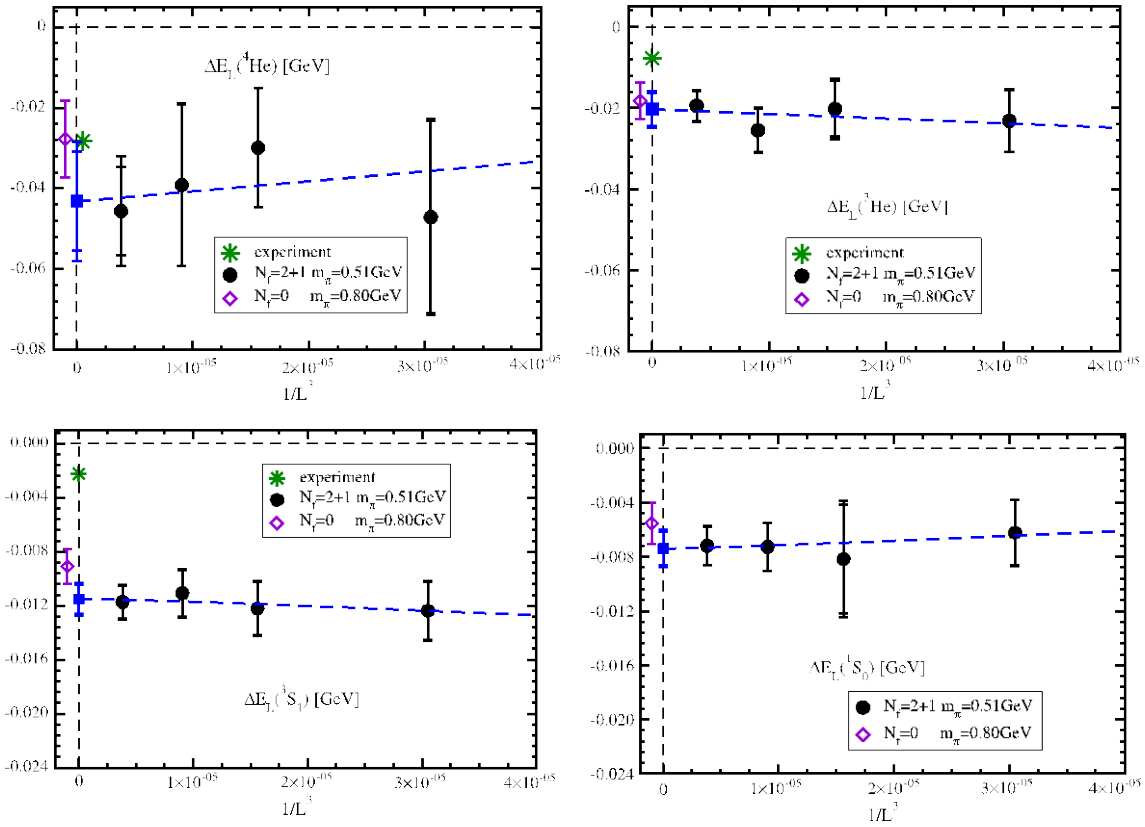

Fig.4. Spatial volume dependence of the energy shift ΔE_L in GeV units for the ^{4}He (top-left), ^{3}He (top-right), $^3S_1$ (bottom-left) and $^1S_0$ (bottom-right) channels.

in the two-nucleon channels is as follows. The binding energy in both channels diminishes monotonically as the up-down quark mass decreases. At some point of the up-down quark mass the binding energy in the $^1S_0$ channel vanishes and the bound state evaporates into the attractive scattering state, while the binding energy in the $^3S_1$ channel remains finite up to the physical point. Thus a next step of primary importance is to reduce the up-down quark mass toward the physical values. This is a dynamical question on the strong interaction, and only lattice QCD could answer it.

4) Determination of effective potentials between baryons based on QCD

Another approach to understand the structure and property of nuclei is extract nuclear potentials from lattice QCD calculations and use them as input in nuclear physics calculations. In 2007 we have proposed a new method to extract a potential between hadrons by measuring the equal-time Nambu-Bethe-Salpeter (NBS) wave function in lattice QCD. An exploratory study of two-nucleon systems with this method in quenched QCD choosing the degenerate up-down quark mass corresponding to 0.53 GeV for the pion mass successfully reproduced empirically known features of the potential: a strong repulsive core at short distances surrounded by an attractive well at medium and long distances. Since then this approach has been applied to various multihadron systems: two-nucleon potentials in even and odd parity sectors including the central, tensor and spin-orbit components, three-nucleon potentials, hyperon-nucleon and hyperon-hyperon

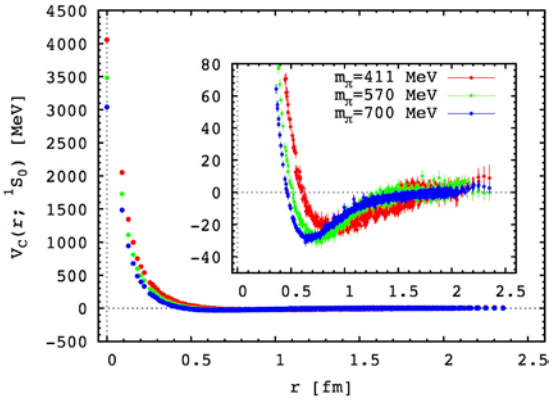

Fig.5. Quark mass dependence of spin-singlet central potential for parity even sector.

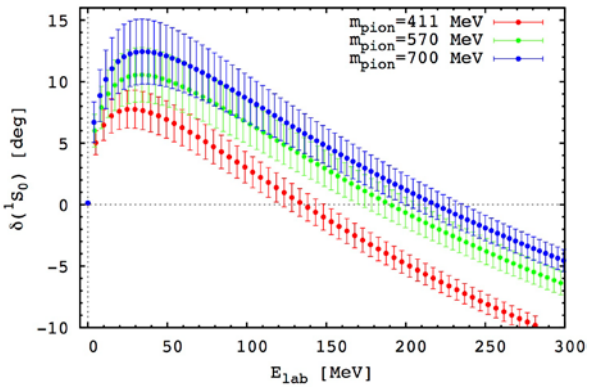

Fig.6. Quark mass dependence of scatteting phase shift for spin-singlet channel.

potentials including the H-dibaryon channel. So far the most extensively studied system is the two-nucleon potentials in even parity sector. Figure 5 shows the up-down quark mass dependence of the spin-singlet central potential in even parity sector obtained by using 2+1 flavor QCD gauge configurations generated in the PACS-CS project. As the quark mass decreases, the repulsive core grows and the attractive pockets in the medium distance become shallower. These potentials are used as input of Schrödinger equation for scattering observables. The resultant scattering phase shift in $^1S_0$ channel is plotted in Fig. 6. Although the interaction is attractive at low energy, it is not strong enough to form a bound state. The $^3S_1$ channel is also in the same situation. This contradicts the observation with the direct method explained above. Furthermore, another concern is that the magnitude of the positive phase shift becomes smaller as the up-down quark mass decreases.

5) Lattice QCD at finite temperature and density

QCD is expected have a rich phase structure as a function of temperature and density. At sufficiently high temperature, quarks and gluons are not confined within hadrons anymore because the effective coupling at the thermal energy scale becomes small due to the asymptotic freedom of QCD. The system will turn into a colored plasma state called “quark-gluon plasma” (QGP), which is considered to play an important role in the creation of matter during the early development of the Universe. Furthermore, QGP is expected to be observed by relativistic heavy-ion collision experiments at RHIC. The deconfinement is also expected at sufficiently high density. The average distance between quarks becomes smaller and the properties of the system will be governed by the asymptotic freedom. At very large densities and low tempeartures, we expect a BCS-like state called “color superconductor” due to the attractive interaction between quarks. At lower densities we expect a nuclear fluid state, which may be realized inside the neutron stars. We have been pushing forward lattice QCD studies at finite temperatures and densities using the Wilson-type quarks. Since it require more computational cost than the staggered-type quarks, various theoretical and computational techniques have been developed: We have introduced a fixed-scale approach armed

with a tempearture-integration method, a Gaussian method based on cumulant expansion, and a histogram method combined with the reweighting technique. With the aid of these methods we have carried out the first study of finite-density QCD with the Wilson-type quarks and the first calculation of the equation of state with 2+1 flavors of Wilson-type quarks.

1.3 Collaboration

Successful numerical simulations heavily depend on an increase of computer performance by improving algorithms and computational techniques. This is achieved in collaboration with applied mathematicians and computer scientists in Division of High Performance Computing Systems. We have developed the mixed precision nested BiCGStab algorithm for code tuning on the PACS-CS machine and the block Krylov subspace algorithms for the Wilson-Dirac equation with multiple right-hand sides. These algorithms have contributed to the significant reduction of the computational cost for the 2+1 flavor QCD and 1+1+1 flavor QCD+QED simulations.

As described in PART I of this report, we have constructed ILDG (International Lattice Data Grid) and JLDG (Japan Lattice Data Grid) in collaboration with Grid and Network group in Division of High Performance Computing System. The former is to share gauge configurations among worldwide particle physics researchers through internet and the latter for the domestic data sharing. Their operation started in 2007 and 2008, respectively. The 2+1 flavor QCD gauge configurations generated in the PACS-CS project were uploaded on ILDG and widely used by particle physics researchers in foreign countries.

We established the Joint Institute for Computational Fundamental Science (JICFuS) in 2009, which is a joint research organization combining the University of Tsukuba's Center for Computational Sciences (CCS), the High Energy Accelerator Research Organization (KEK), and the National Astronomical Observatory of Japan (NAOJ). JICFuS has three major objectives. Firstly, the three organizations collaboratively provide researchers extensive support for improving the algorithms and the computational techniques. Secondly, JICFuS serves as a place for computational fundamental scientists and computer scientists to interact and actively exchange ideas on a routine basis. Thirdly, we will promote collaborative interdisciplinary research between computational fundamental scientists in particle physics, nuclear physics and astrophysics, mediated by computer systems.

1.4 Future Plan

The innovative High Performance Computing Infrastructure (HPCI) plan with the "K computer" at the core was launched by government to actualize an innovative computational environment capable of meeting diverse users needs, and aimed at promoting the exploitation of HPCI. As major policy objectives, building

an organization for promoting computational sciences in major fields (HPCI Strategic Program), and producing revolutionary results through the exploitation of HPCI are cited.

In the HPCI Strategic Program, five potential fields have been identified as strategic fields that not only require K computer resources, but can also be expected to yield significant social and scholarly breakthroughs. "Field 5: The origin of matter and the Universe" is one of these. This field deals with fundamental physics, primarily concerning elementary particles, atomic nuclei, and astrophysics. JICFuS is the institution (strategic institution) that leads research and development in Field 5.

There are four scientific research subjects in Field 5 that are pursued using the K computer. One of them is "Determination of the baryon-baryon interactions using lattice QCD at the physical point". We are currently generating 2+1 flavor QCD gauge configurations at the physical point enlarging the spatial volume by 27 times larger than that in the PACS-CS project. Major physics target is 1+1+1 flavor QCD+QED with the aid of the reweighting technique, the direct construction of light nuclei and the determination of effective baryon-baryon potentials. We also plan to investigate resonance states and measure various hadronic matrix elements taking advantage of large spatial volume.

Lattice QCD studies at finite temperatures and densities will proceed with the Wilson-type quarks. We plan to determine the critical end point/line in 3 and 2+1 flavor QCD with and without densities. For efficient simulation of finite density QCD, we will make further improvement for algorithms and computational techniques.

1.5 Publications

1.5.1 Journal Papers

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2 Division of Astrophysics and Nuclear Physics: *Astrophysics Group*

2.1 Research Activity

In the 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. Recently, we have diversified the research field into the scope of astrobiology based on first-principles simulations. 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, we have performed ultra-high resolution *N*-body simulations of the cold dark matter universe to study the spatial correlation of galaxies, the fine structures of galactic halos, the distribution of subhalos, their structures, and their dependence on the nature of dark matter. To realize high-resolution simulations, we have used the FIRST simulator, T2K-Tsukuba, HA-PACS and K computer. The FIRST simulator is a hybrid computer dedicated for astrophysical RHD, which was developed in the collaboration with the Division of High Performance Computing Systems (see Part I for more details). The FIRST project is initiated by *Grant-in-Aid for Specially Promoted Research* in 2004 (approved by MEXT in Japan), and continued by *Grant-in-Aid for Scientific Research (S)* in 2008. The duration of the project is 10 years (2004~2013) with the total budget of JP405.4 million (US$4.2 million).

2.2 Research Results

2.2.1 Numerical Methods

■ **Trillion-body simulations of dark matter universe on K computer**

Cosmological *N*-body simulations of one trillion particles are performed on the full system of K computer. This is the first gravitational trillion-body simulation in the world and is the winner of the 2012 Gordon-Bell performance prize. Unlike many previous Gordon-Bell prize winners that used the tree algorithm for astrophysical

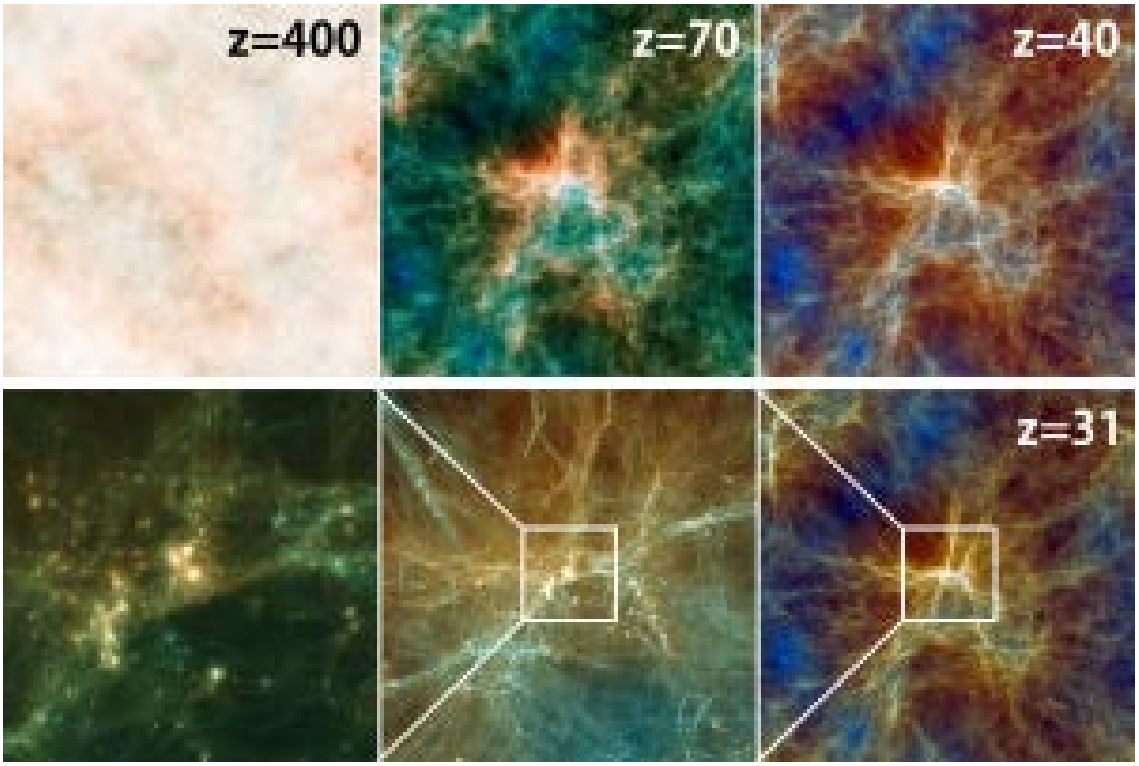


Figure 1. The distribution of dark matter in a 16.8G particles simulation at redshift z=400 (initial), 70, 40, and 31. The distribution is almost uniform at the beginning (z=400, about two million years after the Big Bang, the width of the image corresponds to about five light years). Gradually, dark matter concentrates via the gravity and forms large structures. Bottom-left and bottom-middle images are enlargement of the image of z=31 (about 100 million years after the Big Bang, the width corresponds to about 65 light years).

N-body simulations, we used the hybrid TreePM method, for similar level of accuracy in which the short-range force is calculated by the tree algorithm, and the long-range force is solved by the particle-mesh algorithm. We developed a highly-tuned gravity kernel for short-range forces, and a novel communication algorithm for long-range forces. The execution performance was 5.67 Pflops on the 98% resources of the K computer system.

■ **High performance numerical library for *N*-body simulations: Phantom-GRAPE**

By directly exploiting SIMD (Single Instruction Multiple Data) instruction sets such as SSE (Streaming SIMD Extension) and AVX (Advance Vector eXtension) implemented in the recent x86 processors, we develop a high-performance numerical software library to compute the gravitational forces and potentials in *N*-body simulations, which we call "Phantom-GRAPE". The performance of Phantom-GRAPE on the latest processors with Sandy-Bridge architecture is 20 times higher than that of the implementation without the use of SIMD instructions.

■ **Highly scalable implementation of an *N*-body code on a GPU cluster**

We have developed a highly optimized code for collisionless *N*-body calculations based on direct summation. To improve the scalability of the OpenMP/MPI hybrid parallelized code, we have reduced the number of communications among multiple GPUs and have overlapped communications with computations to hide communication time. The results show excellent scalability with super-linear scaling when the number of *N*-body particles per GPU is less than 10^4 and parallel efficiency approaching unity when the number of *N*-body particles per GPU is greater than 10^4.

■ **Vlasov-Poisson simulations for collisionless self-gravitating systems**

As an alternative to standard *N*-body simulations, for the first time, we develop a numerical scheme to directly solve Vlasov-Poisson equations in the six-dimensional phase space volume. We find that our Vlasov-Poisson simulations have very excellent capability to deal with the collisionless damping, or free streaming effect in collisionless self-gravitating systems. We are now applying this method to the numerical simulations of massive neutrinos in the large-scale structure in the universe.

■ **A new numerical scheme for radiation transfer calculation for a large number of point sources: ARGOT**

We develop a new ray-tracing scheme of radiation transfer calculations on 3D Cartesian grids for very large number of radiating sources, "ARGOT", in which a distant group of radiating sources are regarded as a single bright source using the oct-tree structures. The computational cost is proportional only to a logarithm of the number of radiation sources rather than the number of radiation sources.

■ **GPU acceleration of radiation transfer code**

The calculations of radiation transfer from point radiation sources using the ARGOT scheme, and that from diffuse radiation using the ART scheme are accelerated by exploiting the high-performance computing capability of GPUs. Since the ray-tracing calculation for each light-ray can be performed in parallel, the calculation of radiation transfer based on the ray-tracing scheme can be easily parallelized on highly-parallel architecture like GPUs. The overall performance of the radiation transfer calculation on a single GPU is 10-20 times higher than that on a single recent x86 processor.

■ **Smoothed particle hydrodynamics with tree-based accelerated radiative transfer: START**

We present a novel radiation hydrodynamics code, start, which is a smoothed particle hydrodynamics (SPH) scheme coupled with accelerated radiative transfer. The basic idea for the acceleration of radiative transfer is parallel to the tree algorithm that is hitherto used to speed up the gravitational force calculation in an *N*-body system. It is demonstrated that the radiative transfer calculations can be dramatically accelerated, where the computational time is scaled as $N_p \log N_s$ for N_p SPH particles and N_s radiation sources.

2.2.2 Numerical Simulations

■ Formation of first stars

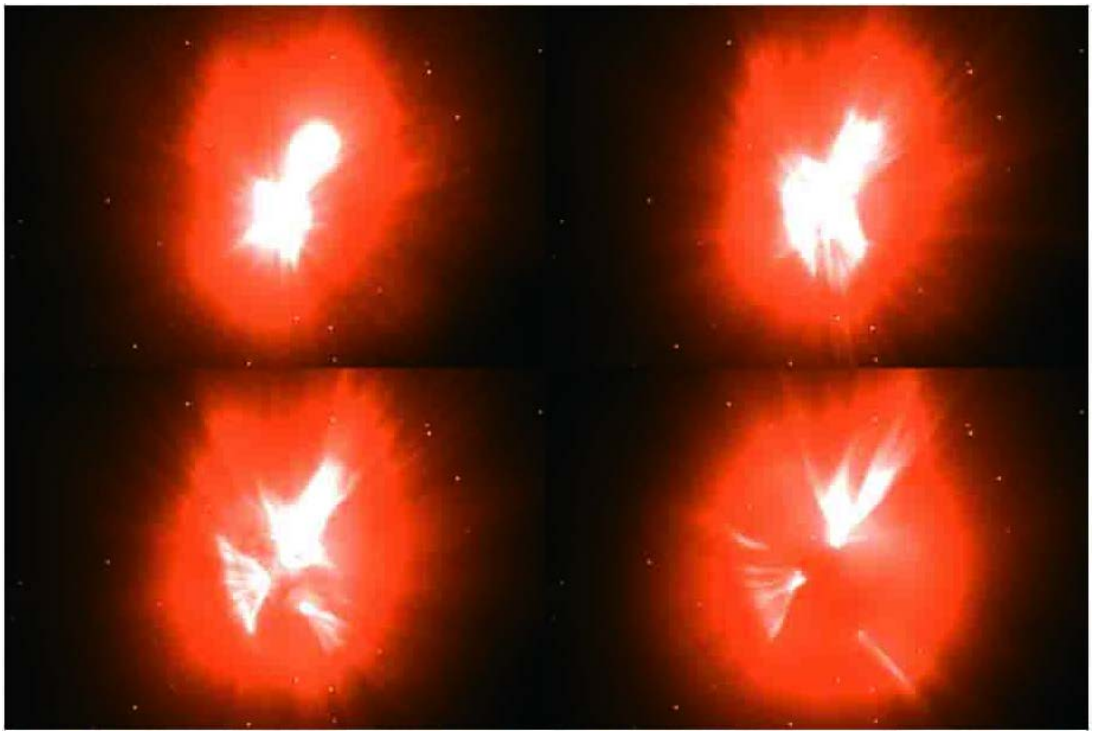


Figure 2. Three-dimensional radiation hydrodynamic simulations of the secondary star formation in the early universe. Using three-dimensional radiation hydrodynamic simulations, we explore the formation of secondary Population III stars under radiation hydrodynamic feedback by a preformed massive star in the early universe. Each panel shows the evolution of a collapsing cloud nearby a first luminous star as a function of time.

We study the dependence of radiative feedback on the mass of source Pop III star. UV radiation from the source star can work to impede the secondary star formation through the photo-heating and photo-dissociation processes. In order to investigate the radiative feedback effects from less massive stars, we perform three-dimensional radiation hydrodynamic simulations, incorporating the radiative transfer effect of ionizing and H_2-dissociating radiation. As a result, we find that if a source star is less massive than $\approx 25\ M_\odot$, the ionizing radiation cannot suppress the negative feedback of H_2-dissociating radiation. Therefore, the fate of the neighbouring clouds around such less massive stars is determined solely by the flux of H_2-dissociating radiation from source stars.

■ Two types of Lyman α emitters (LAEs) envisaged from hierarchical galaxy formation

We model LAEs by three-dimensional cosmological simulations of dark halo merger in a Λ cold dark matter universe. As a result, it is shown that the age of simulated LAEs can spread over a wide range from 2 to 900 Myr. Furthermore, we find that there are two types of LAEs, in one of which the young half-mass age is comparable

to the mean age of stellar component, and in the other of which the young half-mass age is appreciably shorter than the mean age. We define the former as Type 1 LAEs and the latter as Type 2 LAEs. A Type 1 LAE corresponds to early starburst in a young galaxy, whereas a Type 2 LAE does to delayed starburst in an evolved galaxy, as a consequence of delayed accretion of a subhalo on to a larger parent halo.

■ **Galaxy formation and sub-millimetre brightness of early star-forming epoch**

Based on a three-dimensional chemodynamic simulation of an early star-forming galaxy by Mori & Umemura, we explore the evolution of the sub-millimetre brightness. We solve the three-dimensional radiative transfer in the clumpy interstellar media in this model galaxy, taking the size distributions of dust grains into account, and calculate the dust temperature as a function of galactic evolutionary time. We find that the clumpiness of interstellar media plays an important role for the sub-millimetre brightness. In the early phase ($t_{\rm age} \lesssim 0.3$ Gyr), dust grains are concentrated on clumpy star-forming regions that are distributed all over the galaxy, and the grains can effectively absorb ultraviolet radiation from stars. As a result, the dust is heated up to $T_{\rm dust} \gtrsim 35$ K. In the later phase ($t_{\rm age} > 0.3$ Gyr), the continuous supernovae drive dust grains far away from star-forming regions. Then, the grains cannot absorb much radiation from stars, and become a cold state close to the cosmic microwave background temperature. We derive the spectral energy distributions by placing the model galaxy at a given redshift. The peak flux at 850 μm is found to be $S_{850} \sim 0.2$–0.9 mJy if the model galaxy is placed at $6 \geq z \geq 2$. This means that Atacama Large Millimetre/sub-millimetre Array can detect an early star-forming galaxy with SFR of $\sim 10\ M_{\odot}\ {\rm yr}^{-1}$ by less than one hour integration with 16 antennas.

■ **Core-cusp problem in cold dark matter halos and supernova feedbacks**

This study investigates the dynamical response of dark matter (DM) halos to recurrent starbursts in forming less–massive galaxies to solve the core–cusp problem. The cycle of expansion and contraction of the interstellar gas driven by the supernova feedbacks leads to a repetitive change in the gravitational potential of the gas. The resonance between DM particles and the density wave excited by the oscillating potential plays a key role in understanding the physical mechanism of the cusp-core transition of DM halos. DM halos effectively gain kinetic energy from the baryon potential through the energy transfer driven by the resonance between the particles and density waves. We determine that the critical condition for the cusp–core transition is such that the oscillation period of the gas potential is approximately the same as the local dynamical time of DM halos. We present the resultant core radius of a DM halo after the cusp–core transition induced by the resonance.

■ **Galaxy collision and the outer density profile of the dark matter halo in M31**

The cold dark matter (CDM) cosmology predicts that the outer density profile of dark matter halos decreases with the cube of distance from the center. However, so far not much effort has examined this hypothesis. Large-scale stellar structures detected by the recent observations in the halo of the Andromeda galaxy (M31)

provide an attractive window to explore the structure of the dark matter halo. Using an *N*-body simulation of the interaction between an accreting satellite galaxy and M31, we investigate the mass-density profile of the dark matter halo in M31. To reproduce the Andromeda Giant Southern Stream and the stellar shells at the east and west sides of M31, we find the sufficient condition for the power-law slope of the outer density distribution of the dark matter halo. As a consequence, the CDM model fails to reproduce the observational evidences, and the outer density profile of the dark matter halo is steeper (power-law slope of 3.7) than that of the CDM prediction.

■ **Hunting a wandering supermassive black hole in M31 halo**

The hierarchical structure formation scenario posits that galaxies enlarge through multiple mergers with smaller galaxies. Since the centers of all galaxies appear to

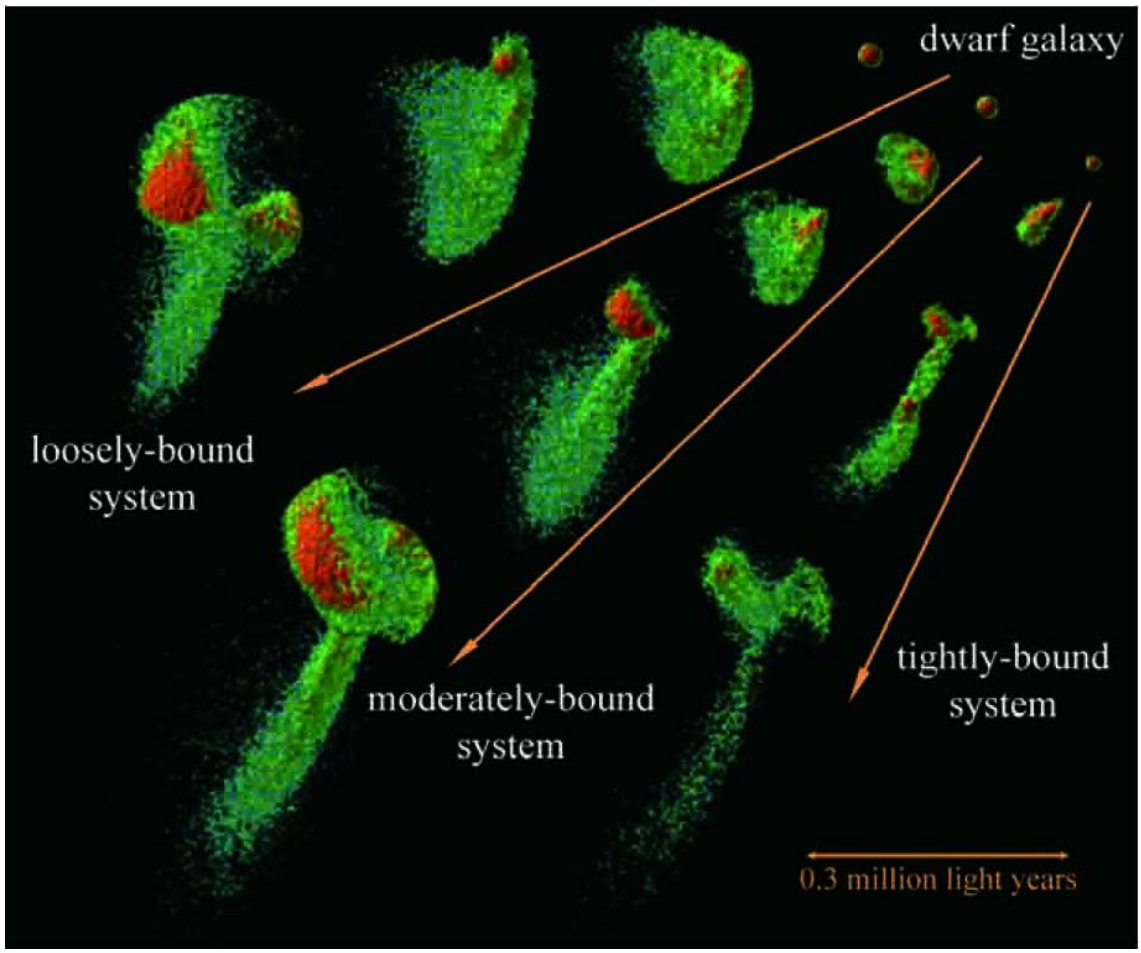


Figure 3. *N*-body simulations of the interaction between an accreting small galaxy and the Andromeda galaxy. Large galaxies such as the Andromeda galaxy are believed to have formed in part from the merger of many less massive galaxies. Here, we have studied the interaction between an accreting small galaxy and the Andromeda galaxy using *N*-body simulations. Each track along an arrow corresponds to the evolution of the projected stellar mass density of the merging small galaxies with the different binding energy.

be occupied by a supermassive black hole (SMBH), collisions should manifest as positional drifts of these SMBHs within their host galaxies. Evidence of such activity, however, is lacking to date. We have conducted numerical simulations to locate the likely positions of SMBHs wandering inside the M31 galaxy, which contains a giant stellar stream. The results of this study will assist observational searches for wandering SMBHs in host galaxies. If such features are observationally verified, they will provide important insights into the formation and evolutionary processes of large galaxies such as M31 and the Milky Way.

■ **Successive merger of multiple massive black holes in a primordial galaxy**

Using highly accurate *N*-body simulations, we explore the evolution of multiple SMBHs in a primordial galaxy. The evolution is pursed with a fourth-order Hermite scheme, where not only three-body interactions of SMBHs but also dynamical friction by stars are incorporated. Initially, 10 SMBHs with equal masses of 10^7 $M_\odot$ are set in a host galaxy with 10^{11} $M_\odot$. It is found that 4-6 SMBHs merge successively within 1 Gyr, emitting gravitational wave radiation. The key process for the successive merger of SMBHs is the dynamical friction by field stars, which enhances three-body interactions of SMBHs when they enter the central regions of the galaxy. The heaviest SMBH always composes a close binary at the galactic center, which shrinks owing to the angular momentum transfer by the third SMBH and eventually merges. The angular momentum transfer by the third SMBH is due to the sling-shot mechanism. The simulations show that a multiple SMBH system can produce a heavier SMBH at the galactic center purely through *N*-body process. This merger path can be of great significance for the growth of SMBHs in a primordial galaxy. The merger of multiple SMBHs may be a potential source of gravitational waves for the Laser Interferometer Space Antenna and pulsar timing.

■ **Non-equilibrium ionization state and two-temperature structures of the ICM in merging galaxy clusters**

Based on a series of hydrodynamic simulations of merging galaxy clusters, we find that the non-equilibrium ionization state of heavy elements in the ICM is significant and can be observed with the next generation X-ray mission with high energy resolution X-ray spectrograph such as ASTRO-H. Furthermore, we show that the observations of merging galaxy clusters with high Mach numbers such as the “bullet cluster” can probe the thermal relaxation processes between ions and electrons and the existence of the two-temperature structure in ICM.

■ **Galaxy formation and effects of AGN feedback**

Our studies of AGN feedback through simulations including a well-resolved multi-phase interstellar medium (grid resolution down to 1 pc) enabled us to determine the dependence of the feedback efficiency and star-formation rate on structural parameters of the dense, warm gas phase. These results naturally explain the M-σ relation and the multi-phase outflows observed in a number of radio galaxies, and inform the implementation of feedback in cosmological simulations. Recently, we focused on predicting the feedback effect of the most powerful disc winds observed, ultra-fast outflows. We found that these may drive

galaxy-wide outflows of several 100 to 1000 km s^{-1}, but also cause star-formation in discs.

- **Effects of the AGN radiation on the evolution of the cloud**

We have performed 3D/1D RHD simulations of a cloud that irradiated by an AGN to investigate the effects of the AGN radiation on the evolution of the cloud and on the gas supply process to the galactic center. We have found that the evolution of the cloud can be classified into two categories: (i) photo-evaporation-driven mode and (ii) radiation pressure-driven mode. In the former case, the cloud is swept by a M-type shock driven by the back-reaction of the photo-evaporation and it collapses into a long massive filament in its final stage because the shock propagates inward spherically-symmetrically. On the other hand, in the latter case, the cloud is swept by a radiation pressure-driven shock and most of the gas in the cloud is collected into a thin massive disc (the post-shock layer), which becomes unstable self-gravitationally on the way of the evolution. We have determined numerically the life time of the cloud for various cloud parameters by 1D spherically-symmetric RHD simulations.

- **Light harvesting and energy transfer in photosystem: Implication for biosignatures**

In searching for Earth-like planets, several planets in the habitable zone have been detected. As detectable signs for lifes in reflection spectra on extrasolar planets, several indicators called as biosignatures have been proposed. One of the biosignatures is red edge, which is a steep change in NIR region in vegetation spectra. On Earth, photosynthetic organisms have developed to optimize the Sun light spectra. However, given photosynthetic organisms on extrasolar planets, it is not strange if they show different absorption spectra. In this study, we focused on the light absorption mechanism in photosynthetic organism and investigated the fundamental properties of the light harvesting complexes (LHCs). To investigate the mechanism, we constructed a theoretical model that can simulate the light harvesting and energy transfer. A dipole-dipole approximation was used for the electronic excitations. We adopted the model to LHC aggregations in purple bacteria., which is known to have a red edge in the longer wavelength region. The calculated oscillator strength and the energy transfer time in LHCs was in a good agreement with the experimental data. We also investigated efficiencies of light absorption in the LHC model under various spectrum of Sun, M star and so on.

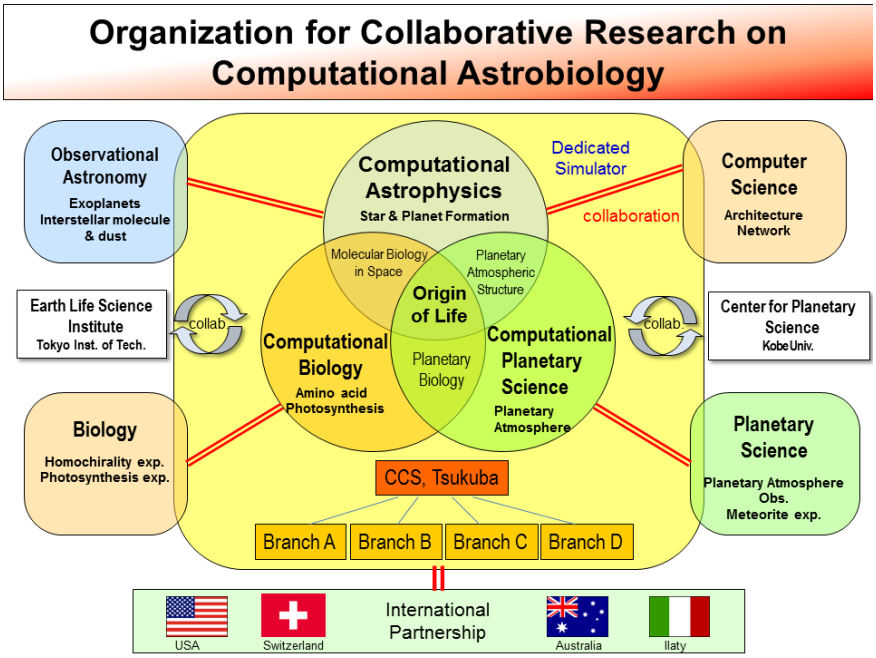
2.3 Collaboration

We have pursued an active role in the Strategic Programs for Innovative Research Field 5 "The origin of matter and the universe", the Ministry of Education, Culture, Sports, Science and Technology of Japan. In addition, we have collaborated with High Performance Computing Systems division at CCS, for development and tuning of simulation codes on FIRST, T2K-Tsukuba and HA-PACS. For the study of the galaxy formation and the reionization of the universe, joint researches have been promoted with the Institute for Cosmic Ray Research at the University of

Tokyo and Astronomical Institute at Tohoku University. Those projects are funded by JSPS Grant-in-Aid for Scientific Research. In the international collaborations, we have partnered with groups at Department of Physics and Astronomy, University of California at Los Angeles, Institute of Astronomy, University of Vienna, Mt Stromlo Observatory, Department of Physics and Astronomy, John Hopkins University, the Institut Astrophysique de Paris, and at the Observatoire de Paris.

■ Organization for Collaborative Research on Computational Astrobiology

Recently, we have initiated "Organization for Computational Astrobiology". Astrobiology has attracted a significant deal of attention owing to advanced observations of extrasolar planets as well as interstellar molecules. This organization aims at exploring key processes related to the origin of life in the universe through *ab initio* calculations based on collaboration among the Computational Astrophysics, Computational Biology, Computational Planetary Science, and Computer Science fields.



These research efforts are targeted on the study of interstellar molecular biology, planetary biology, and planet formation. At present, 54 researchers from 22 institutes are participating in the organization, which was formed at the initiative of the CCS, University of Tsukuba.

One major collaboration is the study of the cosmic origin of amino acid -homochirality, and the hydrodynamic and magneto-hydrodynamic turbulence.

- **Cosmic Origin of Amino acid Homochirality**: Amino acids are produced in the laboratory as racemic mixture, that is, equal quantities of L-amino acids and D-amino acids. Living systems, however, use almost exclusively L-amino acids. This is called the "homochirality" problem. In 1997, the excess of L-amino acids (enantiomeric excess) was discovered in the Murchison meteorite which falled

onto the Earth in 1969. On the other hand, it is demonstrated that circular poralized light can produce the enantiomeric excess of amino acids. Recenltly, circular poralized light has been detected in star-forming regions. The interaction between amino acids and circular poralized light in interstellar space can be explored computationally by the *ab initio* quantum mechanical simulations.

2.4 Future Plan

In a cold dark matter universe, the hierarchical structure formation scenario posits that large galaxies have enlarged through multiple mergers with smaller galaxies. To test the theory, we will promote strongly research in the Numerical Galactic Archaeology using the hydrodynamic/*N*-body simulations of the dynamical, chemical, and spectrophotometric evolution of galaxies. Furthermore, the mass of the spheroidal component of galaxies is correlated with the mass of their central SMBHs. This relation implies that galaxies coevolve with their central SMBHs. However, the coevolution process of galaxies and SMBHs is largely unknown. To solve these problems, we aim to develop a next-generation hybrid computer system that can extract the potentiality of special purpose processor and new-generation acceleration-board to the maximum. Using such a next-generation hybrid computer, we would like to perform the general relativistic radiation hydrodynamics further.

2.5 PUBLICATIONS

2.5.1 Journal Papers

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2.6 GRANTS

- Masayuki Umemura, JSPS Grant-in-Aid for Scientific Research (S), 2008-2013, 95,030,000 yen
- Masao Mori, JSPS Grant-in-Aid for Scientific Research (C), 2013-2018, 5,200,000 yen
- Masao Mori, JSPS Grant-in-Aid for Scientific Research (A), 2009-2013, 27,560,000 yen
- Masao Mori, JSPS Grant-in-Aid for Scientific Research (C), 2006-2009, 3,080,000 yen
- Kohji Yoshikawa, JSPS Grant-in-Aid for Challenging Exploratory Research, 2009-2011, 3,300,000 yen
- Kohji Yoshikawa, JSPS Grant-in-Aid for Young Scientists (Start-up), 2007-2008, 2,975,000 yen
- Takashi Okamoto, JSPS Grant-in-Aid for Young Scientists (B), 2012-2016, 4,550,000 yen
- Takashi Okamoto, JSPS Grant-in-Aid for Young Scientists (Start-up), 2009-2010, 2,340,000 yen
- Kenji Hasegawa, JSPS Grant-in-Aid for Young Scientists (B), 2012-2014, 4,550,000 yen
- Tomoaki Ishiyama, JSPS Grant-in-Aid for Young Scientists (B), 2012-2015, 4,550,000 yen
- Toshihiro Kawaguchi, JSPS Grant-in-Aid for Young Scientists (B), 2007-2011, 3950,000 yen
- Chizuru Akizuki, JSPS Grant-in-Aid for JSPS Fellows, 2007-2009, 2,700,000 yen
- Takayuki Koizumi, JSPS Grant-in-Aid for JSPS Fellows, 2008, 1,800,000 yen

3 Division of Astrophysics and Nuclear Physics: *Nuclear Physics Group*

3.1 Research Activity

In Nuclear Physics Group, we have performed researches on structure and reactions of nuclei as quantum many-body systems composed of nucleons. We put emphasis on development and applications of computational methods based on time-dependent density functional (mean-field) theory which we abbreviate as TDDFT below.

We have developed a few innovative methodologies in the TDDFT. In the linear response TDDFT which is known as RPA and QRPA, we have developed the finite amplitude method which is very useful to achieve linear response calculations including residual interactions fully self-consistently. We have also demonstrated that the canonical-basis time-dependent Hartree-Fock-Bogoliubov (TDHFB) theory provides a computationally feasible and physically sound approximation to the full TDHFB calculations. Although full TDHFB calculations are still very challenging, we have been continuing efforts of code developments and have made a few test calculations of linear responses.

We applied the TDDFT to several problems. They include systematic calculations of nuclear dipole response, QRPA calculations of nuclear matrix elements relevant to neutrino mass determination through double-beta decay, and multinucleon transfer processes in heavy ion collisions.

A unique feature of our group is an interdisciplinary activity. We have been active in computational researches based on the TDDFT in two fields, nuclear physics and condensed matter physics that continues for a long time. In the last five years, we have developed a computational approach for electron dynamics in crystalline solids induced by strong laser pulses. This activity is described in the section of Division of Quantum Condensed Matter Physics.

We would like to mention two other activities on light nuclei. One is a development of a new computational approach for structures of light nuclei, superposing a number of Slater determinants which are generated by a stochastic procedure. Applying it to ^{12}C nucleus, the Hoyle state as well as other states is reasonably described. The other is the quantum three-body calculation of triple-alpha reaction rate. We invented a new theoretical method for radiative capture process, which we call the imaginary-time theory. Using the theory, we

show that the triple-alpha reaction rate can be reliably calculated even at low temperatures.

3.2 Research Results

1.2.1. Nuclear response functions

In RPA and QRPA calculations, some parts of residual interactions have been often ignored since calculations of matrix elements of residual interactions are very cumbersome. We have invented a computational method to overcome the difficulty which we call the finite amplitude method. The residual interaction is defined as the second derivative of the energy functional. In the finite amplitude method, the last step of the functional derivative is evaluated numerically by the finite difference. Therefore, it is sufficient to analytically calculate the first derivative of the energy functional, which is nothing but the mean-field Hamiltonian. It means that, to calculate matrix elements of the residual interaction, we can use computational codes of the mean-field Hamiltonian. The finite amplitude method was first derived in the RPA calculation without pairing, and then extended to QRPA calculations.

We carried out systematic calculations of nuclear dipole responses from light to medium nuclei. The left-panel of Fig. 1 shows RPA calculations of photoabsorption cross sections of Ne and Ca isotopes. As the neutron number increases, dipole strength starts to appear in the low excitations below 10 MeV which is known as the pigmy dipole resonance (PDR). The appearance of the PDR has been attracting much attention for its relevance to the neutron skin, properties of energy functional of neutron-rich matter, and the r-process in the nucleosynthesis. The right-panel of Fig.1 shows fractions of the PDR to the total strength plotted as the number of neutrons and protons, connecting isotopes and isotones. It clearly indicates the importance of the shell effect for the PDR fraction.

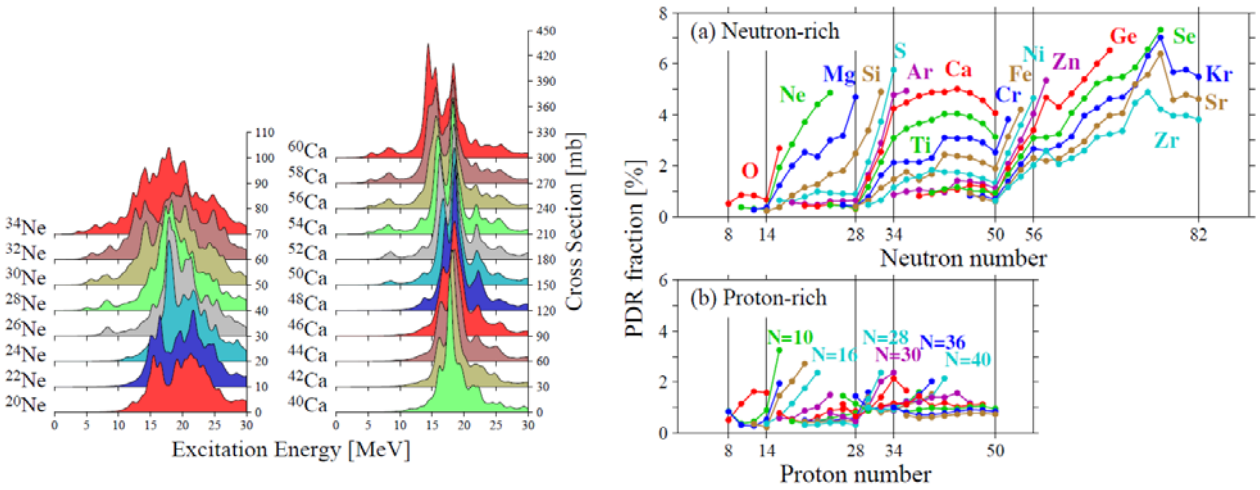

Fig. 1: (Left) Nuclear dipole response of Ne and Ca isotopes. (Right) Fraction of pygmy dipole resonance in the total dipole strength plotted against proton- and neutron-numbers.

1.2.2 QRPA calculation relevant to neutrino mass determination

Terasaki joined our group in 2011 and started a calculation of nuclear transition matrix element of the neutrinoless double-beta (0νββ) decay. This matrix element is one of the key ingredients, along with the experimental decay rate, to determine the effective neutrino mass under the assumption that the neutrino is a Majorana particle.

In this research, QRPA is used which gives virtual intermediate states of the ββ decay. In this approach, the nuclear matrix element is obtained by the trace of the product of four matrices, that is, matrices of the neutrino-potential, transition from the initial to the intermediate states, that from the final state, and the overlap of the two intermediate states. The calculation needs several codes in order to obtain the above matrices. Those codes used specifically for the 0νββ decay have been developed and tested these two years. The QRPA code is used which was developed by Terasaki in the UNEDF project.

An important result obtained so far is the overlap matrix of the intermediate states obtained in the QRPA based on the ground states of the parent and daughter nuclei (Fig. 2). These overlaps were calculated for the first time using the definition of the QRPA ground state; this state is defined as the vacuum to the QRPA quasiboson. The important point is that the QRPA many-body correlations are taken into account correctly by this definition. According to the preliminary result, the correct overlap has an effect to reduce the nuclear matrix element appreciably.

Calculations are now in progress for determining the necessary space size for ^{150}Nd-^{150}Sm. As soon as these calculations are finished, the calculation to obtain the nuclear matrix element will begin. It is very important to investigate how the new nuclear matrix element becomes closer to the values of the shell-model calculations by the reduction effect of the QRPA correlations via the overlap.

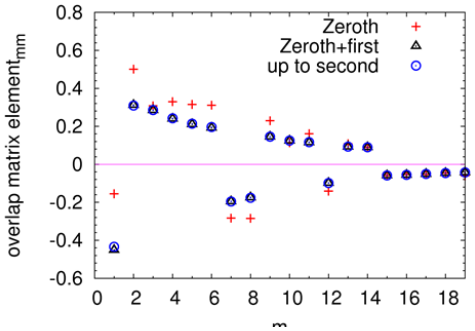

Fig. 2:. Diagonal overlap matrix elements of the intermediate states obtained by the QRPA. The bra states are the QRPA states obtained based on ^{26}Si, and the ket states are based on ^{26}Mg (a fictitious 0νββ decay for a test). The horizontal axis indicates the state number in ascending order of the energy. An expansion method was used with respect to an operator to bring the QRPA correlation to the QRPA ground state, and the good convergence of this expansion is shown by the different symbols; the second-order terms are negligible. The like-particle QRPA is used, which is possible to apply under the closure approximation (this is also the new point of our approach). The Skyrme energy density functional SkM* and the volume pairing energy density functional were used.

1.2.3 Nuclear superfluid dynamics: Canonical-basis TDHFB simulation

TDHFB is expected to provide excellent descriptions of nuclear dynamics including pairing correlations. Although fully three-dimensional simulation solving the TDHFB equation is highly expected to describe low-energy nuclear dynamics such as fusions and fissions, only a few attempts have been reported for such calculations to date.

We have demonstrated the computational feasibility and physical soundness of the approximate scheme which we call the Canonical-basis (Cb-) TDHFB. In this framework, the pairing correlation can be taken into account approximately in a similar way to the BCS approximation. At present, we applied the method to linear response calculations, and have found that it provides results very close to the full TDHFB calculations. The paper reporting the Cb-TDHFB (Ebata et.al, Phys. Rev. C 82, 034306 (2010).) has been taken up as Synopsis of Physical Review C where the Editor noted the potential importance of this approach stating "A possible application of the method, namely, to yield a fully microscopic treatment of fission, could provide a real breakthrough in nuclear physics research."

1.2.4 Toward full TDHFB calculations

We have also conducting an effort to develop a full TDHFB computer codes. At present, we achieved it in the harmonic oscillator basis. Since we do not impose any spatial symmetries, it can describe fully three-dimensional dynamics. The Gogny interaction is used as the effective interaction. Using the code, we have carried out benchmark calculations of the linear response for collective vibrations including quadrupole and isovector dipole modes for oxygen, magnesium, and titanium isotopes. It has been shown that the pairing correlations bring about the adiabatic transitions among the single-nucleon states in the level crossing region when the collective quadrupole vibrations are excited.

To describe large amplitude dynamics such as fusion and fission, we are improving the code to use of the grid (Lagrange mesh) representation, instead of the harmonic oscillator basis. At present, we succeed to carry out calculations in which the Lagrange mesh is used in one direction while oscillator basis is used in other two. An extension to fully three-dimensional grid representation is now in progress.

1.2.4 Multinucleon transfer reaction by TDHF

Multinucleon transfer reactions (MNT) take place in peripheral nucleus-nucleus collisions at low energies. The MNT is expected to be useful to produce nuclei whose production is difficult by other methods. In fact, there is an experimental proposal in RIKEN to produce neutron-rich nuclei of mass number around 200 using the MNT, whose properties are important to understand r-process in the nucleosynthesis.

We have carried out TDHF calculations of MNT for $^{40,\,48}$Ca+^{124}Sn, ^{40}Ca+^{208}Pb, and ^{58}Ni+^{208}Pb reactions for which measurements are available. To our knowledge, this is the first attempt of fully microscopic TDHF calculation for the MNT cross sections, making comparisons with measurements. It was found that the TDHF calculation provides reasonable description for the cross sections. We also find that there are two distinct mechanisms in the MNT: quantum tunneling processes

dominated at large impact parameter collisions, and the formation and breaking of the neck dominated at inner impact parameter region. Figure 3 shows the density profile (left) and the calculated and measured MNT cross sections (right).

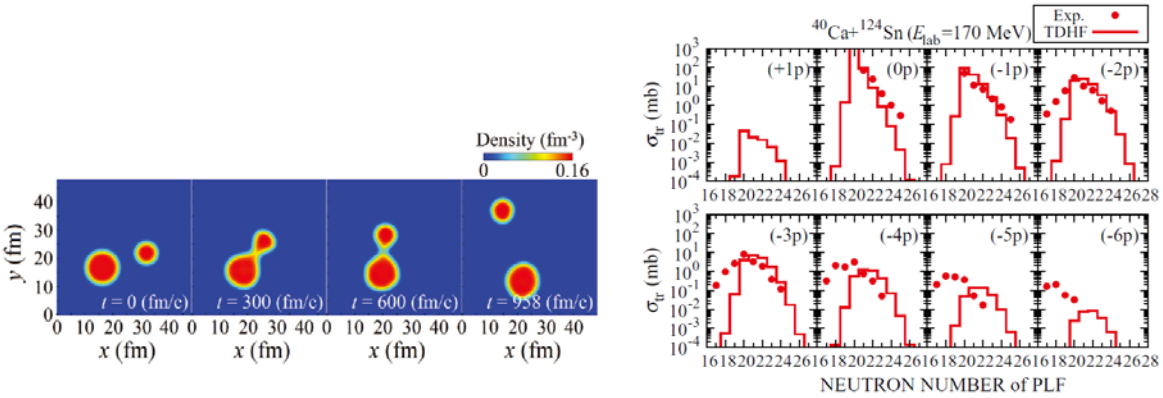

Fig. 3: TDHF calculation of multinucleon transfer processes in ^{40}Ca + ^{124}Sn reaction. (Left) Density profile, and (Right) calculated and measured cross sections.

1.2.5 A new configuration-mixing approach for light nuclei

One of major goals in current computational nuclear theory is to calculate and understand nuclear properties starting solely with a realistic nucleon-nucleon force. Although there have been substantial progresses in the ab-initio descriptions of light nuclei in last two decades, descriptions of excited states which show cluster correlations are still challenging. To describe cluster structures, it is essential to prepare configuration space which may be wide enough to describe long-range cluster correlations.

We have proposed a new computational method which will be suitable to describe cluster states as well as shell-model-like states simultaneously. Our basic idea is to use the imaginary-time method, which is usually used to obtain self-consistent solution in the mean-field theory, to prepare a number of Slater determinants which span a sufficiently large configuration space to describe cluster states. The Slater determinants thus prepared are projected into parity and angular-momentum eigenstates, and then used for configuration mixing calculations diagonalizing the Hamiltonian. We have used the method with the empirical Hamiltonian of Skyrme interaction, and applied to ^{12}C nucleus. We have found that excited states including the Hoyle state as well as the ground state are reasonably described by the method.

1.2.6 Imaginary-time theory for triple-alpha reaction rate

The triple-alpha reaction is a key process that influences the production of all heavy elements in the universe. Accurate knowledge of the reaction rate is essential for understanding stellar evolution and nucleosynthesis. Recently, several theoretical attempts to calculate the rate using quantum theory involving three α-particles have been undertaken. Unfortunately, there is a large degree of scatter in the reported rates at low temperatures, which vary 26 orders of magnitude. One of theoretical difficulties is the lack of formal scattering theory for three-charged particles.

To overcome the difficulty, we have developed a new theoretical method which we call the imaginary-time theory. Using the theory, we can calculate the reaction rates of radiative capture process without solving any scattering problem. Figure 4 shows the calculated reaction rate of triple-alpha process for temperatures of 0.01 to 1 GK. Our calculation supports the empirical rate adopted by NACRE, a standard compilation of astrophysical reaction rates, which assumes a sequential mechanism, first α–α resonance takes place to form ^{8}Be and then ^{8}Be – α collision takes place to produce ^{12}C.

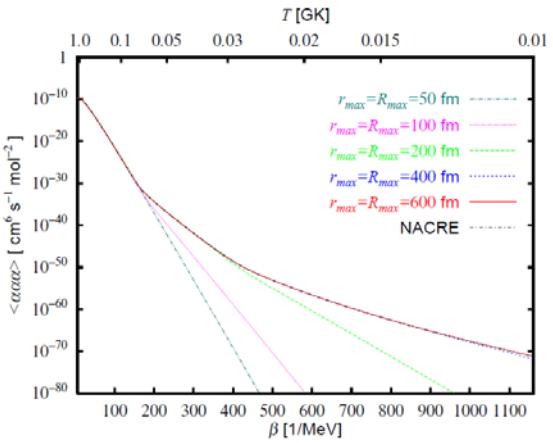

Fig. 4: Triple-alpha reaction rate calculated by the imaginary-time theory. A converged rate can be obtained if calculation is made in sufficiently large space. The empirical rate adopted in NACRE is also shown.

3.3 Collaboration

We have been holding a monthly forum on nuclear density functional theory by three institutes, RIKEN (Dr. Nakatsukasa's group), Niigata Univ. (Dr. Matsuo's group), and ours. Research collaborations on TDDFT have been maintained through the forum, mainly with RIKEN group.

We have several collaborations on TDDFT in the field of condensed matter physics. They are described in the section of Division of Quantum Condensed Matter Physics.

3.4 Future Plan

We plan to further extend our activities of DFT and TDDFT in nuclear physics. After April of 2014, Dr. Nakatsukasa will join our group and is expected to promote strongly the researches in this direction. There are several aspects which we think important for our future plan. We are expecting to extend our research with close relationship with experiments in RIKEN. We are also expecting to promote research collaborations on computational nuclear theories with foreign institutes.

3.5 Publications

3.5.1 Journal Papers

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3.5.2 Proceedings

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4 Division of Quantum Condensed Matter Physics

4.1 Research Activity

Reflecting diverse nature of the field of condensed matter physics, activities of our group extend in several directions. They are classified into three: light-matter interactions by X.-M. Tong, K. Yabana, and N. Maeshima, nano-materials by K. Shiraishi and S. Okada, and strongly correlated systems by H. Koizumi.

COMPUTATIONAL OPTICAL SCIENCES

We have been developing computational approaches and have investigated several aspects of light-matter interactions for atoms, molecules, and solids.

Tong studied on interactions of strong laser pulses with atoms and molecules, aiming to **understand** the mechanism of intense-laser-material interactions and search an effect way to **control** the dynamics in femto-second (10^{-15} second) or even in atto-second (10^{-18} second) time domains by a large scale numerical simulation. To reach the goals, we developed an effective numerical method to solve the time-dependent Schrödinger equation (TDSE) using a split-operator-method in energy representation. The method adapts to modern computer architectures using BLAS and LAPACK and transferred the code to HA-PACS, a super computer of a GPU cluster to speed up the research activities.

Yabana has developed a first-principles computational approach to describe electron dynamics in extended systems based on the time-dependent density functional theory. His group has successful to describe such basic phenomena as the optical breakdown of dielectrics under the irradiation of intense laser pulses, coherent phonon generation by ultrashort laser pulse, and so on. Recently he has developed a formalism and computational method for coupled dynamics of macroscopic electromagnetic fields and microscopic electron dynamics. His group is also active in nuclear physics: activities in that field is described in the section of Division of Astrophysics and Nuclear Physics.

Maeshima has performed numerical study of photoinduced effects on electronic states in condensed matters such as, organic materials, metal-oxides, and semiconductor superlattices. We mainly focus on (1) photoinduced phase transition (PIPT) of correlated electron systems including quasi-one-dimensional organic materials and three-dimensional vanadium perovskites and (2) exciton Fano resonance (EFR) in semiconductor superlattices controlled by CW laser.

COMPUTATIONAL NANO-SCIENCES

One of main achievements was a development of large-scale first-principles calculation using RSDFT program code with PACS-CS computer. In these calculations, Si nano-wires, Si-nano-particles, and SiN films in new generation memories have been performed. Moreover, our group started the collaborative research related to the astro-biology fields with Life Science Group and Astro-Physics Group.

Okada studied the fundamental properties of nanoscale materials and theoretically designed the novel nanostructures based on first-principles total-energy calculations. In particular, we focused on the electronic and geometric structures of hybrid materials consisting of nano-carbon materials, such as fullerenes, carbon nanotubes, and graphene, and foreign materials to investigate the possibility for fabricating these nano-carbon materials in future devices. Okada is conducting research projects supported from government: "Design of graphene-based devices by computational material sciences" (CREST-JST: Leader = S. Okada), "Study of the nano-scale interfaces between C_{60} and semiconductors" (Grant-in-aid MEXT, leader = S. Okada), and "Physical properties and material design of complex structures of carbon nanotubes" (Grant-in-aid, MEXT, leader = S. Okada).

STRONGLY-CORRELATED SYSTEMS

Koizumi has been working on elucidating the mechanism of the high temperature superconductivity in the cuprates.

Understanding the mechanism behind cuprate superconductivity is a very important topic in physics and materials science. It is believed to be a key to achieving room temperature superconductivity, a desired technology for sustainable, environmentally low impact human societies. We are constructing the theory that will lead to a full understanding of cuprate superconductivity.

Another topic is the theoretical study for the realization of the quantum computer using the cuprate. During the effort to elucidate the cuprate superconductivity, it was predicted that a novel loop current exits in the cuprate. This loop current is named, the "spin-vortex-induced loop current (SVILC)"' by us, and will be used as a new current element for nanotechnology. Since each SVILC has a freedom in the circulation direction, clockwise or counterclockwise, it can be used as a qubit in quantum computers. We are doing theoretical studies for the realization of the quantum computer using SVILCs.

4.2 Research Results

COMPUTATIONAL OPTICAL SCIENCES

Mechanism of atomic ionization in mid-infrared laser fields.

We have performed several researches to **understand** and **control** the dynamics in laser-material interactions. Here is an example. We investigated the mechanisms responsible for the fine structures in the photoelectron angular distributions from atoms subject to intense mid-IR laser fields by solving the TDSE

in the integral form. By restricting the ionization to a half-cycle of the laser field and then propagating the liberated electron wave packet during the laser pulse as shown in Fig. 1, we show conclusively that low energy/momenta structure in the photoelectron angular distribution originates from multiple scatterings of the tunnel-ionized electron with the ion. We also show that two conditions must be satisfied simultaneously in order to observe prominent low-energy features. First, multiple scattering of the tunnel-ionized electron wave packet is necessary. Second, tunnel ionization must dominate over multiphoton ionization.

We will develop a general method to solve the TDSE by using split-operator-method. The method mainly uses FFT, BLAS and LAPACK, which are common and efficient packages popularly used in modern computers. Therefore, the codes will be easily transferred to a super-computer of CPU, GPU or MIC system. Combining with the real time, real space density functional method, which was developed by other groups in the center, we will investigate the dynamics of a many-electron system in an ultrashort, intense laser field and search an effective way to control the quantum system in an ultrashort time scale.

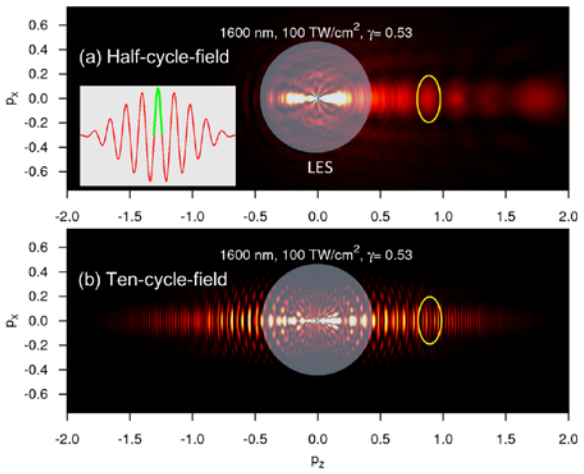

Fig. 1: Photoelectron momentum spectra of H atoms in a midIR field in laser field of (a) a half-cycle and (b) a ten-cycle pulse.

Electron dynamics in dielectrics induced by intense and ultrashort laser pulses

We have been developing a computational method to describe electron dynamics in molecules, clusters, and solids based on the time-dependent density functional theory (TDDFT). In last five years, we concentrated on developments of computational methods and applications for the electron dynamics in crystalline solids. Figure 2 shows electron density in bulk Si under irradiation of the strong laser pulses.

We applied the method to a few phenomena observed in interactions of strong laser pulses with dielectrics. When increasing the intensity of the laser pulse, the strong electric field excites electrons from valence to conduction bands and finally brings the system into a plasma phase, known as the optical breakdown. We numerically simulate the process of the optical breakdown by our first-principles calculation.

We also applied the method to a generation of coherent phonons. When the pulse duration of the laser pulse is shorter than the period of the phonon, a generation of the coherent phonon is widely observed. We have applied our method to Si and Sb, and investigated the microscopic mechanism of the generation of the coherent phonon.

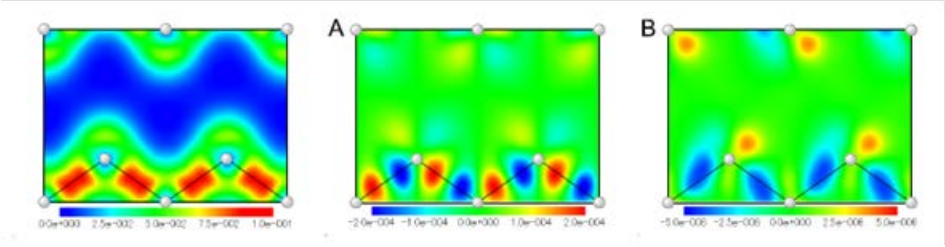

Fig. 2: Electron density distribution of bulk Si under irradiation of strong laser pulse. (Left) Ground state, (A) change of electron density from the ground state when a strong laser puslse is irradiating, and (B) change of electron density when the strong laser pulse ended.

Multi-scale simulation for strong electromagnetic fields in crystalline solids

Propagation of light pulse in extended materials is usually described by macroscopic Maxwell equation. However, for extremely strong electromagnetic fields, one cannot find a convenient form for the constitutive relation since the strong electromagnetic fields induce extremely nonlinear electron dynamics. We have developed a first-principles multiscale simulation method to describe interactions of strong laser pulses with crystalline solids. It solves the Maxwell equation for macroscopic electromagnetic fields and the time-dependent Kohn-Sham equation for microscopic electron dynamics simultaneously where the microscopic electron dynamics calculations substitute the macroscopic constitutive relation. We believe that this new simulation method is quite powerful for any phenomena which involve interactions of strong electromagnetic fields with materials of macroscopic size.

Photoinduced phase transition (PIPT)

We investigate photogenerated midgap states one-dimensional (1D) Peierls –Hubbard model, and demonstrate that there appear novel midgap peaks in optical response spectra of polarons and charged-solitons for large on-site Coulomb interaction U. The origins of these novel peaks are understood in terms of charge-transfer excitations within clusters for each states. These novel midgap states are experimentally observed in pump-probe spectroscopy of quasi one-dimensional (quasi-1D) dimerized Mott insulators, R -tetracyanoquinodimethane (R-TCNQ), where R=K or Rb.

Exciton Fano resonance (EFR)

We examine quantum control of excitonic Floquet states in semiconductor superlattices driven by an intense monochromatic laser. High-resolution optical absorption spectra, calculated using multichannel scattering theory with the R-matrix propagation method, clarified that the EFR structure is induced by the laser field. Each of the physical quantities related to this resonance—such as the spectral intensity, an asymmetry parameter (q-parameter), a resonance width, and so on, are controlled by the laser field.

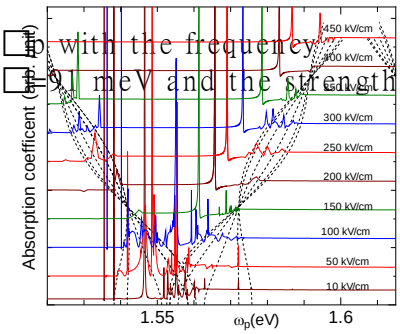

Fig. 3: Absorption spectra as a function of the frequency of the probe laser with the frequency of the driving laser 91 meV and the strength of the driving laser Fac = 50-450 (kV/cm). The dotted lines are quasienergies of Floquet states.

COMPUTATIONAL NANO-SCIENCES

Large-scale calculations of Si-nanowires

Large-scale calculations have been performed especially for Si-nanowires. Over 13000 atom first principles electronic structure calculations have been performed for the first time.

Further, guiding principles for next generation memories (MONOS-type memories) have been obtained by the above first principles calculations. As a result, new-type onboard memories have been developed by Renesas electronics (a Japanese electron device maker) based on our computational science studies. Nowadays, MONOS-type memories become important elements of Japanese and international automobiles.

Moreover, we have proposed a new concept that vacuum ultraviolet light played crucial roles for the homo-chirality in amino acid in bio-materials in early generation of the solar system.

Theoretical study on multiple exciton generation in nano-carbon materials

The multiple exciton generation (MEG) in single-walled carbon nanotubes (SWNTs) is theoretically investigated. We perform the calculation of the MEG rate by considering the direct photogeneration of multiple excitons. In particular, we only consider the generation of two-exciton states. A single photon does not excite two excitons since it is forbidden by the selection rule. However, it is possible to consider the situation where superposed states of multiexciton states are realized because the Coulomb interaction can resonantly couple among multiexciton states. This process was originally proposed for the MEG in nanocrystal. The direct photogeneration produces many excitons by a single photon absorption and thus it is the simultaneous process.

First-principles study on the interface between graphene insulating substrates

First-principles total energy calculations are performed to investigate the energetics and electronic structures of graphene adsorbed on both an oxygen-terminated SiO2 (0001) surface and a fully hydroxylated SiO2 (0001) surface. We find that there are several stable adsorption sites for graphene on both O-terminated and hydroxylated SiO2 surfaces. The binding energy in the most stable geometry is found to be 15

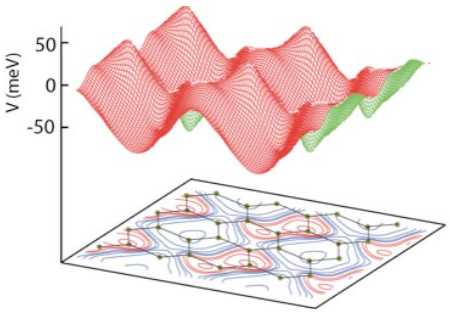

Fig. 4: Electrostatic potential of graphene adsorbed on SiO_2 surfaces.

meV per C atom, indicating a weak interaction between graphene and SiO2 (0001) surfaces. We also find that the graphene adsorbed on SiO2 is a semiconductor irrespective of the adsorption arrangement due to the variation of on-site energy induced by the SiO2 substrate.

STRONGLY-CORRELATED SYSTEMS

High temperature superconductivity in the cuprates:

We have performed the *ab initio* molecular orbital cluster calculation of the CuO_6 unit of the cuprate superconductor. We found that the hole-lattice interaction in the cuprate is very strong; thus, the doped holes become small polarons at low temperatures. We have calculated the spin-wave excitations for an extended Heisenberg model for electrons in the CuO_2 of the cuprate. From this model we have shown that the observed magnetic excitation spectra are explained due to the spin-wave excitation in the presence of spin-vortices with small polarons at their cores.

When spin-vortices are created by itinerant electrons, electrons in the self-consistent field move with twisting their spin directions. In this situation, a nontrivial imposing of the single-valuedness constraint of wave functions is necessary. We have developed a method to impose the constraint, and it has been shown that the spin-vortex induces a loop current, the spin-vortex-induced loop current (SVILC). Using an extended Hubbard model, we have shown that many of the experimental results in the pseudogap phase of the cuprate are explained by the existence of spin-vortices and SVILCs.

A notable point of SVILC is that it has the freedom of the flow direction, either clockwise or counterclockwise.

The SVILC persists as long as the spin-vortex that induces it persists. Since the spin-vortex is a topological object that cannot be destroyed easily, thus, the SVILC is fairly stable. Our result suggests that SVILCs are currents elements of the cuprate superconductivity, and a macroscopic supercurrent is generated as a collection of them. We have developed a method to calculate SVILCs from a microscopic model. With this method, we can routinely calculate electronic states with spin-vortices and SVILCs.

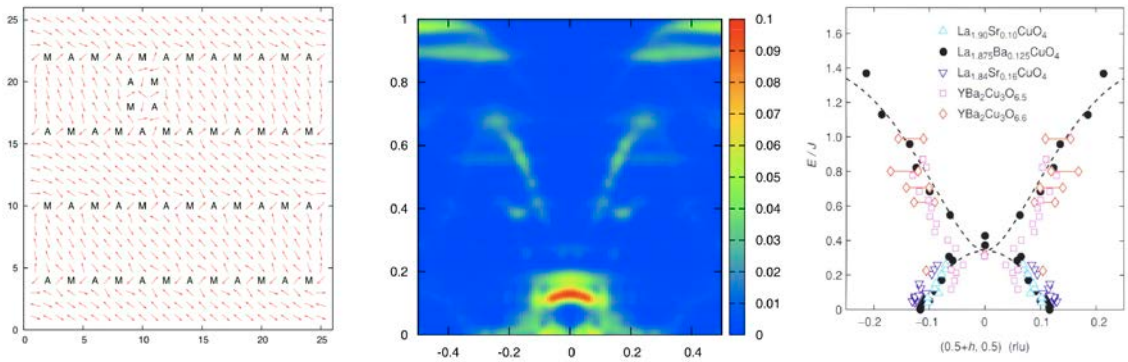

Fig. 5: Left: A spin configuration with spin-vortices embedded in an antiferromagnetic arrangement. Middle: Spin wave excitation spectrum calculated with the left spin configuration. Right Experimentally obtained magnetic excitation spectrum.

Realization of the quantum computer using the cuprate:

We found that SVILCs predicted to exist in the cuprate are suitable as qubits of quantum computers by the following reasons:

- The size of one loop current is a few nm^2; thus, it is easy to accommodate to a large number of qubits in a small space.
- Initialization is expected to be easy, as it can be done by applying strong external fields.
- Our calculations indicate that a gate operation of the order of picoseconds is possible. Therefore, if a decoherence time of 20 μs is achieved, the number of gate operations will be in the order of a million per second.
- The readout is also expected to be easy, since loop current patterns can be detected by feeding external currents.

4.3 Collaboration

Collaborations within Center:

In the development of the RSDFT (Real-Space Density Functional Theory) code, the performance was analyzed and optimizations were carried out with High Performance Computing Group. Moreover, we have started the collaborative research related to the astrobiology with Life Science Group and Astrophysics Group.

Domestic collaborations:

Tong has been collaborating with Prof. N. Nakamura's group of the University of Electro-Communications on investigating the Breit interaction in highly charged ions by comparing our theoretical simulation with their experiment.

Yabana has been collaborating with Prof. Nobusada of Institute of Molecular Sciences in developing large-scale computations based on TDDFT. He also collaborated with Otobe of JAEA, Iwata of Univ. of Tokyo.

Maeshima has collaborated with a condensed matter theory group of Institute of Molecular Science and with experimental study groups in the University of Tokyo and Tokyo Institute of Technology in the study of PIPT..

Koizumi collaborated with Miyaki and Makoshi of University of Hyogo for the ab initio molecular orbital cluster calculation of the CuO_6 unit of the cuprate superconductor. Koizumi is also in the collaboration with Tachiki of Tohoku University on the theory of the cuprate superconductivity.

International collaborations:

Tong has been developing international collaborations with several institutes worldwide:

- Vienna University of Technology, Prof. J. Burgdörfer's group (theory): on investigating the mechanisms of lower energy photon-electron structures of atoms in an intense middle infrared laser field and other dynamic processes of atoms, molecules in an intense laser field.

- University of Colorado Boulder, Profs. H. Kapteyn & M Murnane's group (experiment): on searching an effective way to control atomic, molecular dynamics using atto-second pulse with an infrared laser field.
- The University of Arizona, Prof. A. Sandhu's group (experiment): on the absolute timing of attosecond burst by comparing the measurements with our theoretical predictions.
- Griffith University, Centre for Quantum Dynamics: on calibrating the laser intensity by comparing our quantum simulation with high precision measurements.

Yabana has been continuing and starting collaborations with several groups worldwide.

- Prof. G.F. Bertsch of Univ. of Washington under a long-term collaboration on first-principles electron dynamics simulations.
- Prof. F. Krausz and Dr. V. Yakovlev of Max Planck Institute for Quantumoptics for attosecond electron dynamics in solids
- Prof. K. Varga of Vanderbilt University on electron dynamics simulation, supported by the program of Open Partnership Joint Projects of Japan Society for Promotion of Science.
- Mr. K.-M. Lee and other members of APRI, Korea, on electron dynamics simulation.
- Prof. J. Burgdörfer's group of Vienna Univ. of Tech. on electron dynamics simulation in solids, together with Tong.

4.4 Future Plan

In the field of computational optical sciences, we expect to develop our researches in several directions making real-time quantum dynamics calculations as a common and distinctive feature of our group. For atoms and molecules under intense and ultrashort laser pulses, computational approaches solving time-dependent Schrödinger equation will be further extended, developing computational codes using accelerators such as GPU and MIC. For many-electron dynamics in nanostructures and solids, researches based on time-dependent density functional theory will be further extended. Here a large scale computing using K-computer and next generation supercomputers will be considered. In correlated electron systems, we also expect to develop computational approaches solving time- dependent Schrödinger equation of correlated many-electron systems.

In the field of computational nano-sciences, we are at the stage of reconstruction because of movements of group members.

In the field of strongly correlated systems, we continue to develop researches to elucidate the mechanism of the high temperature superconductivity in the cuprates. We also continue theoretical research aiming at realizing the quantum computer using the cuprate.

4.5 Publications

4.5.1 Journal Papers

- X. M. Tong, P. Ranitovic, D. D. Hickstein, M. M. Murnane, H. C. Kapteyn, and N. Toshima, Enhanced multiple-scattering and intra-half-cycle interferences in the photoelectron angular distributions of atoms ionized in mid-infrared laser fields, Phys. Rev. A **88**, 013410_1-5 (2013)
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- S. A. Sato, K. Yabana, Y. Shinohara, T. Otobe, and G. F. Bertsch, Numerical pump-probe experiments of laser-excited silicon in nonequilibrium phase, submitted to Phys. Rev. B.
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- G. Wachter, C. Lemell, J. Burgdorfer, S.A. Sato, X.-M. Tong, and K. Yabana, Ab-initio simulation of optical-field induced currents in dielectrics, submitted to Phys. Rev. Lett.
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5 Division of Life Sciences: *Biological Function and Information Group*

5.1 Research Activity

All living organisms are composed up of simple molecules and components such as water, proteins, sugar, RNA and DNA, which make the highly sophisticated functions including self-replication and thinking. In biology, there still remain numerous questions regarding the structures and mechanisms, and many important biological phenomena are not clarified yet. We are interested to elucidate the efficient and complicated biological mechanisms through long time scale, longer than microsecond, and with cooperative motions for large numbers of atoms. Modern experimental methods have remarkably developed biological sciences in the 21st century. We are expecting that theoretical approaches will play an important role to derive some novel biological findings in the near future, because remarkably developments in computer technologies made *in silico* approaches more easily applicable.

For quantitative simulations, huge computational resources are recurred for most biological systems. Therefore, we have investigated to utilize supercomputers and have been performed realistic computational simulations. Our research areas are focused on the elucidation of reaction mechanisms and physical properties of biomolecules based on molecular mechanics (MM) and quantum mechanics (QM) methodologies. We have elucidated unresolved characters and chemical mechanisms of biological systems with collaborating with experts in high performance computer systems, related-fields and experimental researchers. We are also interested in applying our results to application fields: chemical industry, drug design and medicals.

5.2 Research Results

1) Quantum mechanical/molecular mechanical(QM/MM) studies on enzymatic reactions

The combination approach of the quantum mechanics/molecular mechanics (QM/MM) is one of the important approaches to investigate the detailed electronic and atomic level mechanisms in large biological systems. In the practical usages of

QM and MM, it is still necessary to speedup the execution. Especially in order to utilize modern supercomputers, more improvements of the parallelization efficiencies are desired. We have performed some investigations to improve the efficiencies both for QM and MM and 2-3 times speedups can be obtained by using the GPU accelerations. Details for our developments are described in the next section.

Efficient parallelization performances of QM/MM were achieved by NWChem program package, we have studied on the enzymatic reaction mechanisms of (1) Nitric Oxide Reductase, (2) DNA topoisomerase, (3) oxygen-evolving complex in photosystem II, (4) Threonine synthase, and (5) Nitrile Hydratase. Their atomic level structures are all solved very recently and the reaction mechanisms of these enzymes have attracted much attention.

Nitric Oxide Reductase (NOR) is a transmembrane protein which catalyzes a reduction of nitric oxide (NO) to nitrous oxide (N_2O). NOR catalytic reaction contains two important chemical reactions of N-N bond formation and N-O bond cleavage. The NOR catalytic process is critical for the denitrification process in the anaerobic respiration. In 2010, first x-ray structure of NOR was reported at the atomic resolution (2.7 Å). It was revealed that the catalytic site is constituted by a non-heme iron FeB and a heme b3, but the reaction mechanism of NOR has not been fully elucidated. We have investigated the NOR reaction mechanism by using QM/MM method. Intermediate states and the reaction energy profile were determined and the catalytic reaction mechanism was clarified. We showed that the N-N bond formation has no activation barrier, but N-O bond cleavage exhibits a 20.9 $kcalmol^{-1}$ activation barrier. The N-O bond cleavage occurs via a characteristic hyponitrous intermediate (FeB(II; s = 4/2) / N_2O_2(-1; s = 1/2) / Feb3(III; s = –1/2)) with bidentate coordination between Glu211 and a non-heme iron atom.

DNA topoisomerase (topo) is a DNA-binding enzyme which catalyzes interconversions of the different topological forms of DNA. This enzyme forms a covalent intermediate in which catalytic tyrosine residue is covalently bonded to the DNA backbone phosphate, after and before cleavage and religation reactions. Recently, one crystal structure of the covalent intermediate of yeast topo II in complexed with single DNA was solved at the 3.0Å resolution. Using the x-ray structure as the initial coordinate, we performed molecular dynamics simulations and QM/MM calculations. We proposed a new reaction mechanism, named Substrate Mediated Proton Relay (SMPR) mechanism, for the DNA religation reaction in topo II.

Oxygen-evolving complex (OEC) is a key reaction center in photosystem II (PSII) which catalyzes "$2H_2O$ –> $4H^+ + 4e^- + O_2$" reaction through five redox states (Si, i = 0-4). J.-R. Shen and co-workers have determined a high-resolution PSII x-ray structure and it was found that OEC is involved in many hydrogen-bonds (H-bonds) with water molecules and neighboring amino acid residues, however, it is still matter of debates for the reaction mechanisms. We investigated the OEC electronic structures by using a high level QM/MM approach. We adopted a large QM region including second coordination amino acids and waters (Total 380 atoms, 3000 basis functions) and investigated possible protonation states and electronic structures. OEC core structures and calculated quantum ground state are in good agreements with experimental results.

Threonine synthase (TS) catalyzes the last step of L-Thr biosynthesis and its reaction is the most complex among the PLP enzymes. To elucidate the detailed mechanism, we performed comparative QM/MM calculations with an exhaustive search for the reaction pathways in the reaction-specificity-determining-process. Satisfactory agreements with the experimental data were obtained. Contrary to the earlier proposal, the base that abstracts a proton from the attacking water was the Lys61 amino group rather than the phosphate ion. We also determined that phosphate ion forms a stable H-bond with the L-Thr moiety, which is critical for the reaction specificity. Additionally, a new mechanism was proposed for the transaldimination process.

Nitrile hydratase (NHase) catalyses hydration of nitrile to the corresponding amide and has been used as a biocatalyst in chemical industry. However, the detailed catalytic mechanism of this enzyme has not been elucidated. We analyzed several proposed reaction pathways of NHase comprising Fe(III) at the active site by using QM/MM method. First we analyze three reaction mechanisms which have been suggested in previous theoretical studies using active-site models (Hopmann et al., 2008) to reveal the effects of surrounding protein environment, especially Tyr72 amino group which is essential for the activity of NHase, on the reaction process.

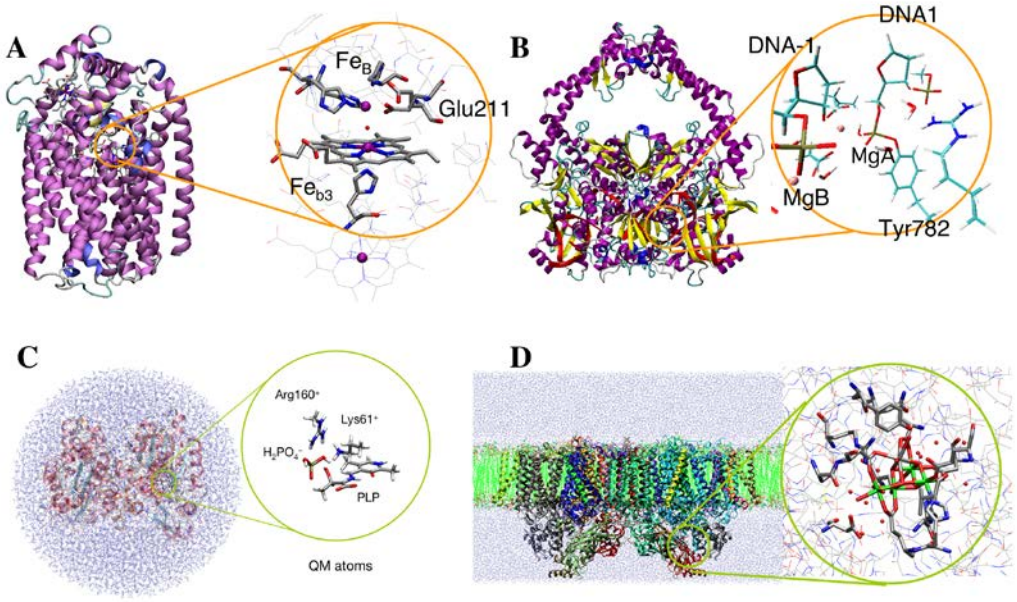

Figure 1. Systems used for QM/MM calculations. QM regions are enlarged. (A) NOR, (B) topo, (C) TS, and (D) OEC-PSII.

2) GPU acceralations for MD and QM calculations

In the bioscience, computational simulations are increasingly important for the detailed analyses. Molecular dynamics method is one of the typical theoretical methods which allow us to elucidate the dynamical mechanism in biomolecular functions, however, it still requires heavy computational costs for the realistic

models and there are still limitations for the total simulation time. For example, in traditional supercomputers such as PACS-CS, nanoseconds are the simulation-limit for typical protein systems composed of 50,000 atoms. For biological functions, microsecond simulations are required to investigate the large-scale conformational changes. Thus, utilization of GPUs to speedup MD simulations is very attractive. Currently, major MD program packages such as Amber, Gromacs, and NAMD, supports GPU accelerations for the non-bonded interactions. We found that replica exchange MDs shows 2.6-3.0 times accelerations by the hybrid usage of GPUs and CPUs in HA-PACS.

The high-speed execution of MD was utilized for the conformational sampling of vitamin D receptor binding domain bound to the natural ligand. Although nuclear receptors (NRs) are important drug targets, it has been unclear for the actual solution conformation, i.e., it has been suggest there exists distinct receptor conformations from crystal structures. We could revealed the "uncharacterized" conformations and an alternative ligand binding pocket, which found out to be an inactive pocket of the natural agonist, as well as the conformation dynamics including helix 12, an activation switch, and the ligand. The calculated major conformation was in good agreements with crystallographic active conformations, and more interestingly, minor conformations exist with very small excitation energies. In the minor conformation, helix 12 adopts disordered conformations, and one conformation is unexpectedly similar to a crystallographic inactive conformation of glucocorticoid nuclear receptor. Expected trypsin digestion site in the minor conformation is consistent with expreiments. We also revealed relations between helix 12 conformations and the ligand bonding modes. In the active pocket, helix 12 maintained the crystallographic/agonistic conformation, on the other hand, in the inactive pocket, helix 12 exhibited large conformational changes. The natural agonist binding mode in the inactive pocket was unexpectedly very similar to that of an antagonist in a VDR crystal structure. This indicates that the antagonist mimics the natural agonist binding mode in the inactive pocket. We examined roles of ligand binding modes in the ligand-specific activities in combinations with experimental results, and we suggested a mechanism that ligands, including antagonits and super agonists, may modulate the VDR activity by selecting the pre-existing active and/or inactive side-chain pockets. This study is important for elucidating the natural agonist bonding modes of NR both in the active and inactive pockets. This study also provides valuable insights for 1) a characterization of the inactive pocket, 2) understanding the effects of physicochemical properties of ligands on NR activities, and 3) a novel strategy of VDR-targeted drug design.

In the QM methodologies, Hartree-Fock (HF) calculation is basic and common process. Thus GPU accelerated Fock matrix preparation is most important. We developed a GPU acceralated Fock matrix preparation routine in OpenFMO program with CUDA. Atomic operation less algorithm was proposed and implemented for the Fock matrix preparation. Applying several speedup techniques, such as screening, dynamic load-balancing, and sorting basis functions, our program showed 13 to 22 times faster timing results against a CPU core. And also, the program has been parallelized with MPI to utilize multiple GPU cards.

Parallelization benchmark was examined and reveals that 16 GPUs execution was 40 times faster than 4 CPU core execution.

3) Astrobiology

The naturally-occurring amino acids in terrestrial life are all the levorotatory (L-) form, none of the D-form. The origin for its selectivity still remains a big mystery. One of the possible scenarios is that the chiral induction of amino acids is formed on meteorites in the early solar systems [3]. In order to validate the hypothesis, we have investigated the mechanisms of photo-induced chirality formation by using the TDDFT method. Circular dichroism and UV- absorbance spectrum were calculated for amino acids and plausible chiral induction mechanisms were discussed

5.3 Collaboration

1) Computational biology researches are performed with fruitful discussions with Prof. Megumi Kayanuma, Prof. Katsumasa Kamiya, Prof. Kenji Shiraishi, Prof Kazutomo Ishida, and Prof. Yasutaka Shigeta.
2) Developments of GPU codes of HF calculations have been mainly performed by Hiroaki Umeda with collaborations of Prof. Taisuke Boku and Prof. Toshihiro Hanawa in the High Performance Computing System Group.
3) Astrobiology studies has been performed with collaborations with Porf. Masayuki Umemura, Prof. Kenji Shiraishi, Prof. Kazuhiro Yabana and Prof. Megumi Kayanuma.

5.4 Future Plan

In living organism, a series of chemical reactions, such as synthetic, degradation, redox reactions, driven by enzymes undergoes to maintain their life. For understanding these chemical reactions by the enzymes, it is dispensable to know their geometric and electronic structures of active sites and their change upon the reactions. One of the most significant problems in the biomaterial science is to combine the information from conventional biochemical and molecular biological experiments with those from the theoretical calculations in order to understand and take advantage of their function in vivo. To investigate the enzymatic reactions at the atomic level, the first-principles calculations are one of the powerful methods in spite of the limitation of the size that the method can handle with. To tackle with the chemical reactions of the large-scale enzymes with complicated electronic structures such as cytochrome *c* oxidase and photosystems II, which are of great importance in the biology, we would like to develop multiscale modeling methods especially for the bio-systems. In particular, we have plans to code and tune following methods:

(1) Fragment molecular orbital methods.

(2) Car-Parrinello molecular dynamics methods based on the real space density functional theory.
(3) QM/MM molecular dynamics simulation methods.
(4) Classical molecular dynamics simulation methods.
(5) Coase-grained molecular dynamics simulation methods.

(1), (2), and (3) are the first-principle-based method so that the chemical reaction analyses are performed with them. On the other hand, (4) and (5) are force-field-based method that can be used to investigate the large amplitude motions of proteins such as protein foldings and domain motions. The latter can be applied to investigate ligand-protein binding and protein-protein binding for the drug discovery. These codes will be implemented and tuned toward the exa-flops computing architecture.

In order to extract the biologically relevant event, we also develop the conformational search methods such as metadynamics, parallel cascade molecular dynamics (PaCS MD), and so on. With these method, we investigate aggregation of proteins that causes diseases known as amyloidosis including Altzheimer's, Pakinson's and prion diseases.

5.5 Publications

5.5.1 Journal Papers

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6 Division of Life Sciences: *Molecular Evolution Group*

6.1 Research Activity

Molecular Evolution Group in Division of Life Sciences has tackled various unsolved problems in evolutionary biology. In particular, we are interested in the evolutionary process which shaped extant molecular mechanisms and genomes in modern eukaryotic cells. During the period from 2008 to 2013, the following topics were intensively investigated.

Global eukaryotic phylogeny

We have no concrete vision regarding the relationship amongst major eukaryotic lineages, which were separated from one another in early eukaryotic evolution, as (i) phylogenetic 'signal' in the sequence data analyzed is insufficient, and (ii) the sequence data are available from only restricted members of eukaryotes. To overcome the two problems, we surveyed and isolated previously unstudied eukaryotes in natural environments, and generated large-scale sequence data from the novel species. We believe that phylogenetic studies analyzing large-scale sequence data ('phylogenomic' data) with an appropriate species diversity advance our understanding of eukaryotic evolution.

This research topic was mainly supported by a grant-in-aid for scientific research B (No. 21370031; awarded to Inagaki for 2009-2012) and a grant-in-aid for challenging exploratory research (No. 21370031; awarded to Inagaki for 2010-2011) from the Japan Society for Promotion of Sciences (JSPS).

Evolution of mitochondria

Diverse eukaryotes possess respiration organelles, mitochondria, which were derived from a single endosymbiosis of an α-proteobacterium. As the first mitochondrion was most likely established in the last common ancestor of eukaryotes, this endosymbiosis should have possessed a huge impact on early eukaryotic cell and genome evolutions. During 2008-2013, we focused on the mitochondrial evolution in the eukaryotes thriving in microaerophilic/anaerobic environments.

This research topic was mainly supported by a grant-in-aid for scientific research B (No. 23405013; awarded to Hashimoto for 2011-2013) from JSPS and a grant-in-aid

for scientific research on innovative areas (No. 23117005; awarded to Hashimoto for 2011-2015) from the Ministry of Education, Culture, Sports, Science and Technology (MEXT) in Japan.

Evolution of plastids

Plastids in photosynthetic eukaryotes were originated from a single endosymbiotic cyanobacterium in the common ancestor of glaucophytes, red algae, and green plants (green algae plus land plants). In the latter evolution, plastids further spread into multiple eukaryotic lineages through multiple endosymbioses of photosynthetic eukaryotes in distantly related heterotrophic eukaryotes. During 2008-2013, we investigated mainly the origin and evolution of the green-colored plastid in a dinoflagellate *Lepidodinium chlorophorum*.

Evolution of bacterial endosymbionts in diverse eukaryotic cells

The evolutionary processes which transformed an α-proteobacterium into the ancestral mitochondrion, and a cyanobacterium into the ancestral plastid are difficult to retrace, as the key information to model these ancient events has already lost in the latter evolution. To overcome the difficulty in studying mitochondrial and plastidal endosymbioses, we started investigating cyanobacterial endosymbionts, which were highly integrated into host (eukaryotic) cells, in rhopalodiacean diatoms and a testate amoeba *Paulinella chromatophora*. As the two systems of our interest are evolutionarily 'younger' than mitochondria or plastids, the careful investigations on these organisms likely provide us valuable clues to reconstruct the process which established mitochondria and plastids.

This research topic was mainly supported by a grant-in-aid for scientific research on innovative areas (No. 23117006; awarded to Inagaki for 2011-2015) from MEXT.

Evolution of translation elongation factors in eukaryotes

Elongation factor-1α (EF-1α) and elongation factor-like (EFL) proteins are functionally homologous to one another, and are core components of the eukaryotic translation machinery. The patchy distribution of the two elongation factor types across global eukaryotic phylogeny is suggestive of a 'differential loss' hypothesis that assumes that EF-1α and EFL were present in the most recent common ancestor of eukaryotes followed by independent differential losses of one of the two factors in the descendant lineages. During 2008-2013, we surveyed EF-1α/EFL genes in diverse eukaryotes to deduce the precise evolution of the two translation factors.

Methodological studies in molecular phylogeny

By taking advantage of our access to the supercomputer T2K Tsukuba System, we carried out phylogenetic studies considering simulation sequence data, which required large computational power. These studied were conducted under the "Interdisciplinary Computational Science Program" in Center for Computational Sciences, University of Tsukuba.

6.2 Research Results

One of our long-term research interests is accurate reconstruction of global eukaryotic phylogeny. In the above framework, we mainly focused on novel microbial eukaryotes mentioned below, *Palpitomonas bilix*, *Tsukubamonas globosa*, and *Carpediemonas*-like organisms in 2008-2013.

6.2.1 *Palpitomonas bilix*

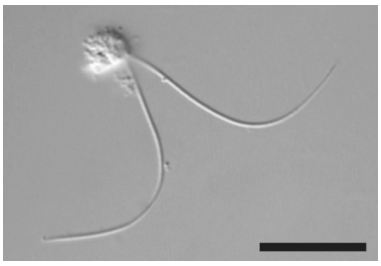

Figure 1. *Palpitomonas bilix*. Scale bar = 10 μm. This image was a part of Yabuki et al. 2010 **Protist** 616:523-538.

We investigated a novel free-living heterotrophic flagellate *Palpitomonas bilix*, which was a free-living heterotrophic flagellate isolated form the sea water collected in Palau, 2006. This flagellate is 3-8 μm in size, and possesses two subequal flagella, approximately 20 μm long (Figure 1). Electron microscopical observations revealed that the flagellar apparatus of *P. bilix* resembles that of members of the green algal class, Charophyceae, while the mastigonemes of the *P. bilix* flagellum share some characteristics with those found in cryptophytes and telonemids. In order to better understand the phylogenetic position of *P. bilix*, we sequenced six commonly used phylogenetic marker genes encoding the small and large subunits of ribosomal RNA, α-tubulin, ß-tubulin, 90 kDa heat shock protein, and translation elongation factor 2. Depending on the genes analyzed, *P. bilix* shows a generally weak phylogenetic affinity to either the newly erected Hacrobia, which includes cryptophytes and haptophytes, or to Archaeplastida. Since either morphological observation or 6-gene phylogenetic analyses identified no clear close relative of *P. bilix*, this novel biflagellate was classified into a new genus *Palpitomonas* with the higher-level classification being unclear, suggesting the possibility that *P. bilix* might provide key information at the early stage of eukaryotic cell evolution. The results describe above were published in Yabuki et al. (2010 **Protist** 210:523-538).

To further pursue the phylogenetic position of *P. bilix*, we here conducted transcriptomic analyses on *P. bilix* by using 454 pyro-sequencing and obtained 104,136 reads, which were assembled into 8,586 contigs. We generated a 'phylogenomic' alignment, which contains 157 genes (41,372 amino acid positions) in phylogenetically diverse 64 eukaryotes including *P. bilix*, and subjected to the maximum-likelihood and Bayesian phylogenetic methods. Our '157-gene' analyses successfully clarified the phylogenetic position of *P. bilix* in the tree of eukaryotes: *P. bilix* branched at the base of the assemblage of Cryptophyceae (cryptophytes), Goniomonadea (goniomonads), and Leucocrypta (kathablepharids) that are the members of the phylum Cryptista with high statistical support (Figure 2). Thus we conclude that *P. bilix* is an early-branching member of Cryptista, and is significant to investigate the plastid evolution in this protist assemblage. The manuscript discussing the position of *P. bilix* and the morphological evolution of members of Cryptista is currently under revision to be published in **Scientific Reports**.

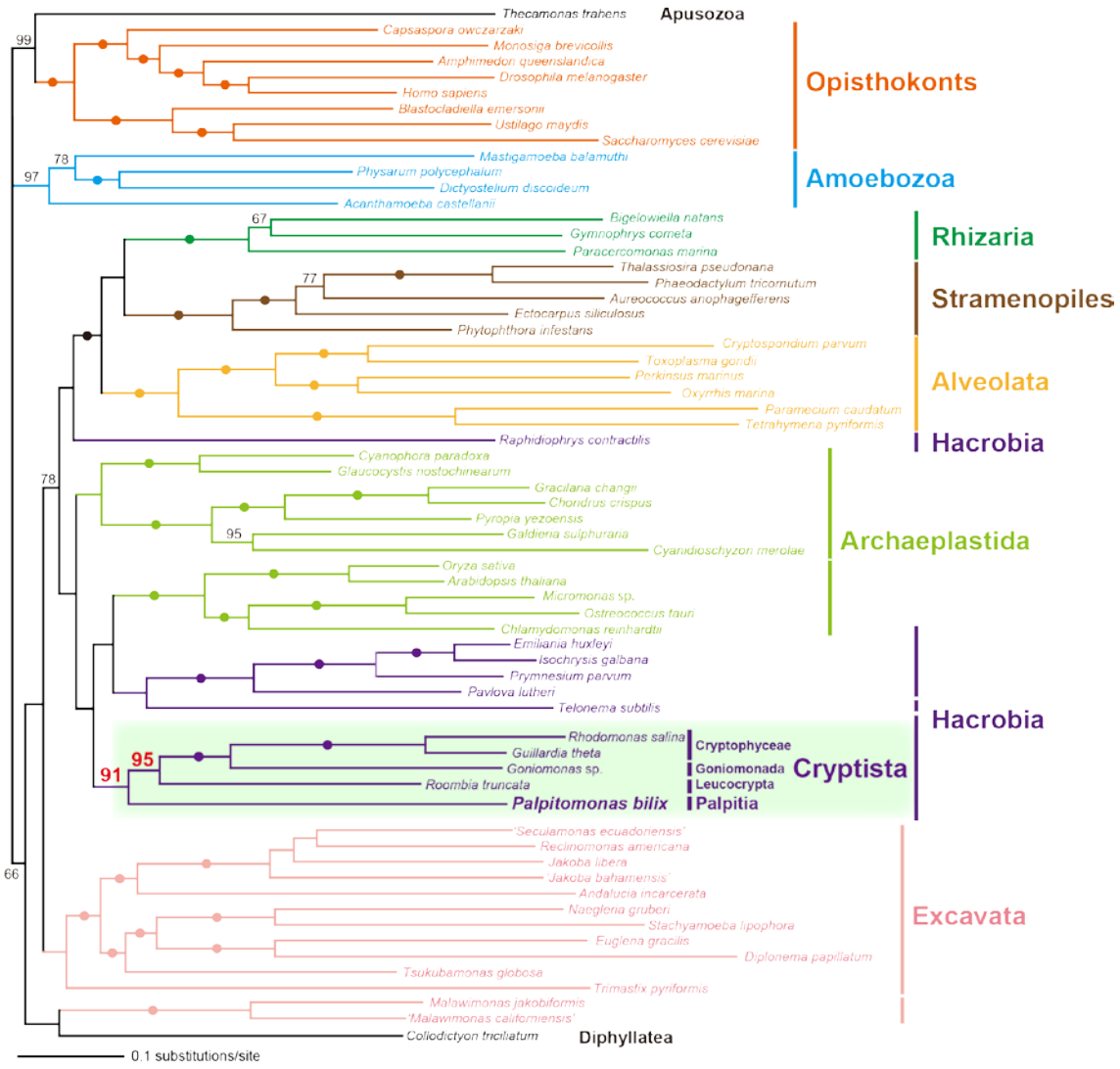

Figure 2. Phylogenetic position of *Palpitomonas bilix* inferred from the maximum-likelihood (ML) phylogenomic analysis. Values at nodes represent ML bootstrap percentage values (MLBPs). Only MLBPs ≥60 % are shown in this figure. Dots correspond to MLBP of 100%.

6.2.2 *Tsukubamonas globosa*

A free-living heterotrophic flagellate, *Tsukubamonas globosa* (Figure 3), was isolated from a pond in the University of Tsukuba, Japan. Under light microscopy, *T. globosa* is a spherical cell, and always swims with rotating motion. Electron microscopic observations revealed that *T. globosa* possessed a ventral feeding groove, which is one of the hallmark characteristics of the supergroup Excavata. The position of *T. globosa* was unresolved in the small subunit ribosomal RNA phylogeny. On the other hand, a multigene phylogeny using α-tubulin, β-tubulin, Actin, heat shock protein 90, and translation elongation factor 2 robustly united *T. globosa* with members of Discoba composed of Jakoba, Euglenozoa, and Heterolobosea, although the precise position of *T. globosa* in this clade remained unresolved. The detailed morphological comparisons elucidated that *T. globosa*

possessed a novel set of morphological features, and could not be classified into any taxa in the Discoba clade. The results describe above were published in Yabuki et al. (2011 **Journal of Eukaryotic Microbiology** 58:319-331).

Figure 3. *Tsukubamonas globosa*. This image was provided by N. Yubuki.

Jakobida is an intriguing protist group to understand the early eukaryotic evolution, since members of this group are known to possess the most gene-rich mitochondrial (mt) genomes known out of all eukaryotes. The most gene-rich mt genome determined so far is of the jakobid *Andalucia godoyi* carrying 100 functionally assignable genes (66 and 34 genes encoding proteins and structural RNAs, respectively; Burger et al. 2013 **Genome Biology and Evolution** 5:418-38). Other jakobids also possess gene-rich mt genomes encoding 91-97 functionally assignable genes (Burger et al. 2013). The gene-rich ancestral (i.e. bacteria-like) nature of jakobid mt genomes has been suggested to support an early-branching position of jakobids amongst eukaryotes (Lang et al. 1997 **Nature** 387:493-497). More recently, the mt genomes of diverse jakobids has been intensively sequenced to elucidate the evolutionary change in mt genomes within the jakobid lineage (Burger et al. 2013). For other lineages in the Discoba clade, complete mt genome sequences are available for two closely related species in Heterolobosea (*Naegleria gruberi* and *Naegleria fowleri*), and several species in Euglenozoa (kinetoplastids; e.g., *Trypanosoma cruzi*). However, prior to our study, no mt genome data was available for *T. globosa*, which represents the novel lineage in the Discoba clade.

In the second part of our study on *T. globosa*, we examined the detailed phylogenetic position of *T. globosa* in the Discoba clade, and determined the mt genome sequence completely. To elucidate the position of *T. globosa* in the Discoba clade, we took a 'phylogenomic' approach based on the transcriptomic data generated by using 454 pyro-sequencing (236,871 reads), which were subsequently assembled into 12,694 contigs. We prepared and analyzed a 'phylogenomic' alignment comprising 157 genes sampled from phylogenetically diverse eukaryotes including *T. globosa* (72 taxa with 41,372 amino acid positions). As expected from the initial study of *T. globosa*, our phylogenomic analyses with the maximum-likelihood method clearly indicated that (i) *T. globosa* was not nested within any of the previously known discoba lineages (i.e. Jakobida, Euglenozoa, and Heterolobosea), and (ii) branched at the base of the subclade of euglenozoans and heteroloboseans (so-called discicristates) with high statistical supports (Figure 4). These results suggest that *T. globosa* represents a genuinely novel lineage in the Discoba clade.

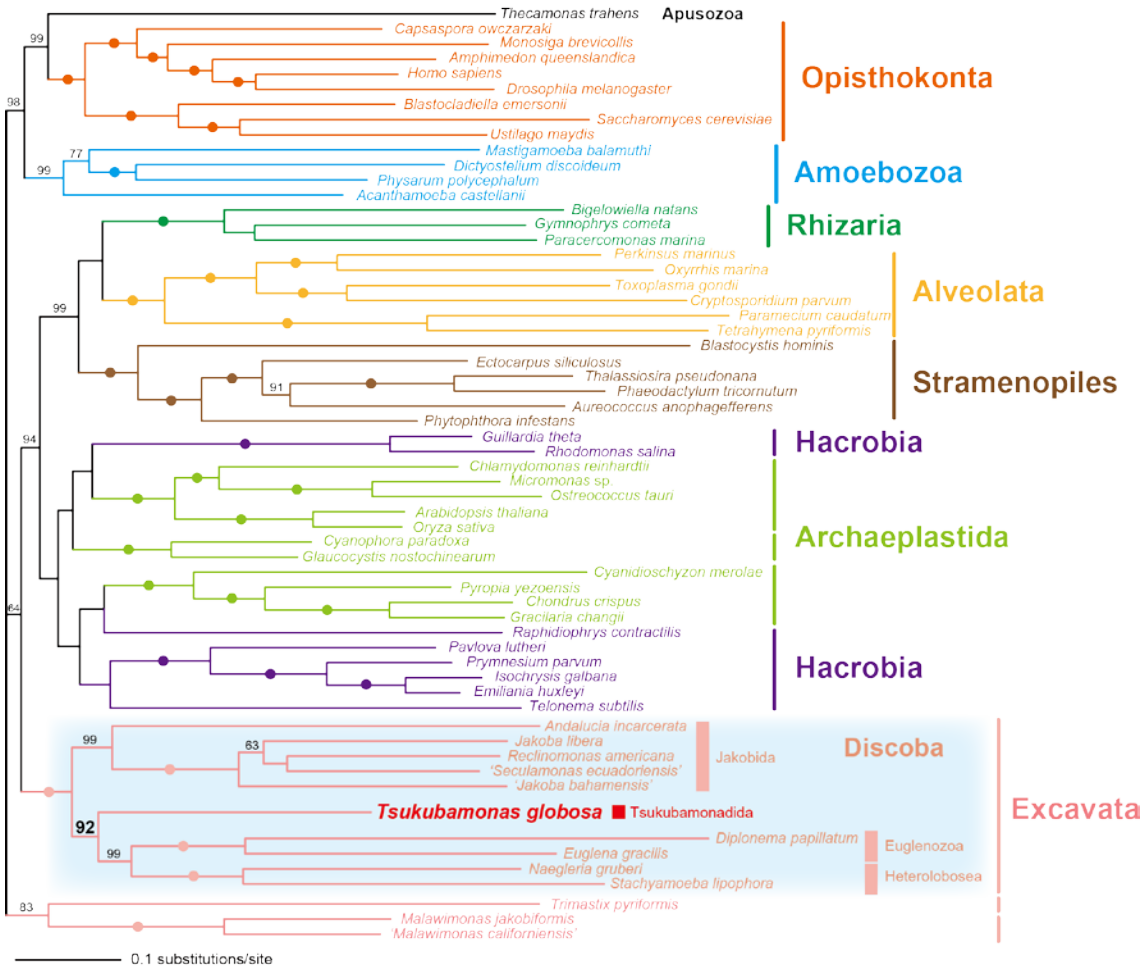

Figure 4. Phylogenetic position of *Tsukubamonas globosa* inferred from the maximum-likelihood (ML) phylogenomic analysis. Values at nodes represent ML bootstrap values (MLBPs). Only MLBPs ≥60 % are shown in this figure. Dots correspond to MLBP of 100%.

We succeeded in sequencing the mt genome of *T. globosa* by combining a whole-genome-amplification technique and 454 pyro-sequencing. *T. globosa* mt genome can be mapped as a circular molecule with 48,643 bp in length, containing three ribosomal RNA genes, 26 transfer RNA (tRNA) genes, and 52 open reading frames (ORFs) of which 41 are identifiable by sequence similarity to orthologues. The complete mt genome data from representative diacobids including *T. globosa*, together with their phylogenetic relationship, revealed that parallel gene loss events shaped the modern discobid mt genomes.

The phylogenetic position of *T. globosa* inferred from the phylogenomic analyses described above, and its complete mt genome data were accepted to be published in **Genome Biology and Evolution**.

6.2.3 *Carpediemonas*-like organisms (CLOs)

Diplomonads, retortamonads, and "*Carpediemonas*-like" organisms (CLOs; Figures 5A-P) are a monophyletic protist group (so-called Fornicata) that are microaerophilic/anaerobic and lack typical mitochondria. Most diplomonads and

retortamonads are parasites, and the pathogen *Giardia intestinalis* is known to possess reduced mitochondrion-related organelles (MROs) that do not synthesize ATP. By contrast, free-living CLOs have larger organelles that superficially resemble some hydrogenosomes, organelles that in other protists are known to synthesize ATP anaerobically. This group represents an excellent system for studying the evolution of parasitism and anaerobic, mitochondrion-related organelles. Understanding these evolutionary transitions requires a well-resolved phylogeny of diplomonads, retortamonads and CLOs. Unfortunately, the deep relationships amongst these taxa were unresolved due to limited data for almost all of the CLO lineages. To address this, we assembled a dataset of up to six genes sampled from representatives from all six CLO lineages. The phylogenetic analyses of the six genes (Figure 5Q) place CLOs as well as the retortamonad *Chilomastix* as a paraphyletic basal assemblage to the lineage comprising diplomonads and the retortamonad *Retortamonas*. In particular, *Dysnectes brevis* was demonstrated with strong support to be the closest relative of the diplomonads + *Retortamonas* clade. The results described above were published in two articles (Kolisko et al. 2010 **Environmental Microbiology** 12:2700-2710; Takishita et al. 2012 **Protist** 163:344-355).

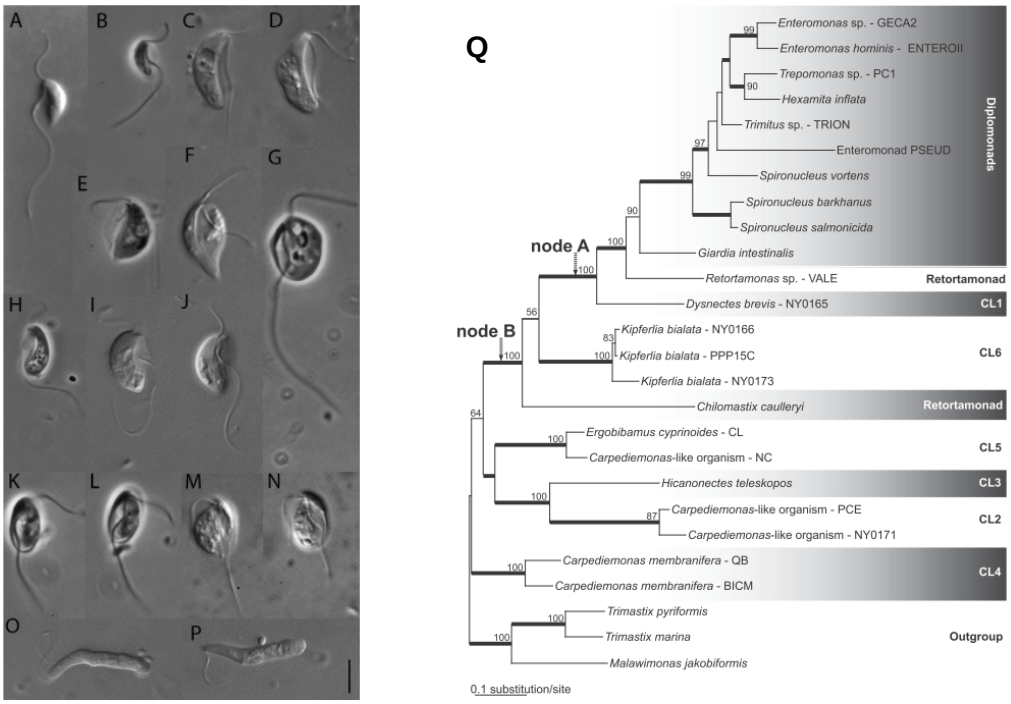

Figure 5. Diversity and phylogenetic relationship of *Caperiemonas*-like organsims (CLOs). **A-B** *Carpediemonas membranifera*, **C-D** *Kipferlia bialata*, **E** *Dysnectes brevis*, **F** *Dysnectes* sp., **G** *Hicanonectes teleskopos*, **H** strain CL, **I-J** strain NC, **K-L** strain PCE, **M-N** strain NY0171, **O-P** strain PCS. Scale bar is 5 mm for all figures. **Q** Maximum-likelihood analysis of members of Fornicata based on the six-gene dataset. Only maximum-likelihood bootstrap values ≥50% are shown. These figures were published as parts of Kolisko et al. (2010) and Takishita et al. (2012).

The Fornicata phylogeny based on the six-gene alignment described above unfortunately failed to provide the robust picture regarding the relationship amongst major CLO lineages, which correspond the basal branching order in the Fornicata clade. To address this issue in the Fornicata phylogeny, we were in collaboration with the groups in Dalhousie University (Halifax, Canada) led by

Drs. Andrew J. Roger and Alastair G. B. Simpson, to generate the transcriptomic data from 9 diverse CLO strains and two diplomonads. We particularly contributed in generating the illumine RNA-seq data from two CLO strains (*D. brevis*, strain NY0171) and a diplomonad *Trepomonas* sp. (approximately 240-290 million reads for each sample). These massive sequence data enabled us to assemble a 'phylogenomic' alignment comprising 163 genes sampled from 12 members of Fornicata, which included CLO strains representing five major subgroups, and six members of Preaxostyla or Parabasalia as the outgroup (39,089 amino acid positions in total). Significantly the 163-gene analysis resolved the backbone of the Fornicata clade with almost full support values. We are currently investigating the evolution of metabolic pathway in mitochondria by mapping the metabolic pathways in MRO in the five CLO strains and the diplomonad *G. intestinalis*, which were also deduced from their transcriptomic data. We are now preparing the manuscript on the phylogenomic analyses described above.

As described in the previous sections, we need large-scale sequence data to elucidate the evolutionary relationship amongst major lineages in eukaryotes. However, most of the extant computer programs for molecular phylogeny have not been developed for analyzing large-scale sequence data originally. At the same time, our knowledge regarding large-scale phylogenetic analyses has yet to be accumulated to date. Thus, we started two projects described below.

6.2.4 Methodologial studies for phylogenetic analyses of nucleotide sequence data which bear across-tree base composition variation

In phylogenetic analyses of nucleotide sequences, 'homogeneous' substitution models, which assume the stationarity of base composition across a tree, are widely used, albeit individual sequences may bear distinctive base frequencies. In the worst-case scenario, a homogeneous model-based analysis can yield an artifactual union of two distantly related sequences that achieved similar base frequencies in parallel. Such potential difficulty can be countered by two approaches, 'RY-coding' and 'non-homogeneous' models. The former approach converts four bases into purine and pyrimidine to normalize base frequencies across a tree, while the heterogeneity in base frequency is explicitly incorporated in the latter approach. The two approaches have been applied to real-world sequence data; however, their basic properties have not been fully examined by pioneering simulation studies. Here, we assessed the performances of the maximum-likelihood analyses incorporating RY-coding and a non-homogeneous model (RY-coding and non-homogeneous analyses) on simulated data with parallel convergence to similar base composition. Both RY-coding and non-homogeneous analyses showed superior performances compared with homogeneous model-based analyses. Curiously, the performance of RY-coding analysis appeared to be significantly affected by a setting of the substitution process for sequence simulation relative to that of

non-homogeneous analysis. The results described above were published in Ishikawa, Inagaki and Hashimoto (2012 **Evolutionary Bioinformatics** 8:357-371)

Our initial simulation study described above demonstrated the superiority of non-homogeneous models over homogeneous models when a target dataset includes sequences evolved under different tempos and modes. However, the analyses under non-homogeneous models (non-homogeneous analyses), in which an enormous amount of model parameters need to be optimized, can be computationally intense. To counter the computational cost for non-homogeneous analyses, we are currently challenging to parallelize a phylogenetic program called as NHML, which implements a non-homogeneous model. We applied two approaches for parallel computing, OpenMP and MPI, into the algorithm for the calculation of the likelihood of a tree. Analyses of the simulated sequence datasets using this HYBRID version of NHML successfully achieved reasonable parallel efficiency for the likelihood calculation of a tree until using 256 CPU cores. Moreover, we divided MPI communicator into multiple sub-communicators to conduct likelihood calculations of multiple trees in parallel. The current version of this program achieved the suitable performance of parallelization with more than 1024 CPU cores. This achievement was reported as Ishikawa et al. (2013 **Proceedings of High Performance Computing Symposium**).

6.2.5 Potential bias in bootstrap support values in the maximum-likelihood methods

In this work, we examined the potential bias in bootstrap support (BS) values stemming from heuristic tree search under the maximum-likelihood criterion by using simulated datasets. We compared the results from the bootstrap analysis with single heuristic tree search (sHTS) path with that from the same analysis with multiple heuristic search (mHTS) paths. The support values for bipartitions calculated from sHTS-path bootstrap analysis—regardless of the method for generating the starting trees—have a clear trend of being smaller than the corresponding values form mHTS-path analysis. The log-likelihoods of the trees inferred from sHTS-path were found to be smaller than those from mHTS paths, suggesting that BS values were affected by the efficiency of heuristic tree search. We observed that the difference in the BS values between sHTS-path and mHTS-path analyses was magnified in larger-size simulation datasets.

6.3 Collaboration

6.3.1 Collaboration within Division of Life Sciences

We are collaborating with Dr. Mitsuo Shoji in Biological Function and Information Group to predict the tertiary structure and protein-protein interactions of translation elongation factors in eukaryotes.

6.3.2 Collaboration with Division of High Performance Computing System

In order to develop the hybrid MPI/OpenMP parallelization of a phylogenetic program with non-homogeneous models, we are in close collaboration with members of Division of HPCS. Sohta Ishikawa, one of our graduate students, has been co-supervised by Dr. Mitsuhisa Sato (Division of HPCS) as a part of the dual-degree program between the Graduate schools of Life and Environmental Sciences, and Computational Sciences.

6.3.3 Collaboration with Division of Computational Informatics

We are currently collaborating with the CI group to develop a database to handle the next-generation sequence data generated from phylogenetically diverse microbial eukayrotes by our group. Yuki Nishimura, one of our graduate students, has been co-supervised by Drs. Hiroyuki Kitagawa and Toshiyuki Amagasa (Database group in Division of CI) as a part of the dual-degree program between the Graduate schools of Life and Environmental Sciences, and Computational Sciences.

6.4 Future Plan

6.4.1 Phylogenomic analyses of novel microbial eukayrotes

We continue challenging to resolve the global eukaryotic phylogeny by subjecting microbial eukaryotes, which may hold keys to understand questions in the cellular and genome evolutions in eukaryotes, to 'phylogenomic' analyses. As the first step, large-scale sequence data will be retrieved from the following eukaryotic organisms.

Microheliella maris ……This 'marine microheliozoan' (Figure 6, left) was proposed to be related to centrohelids, and formally described in Yabuki et al. (2012) **Protist** 163:356-388.

Strain SRT127 ……Strain 127 is an undescribed member of Centrohelida.

Rigifila ramosa ……*R. ramosa* (Figure 6, Center) is a heterotrophic filose flagellate, and formally described in Yabuki, Ishida, Cavalier-Smith (2013) **Protist** 164:75-88. This flagellate is the closest relative of Micronuclearia, and possesses a phylogenetic affinity to Apusozoa and Diphyllatea (e.g., *Diphylleira* sp. strain SRT116; see below).

Strain SRT116 ……*Diphylleira* sp., a member of Diphyllatea.

Strain SRT149 ……This heterotrophic flagellate (Figure 6, Right) is an undescribed eukaryote, which is a close relative of cryptophytes and goniomonads and represents an

'environmental clade' CRY-1 (e.g., Shalchian-Tabrizi et al. 2008 **Environmental Microbiology** 10:2635-2644).

Strain PAP020 ····· Undescribed anaerobic flagellate. This flagellate showed no special affinity to any known eukaryotes in a 18S ribosomal RNA phylogeny (data not shown).

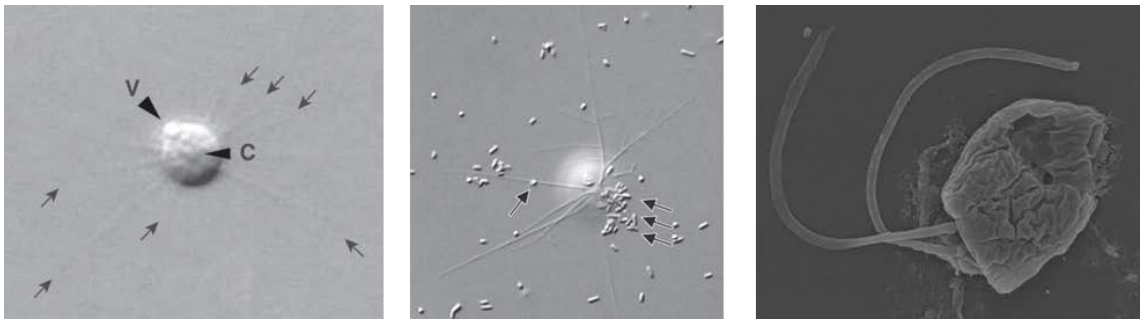

Figure 6. Microbial eukaryotes of our interest. **Left**, *Microheliella maris*. This image was a part of Yabuki et al. (2012). **Center**, *Rigifila ramosa*. This image was a part of Yabuki et al. (2013). **Right**, Strain SRT149. This image was taken by T. Shiratori.

6.4.2 Methodology for large-scale phylogenetic analyses

For our methodological projects, we will maintain the close cooperation with Division of High Performance Computing System and Division of Computational Informatics to develop phylogenetic programs for large-scale maximum-likelihood analyses, and basic databases required for handling massive sequence data from next-generation sequencing.

6.5 Publications

6.5.1 Journal Papers

- R. Kamikawa, M. Kolisko, Y. Nishimura, A. Yabuki, M. W. Brown, S. A. Ishikawa, K. Ishida, A. J. Roger, T. Hashimoto & Y. Inagaki. Gene-content evolution in discobid mitochondria deduced from the phylogenetic position and complete mitochondrial genome of *Tsukubamonas globosa*. **Genome Biology and Evolution**, in press.
- R. Kamikawa, M. W. Brown, Y. Nishimura, Y. Sako, A. A. Heiss, N. Yubuki, R. Gawryluk, A. G. B. Simpson, A. J. Roger, T. Hashimoto & Y. Inagaki. Parallel re-modeling of EF-1α function in eukaryotic evolution: Divergent, low-expressed EF-1α genes co-occur with EFL genes in diverse distantly related eukaryotes. **BMC Evolutionary Biology**, 13, 131 (2013)
- E. Nagayasu, S. Ishikawa, S. Taketani, T. Ooka, G. Chakraborty, A. Yoshida, Y. Inagaki, T. Hayashi & H. Maruyama. Identification of a bacteria-like ferrochelatase gene in *Strongyloides venezuelensis*, an animal parasitic nematode. **PLoS ONE**, 8, e58458 (2013)

- T. Matsumoto, M. Kawachi, H. Miyashita & Y. Inagaki. Prasinoxanthin is absent in the green-colored dinoflagellate *Lepidodinium chlorophorum* strain NIES-1868: Pigment composition and 18S rRNA phylogeny. 2012 **Journal of Plant Research**, 125, 705-711 (2012)
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- A. Yabuki, T. Nakayama, N. Yubuki, T. Hashimoto, K. Ishida & Y. Inagaki. *Tsukubamonas globosa* n. g., n. sp., a novel excavate flagellate possibly holding a key for the early evolution in "Discoba." **Journal of Eukaryotic Microbiology**, 58, 319-331 (2011)
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6.5.2 Proceedings

- S. A. Ishikawa, H. Nakao, Y. Inagaki, T. Hashimoto & M. Sato. Non-homogeneous 置換モデルを搭載した系統解析プログラムの MPI/OpenML ハイブリッド並列化 : 大規模遺伝子データセットへの適応に向けて. **Proceedings of High Performance Computing Symposium** pp. 10-20 (2014).
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7 Division of Global Environmental Science: *Atmospheric Science Group*

7.1 Research Activity

In the Division of Global Environmental Science, Atmospheric Science Group is the only one group formed for the research activity in the Center for Computational Sciences (CCS). Prof. Hiroshi L. Tanaka, the Division head, and Associate Prof. Hiroyuki Kusaka are the members of the Atmospheric Science Group. In addition to these two scientists, there are two affiliated research members within the university campus: Prof. Hiroaki Ueda of Life and Environmental Science, and Assistant Prof. Yasutaka Wakazuki of the Center for Research in Isotopes and Environmental Dynamics. They are highly involved in numerical simulations of the atmospheric science studies. Dr. Tanaka's expertise is in the general circulation of the atmosphere; Dr. Kusaka's expertise is in urban climate; Dr. Ueda's expertize is in climate system; and Dr. Wakazuki's expertise is in meso-scale weather system. We also invite Dr. Fujio Kimura of JAMSTEC and Dr. Akio Kitoh of Meteorological Research Institute (MRI) for the collaborative research members from outside campus. Following is the list of the research activities for 2008 to 2013.

Activity in 2008
1) Field experiment of urban heat island in Tsukuba city
2) Development of Multi-layer Urban Canopy Model
3) Analysis of Arctic Oscillation simulated by global warming prediction models

Activity in 2009
1) Installed the WRF model in the T2K-Tsukuba supercomputer
2) An inter-comparison study between the WRF-UCM and WRF-Slab Model
3) Detection of pressure patterns using support vector machine

Activity in 2010
1) Numerical simulation of urban precipitation using the WRF model
2) Applying the LETKF data assimilation code to the NICAM
3) Diagnostic analysis of the Arctic Oscillation using the AOI equation

Activity in 2011
1) Development of Local Meteorological Model (LMM) based on LES Model
2) Urban climate projection by the WRF model. Dynamical downscaling and predicting heat stress in the 2070's August for Tokyo, Osaka, and Nagoya.
3) Development of 3D spectral linear baroclinic model and the application to the baroclinic instability

Activity in 2012
1) Formation mechanism of the extreme surface air temperature of 40.9 C observed in the Tokyo metropolitan area
2) Analysis and numerical simulation of Arctic cyclones using NICAM.

Activity in 2013
1) Proposal of a new equation to estimate globe temperature
2) Parameter sensitivities of the dual-localization approach in the local ensemble transform Kalman filter

7.2 Research Results

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

ACTIVITY IN 2008

A field experiment is performed in Tsukuba City, Ibaraki Prefecture, on the early morning 17 Feb 2008. As a result, the center of heat island is found in the Takezono area. The heat island intensity at 0600 Japan Standard Time (JST) is 5 ℃. Observed vertical profile of the temperature reveals that the atmospheric stability is almost neutral over the central park near the station although it is strong stable over the open space in the University of Tsukuba. The temperature difference between the two sites is 4℃.

Secondly, our group has started to develop Multilayer Urban Canopy Model (MUCM), in order to better represent the physical process in urban environment in mesoscale model. Then, four types of multilayer urban canopy models—level 4, level 3, level 2, and level 1—are developed to reduce the computational load of the heat budget calculations at the wall surface. From the simplification, the performance of the Level 3 model is almost equal to the Level 4 model, and the amount of memory is reduced by 57%, the CPU time is reduced by 67%.

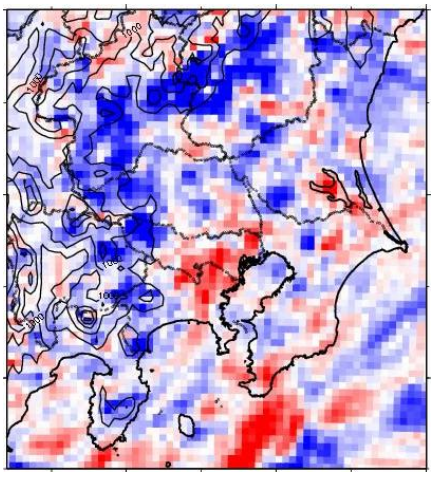
We analyzed the Arctic Oscillation (AO) under the global warming for the 20th and 21th century using data sets of 10 AOGCM for IPCC-AR4. The long-term variability of the atmosphere superficially looks like to correspond with the climate

warming. However, its spatial pattern didn't necessarily represent the AO. And the global mean surface temperature simulated by the models reproduces the observation responding to external forcing. However, none of the models could reproduce accurately the observed AOI. Therefore, it is concluded that the observed decadal variability like the AO is not the forced response, but can be explained mostly by the natural variability of the atmosphere.

Activity in 2009

An inter-comparison study between the WRF UCM and Slab model was performed. In the Tokyo metropolitan area, UCM accurately captures the observed monthly mean daytime and nocturnal UHI, whereas slab model does not show a nocturnal UHI. In addition, WRF_UCM accurately reproduces the frequency distribution of surface air temperatures, whereas the simulation results of WRF_SLAB have shown poor performance.

Secondly, we developed automatic pressure pattern detection technique using Support Vector Machine (SVM). In climate research, a huge number of surface weather charts must be scanned visually. To solve this problem, we propose an automatic detection method using pattern recognition developed in the computer science field. Using this technique, we classified pressure patterns into the "winter type" and "not winter type". In our experiments, we used the JRA-25 data from 1981 to 2000 for training data and test data. The results showed that our SVM method achieves greater than 90% accuracy.



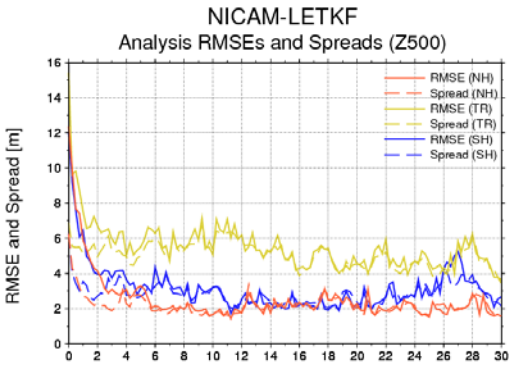
Activity in 2010

Urban climate projection for the 2070's August for the three major Japanese metropolitan areas was performed by the WRF model coupled with un Urban Canopy Model (UCM). Dynamical downscale approach is adopted to simulate 2070's urban climate. The observed characteristics of heat island at early morning is well simulated on the three major metropolitan area. Surface air temperatures at 5 Japan Standard Time (JST) in 2070's in Nerima (Tokyo), Nagoya, and Osaka are 3.1ºC, 2.9ºC, and 3.2ºC higher than that of 2000's, respectively.

Secondly, we performed a sensitivity analysis on the WRF model to investigate the impact of rainfall over a city. We performed the numerical integration for not only a certain case but also several summer months from 2001-2008. Furthermore, we performed an uncertainty experiment using the different boundary conditions. As a result, we were able to understand that the heavy rainfall was higher in the urban area when the urban effect was considered in the model than no urban effect was considered. Moreover, we found that the impact of rainfall was strengthened when the urban effect became strong.

We apply the local ensemble transform Kalman filter (LETKF) to the NICAM to develop the NICAM-LETKF. The feasibility and stability of the NICAM-LETKF are investigated under the perfect model scenario. According to the results, we confirm that the converged analysis errors of the NICAM-LETKF are smaller than

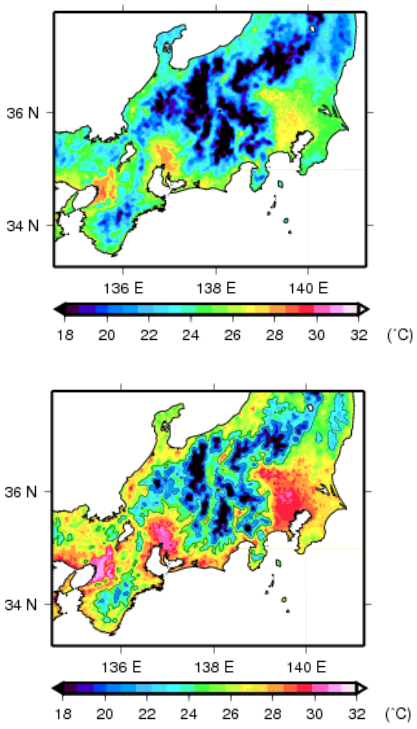
the observational errors, and the magnitude and distribution of the root mean square errors (RMSEs) are comparable to those of the ensemble spreads. It is concluded that the NICAM-LETKF works appropriately and stably under the perfect model scenario even if the inflation parameter and the observational errors are adaptively estimated within the LETKF.



We investigated the abnormal weather associated with negative Arctic Oscillation Index (AOI) in the winter of 2009/2010 using the AOI equation. AO is defined as the EOF-1 of sea level pressure variation, which is dynamically connected to the variation of the barotropic height. We consider that the barotropic component of the atmosphere governs the essential part of the low-frequency variability of the general circulation of the atmosphere. With this method, the abnormal winter of 2009/2010 is analyzed diagnostically. According to the result, it is found that (1) the abnormal AOI is caused by the linear internal process, (2) AOI is triggered by the nonlinear transient eddy forcing, (3) the barotropic external forcing is unimportant.

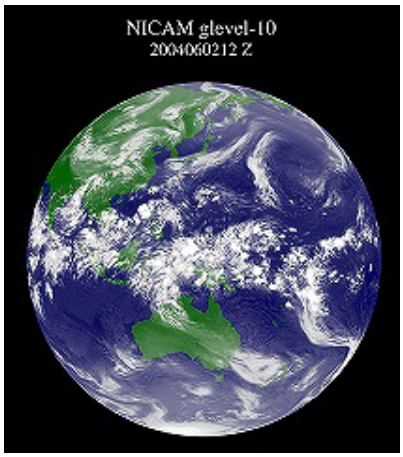
Activity in 2011

We have carried out future prediction experiments for urban climate for 2070s, targeting the Tokyo, Osaka and Nagoya metropolitan area, using the WRF model. Furthermore, by using this prediction results, we evaluated heat stress effect on the residents of Tokyo, Osaka and Nagoya. As a result shows that 2070s will become hotter than recording average air temperature in August 2010. Also , it was suggested that sleep disorder may occur almost every day in the future as it was in August of 2010. Furthermore, the time recommended to suspend taking strenuous exercise outdoors, which was 30% during the day in August 2000s, was suggested to raise to 63% in 2070s. Secondly, in order to evaluate the degree of impact of buildings, parks, and trees on the local temperature distribution, our group has started to develop Urban Meteorological Model based on LES Model.



A linear baroclinic model (LBM) is developed from a three-dimensional (3D) spectral primitive equation model. With this LBM we investigated the linear stability problem for various zonally-varying basic states on a sphere. For a zonal climate basic state, we confirm that the traditional Charney mode and dipole-Charney mode appear as the most dominant unstable modes in the synoptic

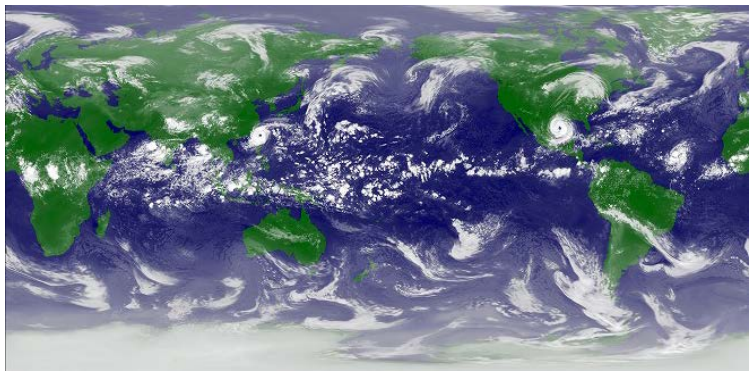
to planetary scales. For a zonally varying basic state, we find that these unstable modes are modified by the regionality of the local baroclinicity of the basic state. Given the zonally varying barotropic basic state, we find that the barotropically most unstable standing mode appears to be the Arctic Oscillation (AO) mode. The eigensolution of the LBM in this study is regarded as a generalized extension at the 3D normal mode at the motionless atmosphere to those of an arbitrary climate basic state.



ACTIVITY IN 2012

The formation mechanisms of extreme high temperature events at Kumagaya are investigated using the Weather Research and Forecasting (WRF) model. The results show that extreme event in Kumagaya on 16 August 2007 was mainly caused by a new type of foehn wind with diabatic heating from the ground surface which is different from typical thermodynamic foehn (wet foehn) and dynamic foehn (dry foen).

We conducted a numerical simulation of a rapid development of an arctic cyclone (AC) appeared in June 2008 using a cloud resolving global model NICAM. We investigated the 3D structure and intensification mechanism of the simulated AC that developed to the minimum sea level pressure of 971 hPa in the model. According to the result, the AC indicates a barotropic structure with a warm core in the lower stratosphere and a cold core in the troposphere. The development of the AC is accompanied by an intense mesosclae cyclone (MC) showing baroclinic structure with a marked local front.



Activity in 2013

Globe temperature is one of important element of the heat stress index, the Wet Bulb Globe Temperature, which is used to evaluate how radiation adds to thermal discomfort in the workplace. As the measurement of globe temperature is not standardized. We derived a new equation based on the heat balance equations of the globe with its numerical constants experimentally determined. This equation was able to predict the curvilinear dependence of the globe temperature on global solar radiation without any discontinuity, and it also showed the globe temperature response to wind speed.

In the ensemble Kalman filter, covariance localization plays an essential role in treating sampling errors in the ensemble-based error covariance between distant locations. We may limit the influence of observations within a narrower region than the range that the observations should impact, particularly when the model resolution is very high, since larger-scale structures than the localization scale are removed due to tight localization for the high-resolution model. To retain the larger-scale structures with a limited ensemble size, the dual-localization approach, which considers two separate localization scales simultaneously, has been proposed. The dual-localization method analyzes small-scale and large-scale analysis increments separately using spatial smoothing and two localization scales.

7.3 Collaboration

1.Collaborative Research with Japan Weather Association (JWA)
Collaborating in improvement of WRF, weather prediction, disaster analysis, renewable energy.

2. Collaborative Research with Toshiba
Collaborating in improvement of weather prediction.

3. Collaborative Research with Tajimi City
We concluded a cooperation agreement with Tajimi City to clarify the formation mechanism of the extreme heat.

4. Collaborative Research with Academia Science, Taiwan
Collaborating in regional future climate projection for Taipei, Taiwan.

5. Collaborative Research with Weather News Inc. (WNI)
We are studying about the fog forecast and the discrimination of precipitation (rainfall, snowfall forecast) in the Kanto region with weather forecasters of global forecast center. We can benefit from the forecasters needs in the field (such as road weather) and their valuable experience for forecasts through this work.

6. Collaborative Research with Nippon Telegraph and Telephone Corporation. (NTT)
Collaborating in Research about down scalar using WRF with NTT.

7. Collaborative Research with Meteorological Research Institute for Technology Corporation. (MERIT)
Collaborating in Research about prediction of snow damage to influence on power line.

8. Collaborative Research under GRENE Arctic Research Project of MEXT
Collaborating in Research about Arctic climate system and its prediction. Arctic amplification and Arctic Oscillation are the main targets of our study.

9. Collaborative Research with AORI for the Arctic Process using NICAM
Collaborating in Research with Atmosphere Ocean Research Institute (AORI) of the University of Tokyo about Arctic climate system and its process, using the cloud resolving global model NICAM.

10. Collaborative Research with DPRI for the Volcanic Ash Dispersion in the Air.
Collaborating in Research with Disaster Prevention Research Institute (DPRI) of Kyoto University about the volcanic ash dispersion using PUFF model developed by the AVO of the University of Alaska.

11. Collaborative Research with Meteorological Research Institute for Atmosphere-Ocean coupled model
Collaborating in Research about future projection including paleo-climate study

12. Palaeoclimate Modeling Intercomparison Project (PMIP)
Collaborating in Research about paleo-climate modeling across the globe

13. Pliocene Model Intercomparison Project (PlioMIP)
Collaborating in Research about Pliocene (3Ma) modeling study with proxy data

7.4 Outside Fund

1. Environment Research and Technology Development Fund of the Ministry of the Environment, Japan 2010-2014. (S-8-1). (JPY 115,586,000)

2. Research Program on Climate Change Adaptation, Initiative for Strategic Adaptation to Climate Change (RECCA). The Ministry of Education, Culture, Sports, Science and Technology of Japan (MEXT). 2010-2014. (JPY 56,200,000)

3. Analysis of urban air temperature.
Grant-in-Aid for Scientific Research B of the Japan Science and Technology Agency (JST), Japan. 2010-2012. (JPY 1,400,000)

4. Urban precipitation observations.
Grant-in-Aid for Scientific Research B (22300316) of the Japan Science and Technology Agency (JST), Japan.2010-2012. (JPY 800,000)

5. Urban precipitation observations.
Grant-in-Aid for Scientific Research A of the Japan Science and Technology Agency (JST), Japan.2013-2017. (JPY 20,000,000)

6. Environment Research and Technology Development Fund of the Ministry of the Environment, Japan.2007-2011. (S-5-3) (JPY 74,138,000)

7. Actual condition and mechanism of urban heat island of Tsukuba city.
   The Grant-in-Aid for Young Scientists B of the Japan Science and Technology Agency (JST), Japan. 2007-2010. (JPY 4000,000)

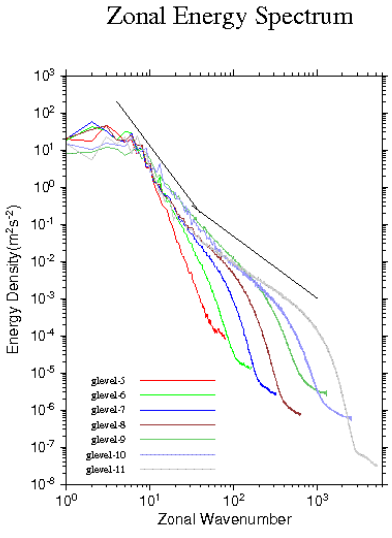
8. Green network of excellence (GRENE) of Arctic Climate Study under Ministry of Education, Culture Sports, Science and Technology (MEXT), Japan. 2011-2015. (PI: J. Ukita, JPY 500,000,000)

9. Environment Research and Technology Development Fund of the Ministry of the Environment, Japan 2008-2013. (S-5-2; A1201). (JPY 45,000,000)

10. Program for Risk Information on Climate Change, Ministry of Education, Culture, Sports, Science and Technology, 2012-2013. (JPY 440,000,000).

7.5 Future Plan

- We plan to develop new multi-layer vegetation canopy model considering rainfall interception and dew deposition. Furthermore, we will introduce this vegetation model to our LES model.
- We plan to evaluate the degree of impact of buildings, parks, and trees on the local temperature distribution using our LES model.
- We have been endeavoring interdisciplinary research activities in climate-health interaction. We are planning on expanding our research activities in this arena, especially in conjunction with global warming projections and mitigation/adaptation planning.
- We plan to use the cloud resolving global mode NICAM for the study of arctic climate change, especially for the arctic amplification, arctic oscillation, and arctic cyclone under the collaboration with AORI of the Tokyo University.
- We pane to expand the 3D normal mode energetics study not only for Rossby wave world, but also for gravity wave world. The tropical low-frequency variability, like MJO, is expected to be one of the normal mode solutions.
- International collaboration is planned for implementing the volcanic ash dispersal model PUFF for volcanos in Indonesia under



the collaboration with DPRI of Kyoto University.

7.6 Publications

7.6.1 Journal Papers

- A. Surname1, B. Surname2, & C. Surname3, Name of Journal, vol.123, 45-67 (2013)
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7.6.4 Press Release

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2010.05.28 The Chunichi NewsPapers Ver.Gifu

「Extreme high temperature events in Tajimi」

The Gifu Newspapers

「Extreme high temperature events in Tajimi」

2010.07.22 Tokyo Broadcasting System Television, Inc.「NSUTA」

「Formation Mechanism of Heat-Island Phenomenon」

2010.07.23 The Asahi Shimbun Comapany Ver.Nagoya Morning edition

「Extreme high temperature events in Tajimi」

2010.07.24 Kyodo News

「Extreme high temperature events in Tajimi」

2010.07.26 Tokai Televison Broadcasting Co., Ltd.「PI-KAN TV」

「Extreme high temperature events in Tajimi」

2010.07.29, 2010.08.16 Chubu-Nippon Broadcasting Co.,Ltd.「IPPOU」

「Extreme high temperature events in Tajimi」

2010.07.30 Chukyo TV Broadcasting Co., Ltd.「news every.」

「Extreme high temperature events in Tajimi」

2010.07.30 Gifu Broadcasting System, Inc.「NEWS FIVE」

「Extreme high temperature events in Tajimi」

2010.07.31 The Chunichi Shimbun

「Extreme high temperature events in Tajimi」

The Gifu Newspapers

「Extreme high temperature events in Tajimi」

2010.08.02 The Yomiuri Shimbun Morning edition

「Extreme high temperature events in Tajimi」

2010.08.15 The Asahi Shimbun Comapany Ver.Nagoya

「Extreme high temperature events in Tajimi」

2010.08.17 The Chunichi Shimbun

「Extreme high temperature events in Tajimi」

2010.08.17 NHK「HOTTOEVENING」Nagoya

「Extreme high temperature events in Tajimi」

2010.08.17 NHK「NEWS7」Nationwide

「Extreme high temperature events in Tajimi」

2010.08.25 NHK「OGENKIDESUKA NIHONRETTOU」Nationwide

「Extreme high temperature events in Tajimi」

2010.08.28 The Asahi Shogakusei Newspapers

「Extreme high temperature events in Tajimi」

2010.10.02 InterFM (76.1FM)「GREEN STATION」

「Global Warming Heat-Island」

2010.12.24 Radio First「TUNAGARURADIO」

「Extreme high temperature events in Tajimi」

Press Release 2011

2011.06.30 Chubu-Nippon Broadcasting Co.,Ltd.「IPPOU」

「Extreme high temperature events in Tajimi」

The Gifu Newspapers

「Extreme high temperature events in Tajimi」

July, August issue Free Magazines

「Introduction of Environmental technique」

Introduction of Our Research activities

2011.07.01 The Gifu Newspapers

「Extreme high temperature events in Tajimi」

The Chunichi Shimbun

「Extreme high temperature events in Tajimi」

2011.07.17 Nikkei Inc.

「Short-time heavy rainfall in Urban Areas」

2011.07.21 Sanspo（Kyodo News）

「Extreme high temperature events in Kumagaya」

Jiji Press Ltd.

「Extreme high temperature events in Kumagaya」

Nikkei Inc.

「Extreme high temperature events in Kumagaya」

2011.07.22 The Mainichi Newspapers　Evening paper

「Extreme high temperature events in Kumagaya」

The Ibaraki Shimbun

「Extreme high temperature events in Kumagaya」

The Asahi Shimbun Comapany

「Extreme high temperature events in Kumagaya」

The Tokyo Shimbun

「Extreme high temperature events in Kumagaya」

Nikkei Inc.

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2011.07.23 Nikkei Inc. Morning edition

「Short-time heavy rainfall in Urban Areas」

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「Extreme high temperature events in Kumagaya」

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「Extreme high temperature events in Kumagaya」

2011.07.26 Nippon Television「ZIP!」

「Short-time heavy rainfall in Urban Areas」

2011.07.27 Nippon Television「SUKKIRI!!」

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2011.07.28 TV Asahi「MORNINGBIRD」

「Short-time heavy rainfall in Urban Areas」

2011.08.02 Yomiuri Telecasting Corporation「MIYANEYA」

「Short-time heavy rainfall in Urban Areas」

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2011.09.22 The Saitama Shimbun

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Press Release 2012

2012.02.06 The Asahi Shimbun Comapany

「Description of the temperature in Ibaraki」

2012.03.04 NHK「OTENKI VARIETY KISHOUTENKETSU」

「Description of the foehn phenomenon」

2012.05.10 Nikkei Inc.

「Evening papers　Introduction of research on downscaling of global warming」

TV Asahi「HOUDOU Station」

「Comment on the future projection of the heavy rain　fall.」

2012.05.13 Fuji TV「Mr. Sunday」

「Comment on urban city and tornado.」

2012.05.15 Nikkei Inc.

「Projection of global warming」

2012.05.26 The Mainichi Newspapers.Evening papers

「Projection of global warming」

2012.06.29 The Ibaraki-Shimbun

「Projection of global warming in Augut of 2070's」

The Chunichi Shimbun

「Projection of global warming in Augut of 2070's」

The Yamagata Shimbun

「Projection of global warming in Augut of 2070's」

The Hokkoku Shimbun
「Projection of global warming in Augut of 2070's」
The Gifu Newspapers
「Projection of global warming in Augut of 2070's」
The Ise Shimbun
「Projection of global warming in Augut of 2070's」
The Sanin Shimbun
「Projection of global warming in Augut of 2070's」
The Fukui Shimbun
「Projection of global warming in Augut of 2070's」
The Shinano Mainichi Shimbun
「Projection of global warming in Augut of 2070's」

2012.07.08 The Mainichi Newspapers Gifu Ver.
「Extreme high temperature events in Tajimi」

2012.07.08 Radio Inter FM「GREEN STATION」
「Projection of global warming」

2012.07.18 The Asahi Shimbun Comapany
「Projection of global warming」

2012.07.26 Nikkei Inc.「Sentanjin」
「Introduction of Prof. Kusaka」

2012.07.28 CBC Radio「Takashi Hirose Let's go on the radio!」
「Projection of global warming」

2012.08.21 NHK「NEWS WATCH」
「Extreme high temperature events in Tajimi」

2012.08.21 NHK Radio1「NHK Journal」
「Extreme high temperature events in Tajimi」

2012.08.22 The Chunichi Shimbun
「Extreme high temperature events in Tajimi」

Press Release 2013

2013.02.10 Tokyo Broadcasting System Television, Inc.
「N suta」 「Mt. Tsukubasan Weather Station」

2013.05.26 Asahi National Broadcasting.(TV Asahi)

「Climatic classification」

2013.07.10 Japan Broadcasting Corporation.(NHK)

「Heat-Island Phenomenon abount This summer」

2013.08.12 NHK Gifu

「Observation of　feeling temerature」

2013.08.12 CBC「N　sta」

「Observation of　feeling temerature」

2013.08.13 The Chunichi Shimbun

「Explanation of heating about Shimanto city,Kouchi Prefecture」

2013.09.09～09.13 Radio Nikkei daini.

「Heating,Guerrila rainfall,Warming」

7.6.5 Awards

- **Best Presentation Award.**

Takane,Y.,H.Kusaka,M.Hara,S.A.Adachi,andF.Kimura,2008:

Formation mechanism of extreme hot conditions

-a case study on 16 August 2007-.3rd Conference on heat island Japan,2008.

- **Best Presentation Award.**

Y. Takane., Kusaka, H., Kondo, H. Formation mechanism of extreme hot conditions and foehn –a case study on 24 June, 2011. 8th Conference on heat island Japan, 2013.

- **Students and Young Scientists Award.**

Suzuki-Parker, A., H.Kusaka,S.Abe,2013:

Climatological perspective and future projection of thermal environment in Japan using WBGT. 52nd Annual Meeting of Japanese Society of Biometeorology,2013.

- **Best Presentation Award.**

Ohashi, Masahiro, and H. L. Tanaka, 2008:

Analysis of Arctic Oscillation simulated by global warming prediction models. First International Symposium on the Arctic Research (ISAR-1), Tokyo, Japan. 4-6 Nov. 2008.

8 Division of High Performance Computing Systems: *High Performance Computing Systems Group*

8.1 Research Activity

8.1.1 Accelerated Computing System

For the research on next generation accelerated computing systems, Prof. Sato carried out the project "Interdisciplinary Research and Education on Advanced Computational Science based on Exascale Computing Technology" funded by Ministry of Education, Sports, Culture, Science and Technology (MEXT), from 2011 to 2013. In this project, we investigate the next generation of accelerated computing based on a novel technology to realize direct communication between accelerators such as GPUs among multiple computation nodes on large scale PC clusters. Due to the memory capacity limitation and power consumption ceiling, it is considered that a weak scaling approach on past few decades of HPC system development is going to face with its limit and a strong scaling will be a serious issue on next generation HPC. On the other hand, the accelerating devices have been very powerful and essential components with high performance/cost ratio as well as high performance/energy ratio. However, these devices are the slave peripherals under CPU control where the interconnection network becomes a serious performance bottleneck on large scale parallel systems.

For a solution to this problem, we have been developing a novel technology to realize the direct communication between accelerators over computation nodes, named TCA (Tightly Coupled Accelerators) based on our original chip named PEACH2 (PCI Express Adaptive Communication Hub ver.2). For the prototyping and performance evaluation of TCA concept, we have developed a large scale GPU cluster HA-PACS (Highly Accelerated Parallel Advanced System for Computational Sciences) with 332 nodes with 1328 GPUs, including 64 nodes equipped with PEACH2 communication board. PEACH2 is implemented with FPGA chip to provide intelligent, low-latency and high-bandwidth communication between multiple PCI Express channels to connect host CPU, GPU and over-node external

PCI-E links. The project is also supported by application users' community in CCS to support various applications such as QCD, Astrophysics, Bio-Science, etc.

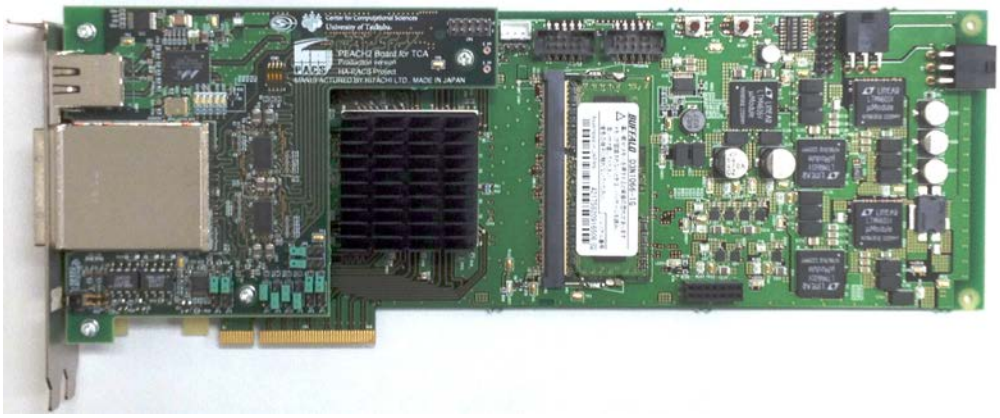


Fig. 1.1-1 PEACH2 PCIe card by TCA architecture

During three years of project terms, Prof. Boku launched the follow-up project "Unified Environment of Computing and Communication towards Post-Petascale Era" as a part of JST-CREST program field "System Software Development for Post-Petascale Era", from 2012 to 2017. This project is mainly focuses on the development of system software including firmware on PEACH2 chip, device driver and library, extension of XcalableMP language (see 1.1.3) and applications on this framework.

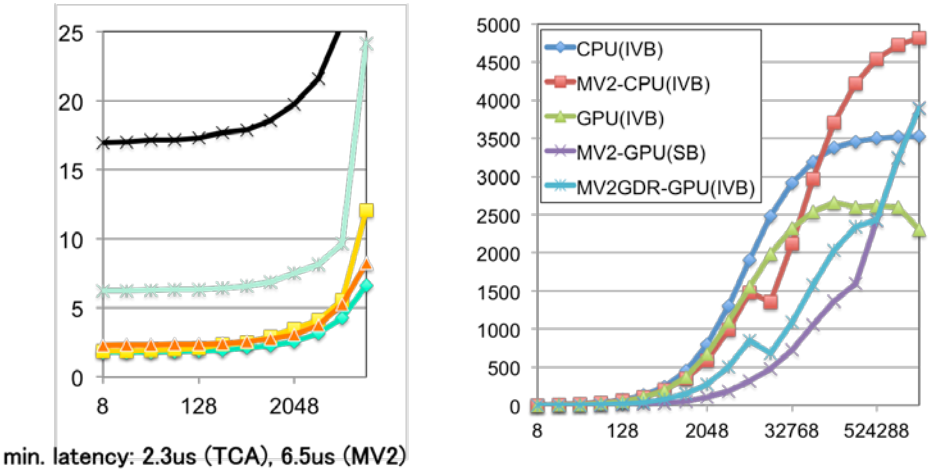


Fig. 1.1-2 Memory-to-memory copy on GPUs in different nodes, comparison between PEACH2 and InfiniBand+MVAPICH2 (left: latency, right: throughput)

8.1.2 Dependable System Design for Embedded Systems

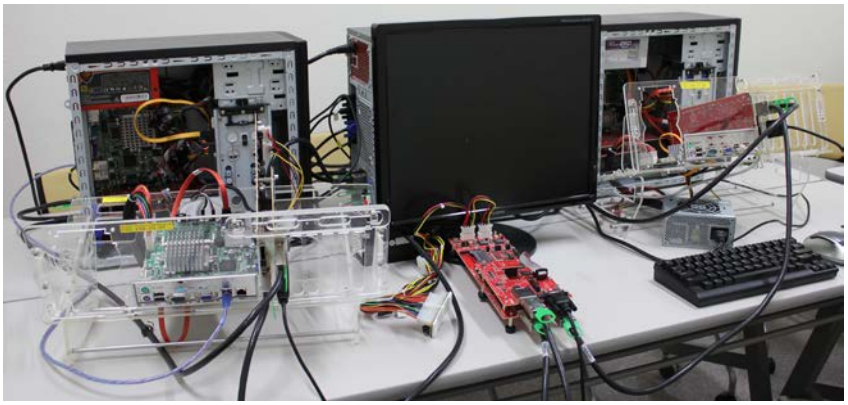


Fig. 1.1-3 PEACH Test Environment

For the research on next generation computing system, Prof. Sato with colleagues of HPC division carried out the project “Low-power and highly-reliable embedded parallel platform” under JST-CREST program on "Dependable Operating Systems for Embedded Systems Aiming at Practical Applications", from 2006 to 2011. In this project, we investigated dependable technologies for high-performance parallel embedded platforms of multi-core and multiprocessors systems. We designed the reliable software distributed memory system with redundant remote page management to provide fault-tolerance for embedded parallel programs, and the power management run-time system for parallel execution to optimize performance and power consumption under real-time constraints. The communication facility using multiple network links was also developed to provide fault-tolerance and trade-off between power and performance in the communication layer of the embedded parallel system. In this project, we have developed PEACH communication Link using PCIe as a near-distance low-power communication device, which was a predecessor of PEACH2 developed in HA-PACS project.

DS-Bench Toolset

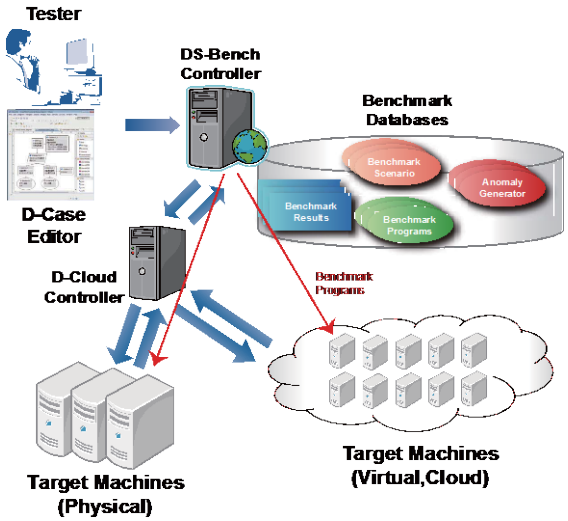


Fig. 1.1-4 DS-Bench Toolset

In addition, we also developed “D-Cloud”, which is an execution platform for testing and simulating dependability of the computing system using a cloud computing environment, and we integrated D-Cloud with “DS-Bench”, a benchmark test framework for system dependability, and “D-Case Editor”, a description and agreement support tool, into a tool chain as DS-Bench Toolset, collaborated with the research team of The University of Tokyo.

8.1.3 Next Generation Parallel Language

We conducted XcalableMP parallel programming language project as a part of “Seamless and Highly-productive Parallel Programming Environment for High-performance computing (e-science)” project funded by Ministry of Education, Culture, Sports, Science and Technology, from 2009 to 2012 led by Prof. Sato. The objective of this project was to improve the productivity of parallel programming for large-scale parallel system of Petascale by designing a new programming language. XcalableMP is a directive-based language extension which allows users to develop parallel programs for distributed memory systems easily and to tune the performance by having minimal and simple notations. The specification is being designed by XcalableMP Specification Working Group (XMP Spec WG) which consists of members from academia and research labs to industries in Japan. In this project, we have developed Omni XMP compiler as a reference implementation with discussions in XMP Spec WG. After this project, XMP Spec WG was organized by PC Cluster Consortium. The development of the Omni XMP compiler is still continued with RIKEN AICS programming environment research team for several platforms including the K computer.

```
int a[N], b[N];
#pragma xmp align [i] with t(i) :: a,
b
#pragma xmp shadow a[*]
void main(void) { . . .
int i, j;
#pragma xmp loop on t(i)
for (i = 0; i < N; i++) {
      b[i] = 0; a[i] = i;
#pragma xmp reflect a
#pragma xmp loop on t(i)
for (i = 0; i < N; i++) {
      b[i] = 0;
      for (j = 0; j < N; j++) {
            b[i] += a[j] ;
      }
```

Fig. 1.1-5 Example code of XcalableMP

XcalableMP is also used as a research vehicle for the next generation parallel programming and languages. “FP3C (Framework and programming for Post Petascale Computing)” project is a Japan-French collaboration to investigate languages, programming paradigms, runtime technologies and parallel algorithms for post-petascale system from 2010 to 2014. In this project, we proposed the multilevel programming paradigm (called FP2C) as a solution for post-petascale system to make use of a huge number of processors and attached accelerators in an efficient and hierarchical way. The users may program theirs parallel algorithms in YML workflow language with parallel components written by XcalableMP (XMP) and its accelerators extensions supported by StarPU runtime technology, where YML, StarPU developed in France, and XcalableMP (XMP), developed by us.

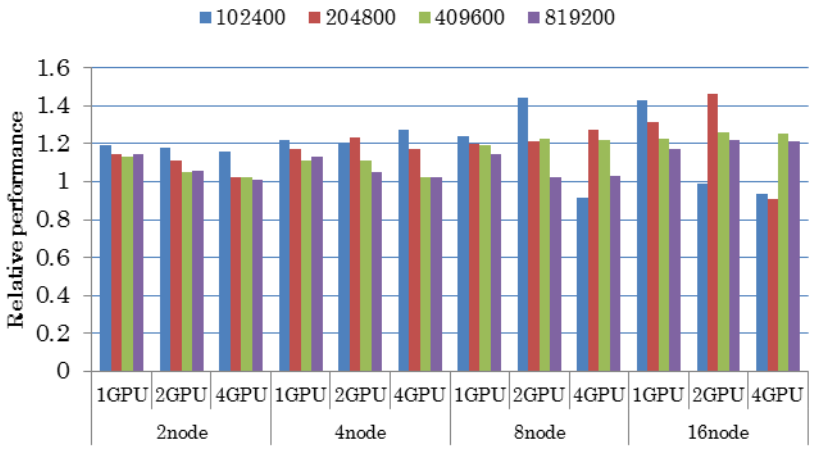


Fig. 1.1-6 Performance improvement by “GPU + multicore CPU” compared with “GPU-only” running, by XcalableMP accelerating device extension with StarPU resource scheduling

Prof. Sato joined “ECS (Enabling Climate Simulations at Extreme Scale)” project as a part of G8 Research Council Initiative International Collaboration, from 2011 to 2014, which is to investigate how to run efficiently climate simulations on future Exascale systems and get correct results. In this project, we are working on supporting fault resilience by designing programming languages constructs as an extension of XMP, and performance study of climate codes using one-sided communications of XMP PAS programming model.

8.1.4 Wide Area Distributed File System

Research of system software for data-intensive computing has been supported by the MEXT Grant-in-Aid for Scientific Research on Priority Areas, “New IT Infrastructure for the Information-explosion Era” (PI: Osamu Tatebe) from 2007 to 2011, and the MEXT Promotion of Research and Development for Key Technologies “Research for Next Generation IT Infrastructure, Resources Linkage for e-Science (RENKEI)” (PI: Ken Miura) from 2008 to 2012, JST/CREST “System Software for

Post Petascale Data Intensive Science" (PI: Osamu Tatebe) from 2011 to 2016, ANR-JST "Framework and Programming for Post Petascale Computing (FP3C)" (PI: Mitsuhisa Sato) from 2012 to 2014, and JST/CREST "Extreme Big Data (EBD) – Next Generation Big Data Infrastructure Technologies Towards Yottabyte/Year" (PI: Satoshi Matsuoka) from 2013 to 2019. The objective is to develop scaled-out file system architecture and system software, and to develop distributed object store for extreme big data.

System design for HPCI shared storage was supported by MEXT grant "System design for HPCI shared storage" in 2011. HPCI shared storage is 20PByte Japanese nation-wide shared storage shared from 9 national supercomputer centers and AICS.

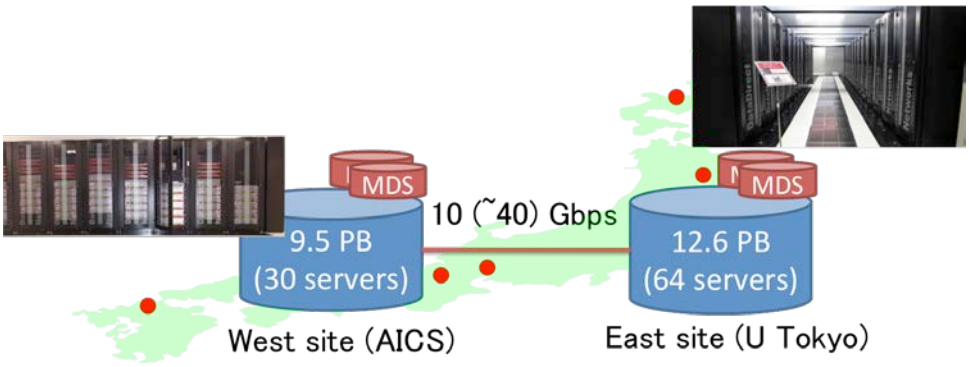


Fig. 1.1-7 HPCI Shared Storage System by Gfarm

HPCI Shared Storage - A 22.1PB single distributed file system consisting East and West sites that can be accessible from "K" computer site, Hokkaido, Tohoku, Tsukuba, Tokyo, Titech, Nagoya, Kyoto, Osaka, and Kyushu Universities.

System design for Japan Lattice Data Grid (JLDG) and International Lattice Data Grid (ILDG) was supported by NII grant "Cyber Science Infrastructure (CSI)" from 2006 to 2010. JLDG is a Japanese nation-wide storage system and ILDG is an international storage system, which is a joint research with the division of particle physics and astrophysics.

8.1.5 Energy Effective System Design

As a research on power efficient server system, Prof. Sato and Prof. Kodama joined to a project of "research and development project for green network/system technology (Green IT Project)" (led by Satoshi Sekiguchi, AIST) as a NEDO program from 2008 to 2012. In the project, we contributed to the development of evaluation framework for energy-saving operation in the server system.
We researched the environment of existing server system and the trend in aspect of energy use, and made a model of power consumption of a server. Because simple measurement of power consumption is not enough to evaluate the efficiency of power consumption, it should be consider the performance of applications. We

developed a framework for evaluating energy efficiency of server system with changing the workload. We made it clear that it is possible to improve the index of performance per watt by appropriately selecting their system parameters depending on the load, and proposed a Green SLA with the consideration.

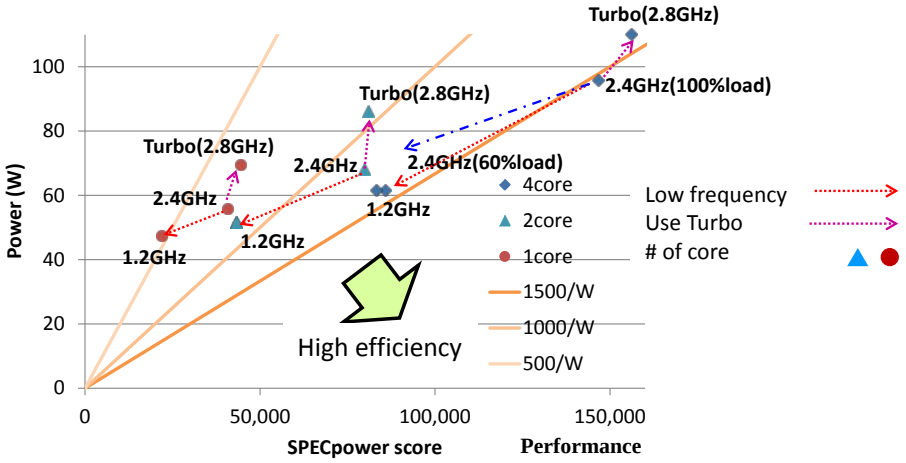


Fig. 1.1-8 **Power efficiency with several parameter**

8.1.6 High Performance Parallel Numerical Algorithm

As a research on development of high-performance numerical library, Prof. Takahashi joined to a project of "An Evolutionary Approach to Creation of a Software Development Environment for Massively-Parallel Computing Systems" (led by Prof. Takizawa, Tohoku University) as a JST-CREST program from October 2011 for five years. In the project, we are developing numerical libraries to fully exploit the performance of large-scale heterogeneous computing systems.

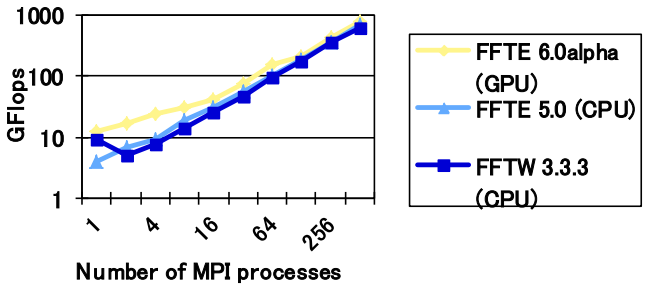
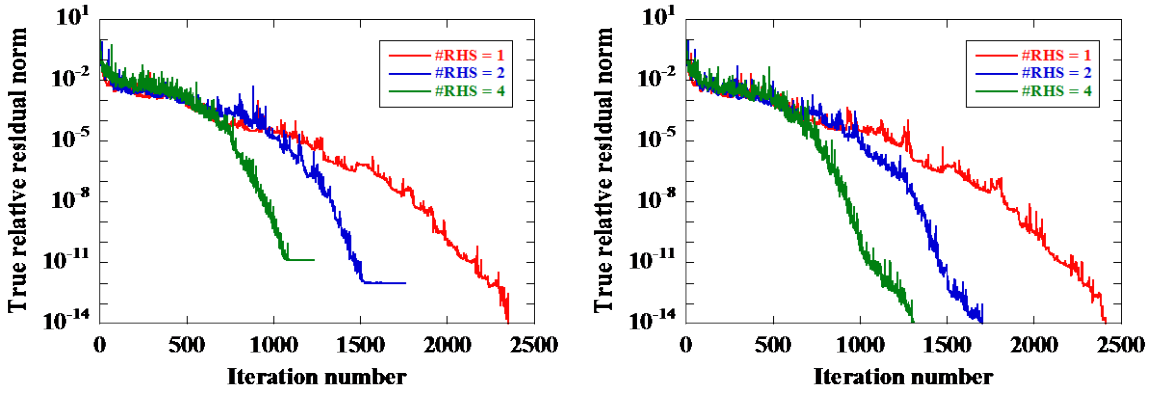


Fig. 1.1-9 **Performance of Parallel FFTs on HA-PACS, N=2^25×number of MPI processes.**

As a research on development of numerical computation methods, we studied Block Krylov subspace methods for linear systems with multiple right hand sides. The test problem is a linear system derived from lattice QCD calculation (n = 1,572,864).



(a) Block BiCGSTAB (b) Block BiCGGR

Fig. 1.1-10 True relative residual history of the Block Krylov subspace methods.

8.1.7 Development of Computational Science Codes

We have developed several real application codes for large scale parallel systems including K Computer and HA-PACS system under a number of internal, domestic and international collaboration.

In the collaboration with RIKEN AICS, University of Tokyo and Fujitsu, we have developed a large scale material simulation code with first principle simulation named RS-DFT (Real Space Density Function Theory) on K Computer. This code was originally developed in CCS on PACS-CS cluster, and then ported to K Computer to realize world largest simulation on material with DFT. We could successfully run the code on approximately 70% of K Computer's resource and achieved 3.4 PFLOPS of sustained performance.

We also have been porting several Nuclear Fusion simulation code under international collaboration "NuFuSE - Nuclear Fusion Simulation for Exascale" as a project in G8 Research Council Initiative International Collaboration under JSPS. We ported a magneto-hydrodynamics code GTC-P developed at Princeton Plasma Physics Laboratory in XcalableMP language towards next generation high level parallel programming as well as its GPU porting. Another work is to port GT5D code developed at Japan Atomic Energy Agency as the largest code in Japan for nuclear fusion simulation with CUDA Fortran to run on HA-PACS with GPU acceleration.

8.2 Research Results

- We carried out the JST-CREST project "Low-power and highly-reliable embedded parallel platform" and performed several researches on reliability and low-power technologies of systems and communications for embedded systems. Especially, we developed a communication link device PEACH, which was a predecessor of PEACH2 developed in HA-PACS project. And we proposed D-Cloud system, a cloud system to test system software using virtual machine technologies.

- We designed and implemented Omni XcalableMP compiler as a reference implementation of XcalableMP parallel programming language. It is ported to several platforms including the K computer. We have submitted some results of the K computer to HPCC Class2 competition in SC13, and won the award of HPCC Class2.

- Under the collaboration with RIKEN AICS, University of Tokyo and Fujitsu, we successfully ported RS-DFT code originally developed at CCS, and executed it on K Computer with approximately 70% of entire system to achieve 3.4 PFLOPS of sustained performance. This work was prized as the best performance award of 2012 ACM Gordon Bell Prize.

- Using XcalableMP as a research vehicle, we joined several international projects such as FP3C with France, G8 ECS and G8 NuFuSE. In FP3C, we have proposed the multilevel programming paradigm (called FP2C) by integrate XMP and YML flow language and StarPU runtime for GPU, to make use of post-petascale system in an efficient and hierarchical way. In NuFuSE, we ported Princeton's GTC-P nuclear fusion simulation code to XMP to demonstrate the coding for large scale distributed memory system without MPI.

- We have proposed the concept of PEARL (PCI Express Adaptive and Reliable Link) as a novel low-power, power-aware, and dependable interconnect using PCI Express and developed PEACH (PCI Express Adaptive Communication Hub) chip manufactured by Renesas Electronics, and PCI Express board using PEACH chip in the JST-CREST project of "Low-Power and Dependable Parallel Processing Platform with Embedded Technology" (P.I. Mitsuhisa Sato). We demonstrated the cluster using PEACH as the interconnect in the research exhibition on SC10, ISSCC2011, and so on.

- We have developed a novel interconnection network technology which enables a direct communication between accelerators such as GPUs not depending on host CPU's interconnection such as InfiniBand, with PEACH2 chip under TCA concept. It shortens the latency for GPU-to-GPU direct memory copy among

different nodes to approximately 30% of traditional technologies. This feature of low latency communication is effective especially for strong scaling on fixed size of problems.

- We have developed "D-Cloud," which is an execution platform for testing and simulating dependability of the computing system using a cloud computing environment in the JST-CREST project of "Low-Power and Dependable Parallel Processing Platform with Embedded Technology" (P.I. Mitsuhisa Sato), and "DS-Bench Toolset", tools for dependability benchmarking with simulation and assurance. We demonstrated the use case of "DS-Bench Toolset" and "D-Cloud in the research exhibition on PRDC'10, ET (Embedded Technology) 2010, ET2011, ET2012. These tools are available for download at http://www.dependable-os.net/osddeos/en/tech.html .
- Research of system software for data-intensive computing has developed Gfarm file system. It is available at http://sourceforge.net/projects/gfarm. HPCI shared storage has being in operation since 2011. JLDG has being in operation since 2008.

- We joined to NEDO "Green IT" project, and we developed a framework for evaluating energy efficiency of server system with changing the workload. We made it clear that it is possible to improve the index of performance per watt by appropriately selecting their system parameters depending on the load.

- We performed a collaborative research with RIKEN and Fujitsu on fast Fourier transform (FFT) for the K computer. As a result, Global FFT on the K computer achieved first place in the 2012 HPC Challenge Class 1 Awards.

8.3 Collaboration

- XcalableMP project is a part of "Seamless and Highly-productive Parallel Programming Environment for High-performance computing" (e-science) project in collaboration with University of Tokyo and Koto University (T2K collaboration).

- The FP3C project is a French-Japanese research project coordinated by INRIA Saclay in France and by the University of Tsukuba in Japan (PI from Japan: Mitsuhisa Sato). It associated CNRS, CEA, INRIA, University of Tsukuba, University of Tokyo, Institute of Technology of Tokyo and the University of Kyoto.

- The G8 ECS (co-PI from Japan: Mitsuhisa Sato) is an international project with research institutes and university of G8 countries including NCSA, NCAR, U. Tennessee in US, INRIA in France, and JSC in Germany.

- The G8 NuFuSE (PI from Japan: Taisuke Boku) is an international project with research institutes and universities of G8 RCI countries including

University of Edinburgh in UK, Princeton University in USA, CEA in France, Forschungszentrum Juelich GmbH in Germany, IPP in Germany, and Keldysh Institute of Applied Mathematics of Russian Academy of Science in Russia.

- JST/CREST "Low-Power and Dependable Parallel Processing Platform with Embedded Technology" (PI: Mitsuhisa Sato) was a joint research with Renesas Electronics Corp. In this project, we collaborated with Toshiba Solutions Corp. for developing a framework for customizing virtual machine with fault injector by integrating with SpecC device model for a software testing environment "D-Cloud."

- In the JST/CREST research area of "Dependable Embedded Operating Systems for Practical Use," we collaborated with the research team of The University of Tokyo (PI: Yutaka Ishikawa) and Fuji Xerox Co. Ltd. for developing "DS-Bench Toolset," tools for dependability benchmarking with simulation and assurance.

- MEXT Promotion of Research and Development for Key Technologies "Research for Next Generation IT Infrastructure, Resources Linkage for e-Science (RENKEI)" (PI: Ken Miura) is a joint research with NII, Osaka University, Tokyo Institute of Technology, Tamagawa University, KEK, AIST, and Fujitsu.

- JST/CREST "System Software for Post Petascale Data Intensive Science" (PI: Osamu Tatebe) is a joint research with University of Electro-Communications.

- JST/CREST "Unified Environment of Accelerated Computing and Communication towards Post-Petascale Era" (PI: Taisuke Boku) is a joint research with RIKEN AICS.

- JST/CREST "Extreme Big Data (EBD) – Next Generation Big Data Infrastructure Technologies Towards Yottabyte/Year" (PI: Satoshi Matsuoka) is a joint research with Tokyo Institute of Technology, NII and RIKEN.

- System design of HPCI system is a joint research with Hokkaido University, Tohoku University, University of Tokyo, Tokyo Institute of Technology, Nagoya University, Kyoto University, Osaka University, Kyushu University, and RIKEN.

- JLDG is a joint research with KEK, Nagoya University, Osaka University, Hiroshima University and RIKEN.

8.4 Future Plan

In our Division of HPC Systems, we have two primary purposes: (1) R&D on high performance computing system including hardware, system and application level software, algorithm, language, library, storage and network, and (2) supporting application research groups under collaboration towards higher performance and larger problem size on real-world problems.

For the R&D on HPC systems, we are focusing on a serious limitation on the computing capability and capacity which are different from past 20 years of history in HPC system. The performance improvement so far has been mainly achieved by weak scaling, that is, to enhance the system size such as number of processors, memory capacity, storage capacity and network bandwidth under a fixed cost of total system. However, the next generation system towards Exascale computing is facing the serious issues on power, footprint and system resiliency while the requirement on computing performance and data capacity is still growing. In next decade, we have to focus especially on large capacity of data handling both on storage and networking as well as computation performance, that is, so called big data and extreme computing. One of the promised key technologies on extreme computing is the accelerating technologies by extreme SIMD processors, GPUs, many-core processors, etc. For low power storage solution, we need to care on memory hierarchy expanded from cache level to permanent storage. In our division, we have a strong team to cover these issues, but we need more strong collaboration within CCS and world wide scale.

To solve widely spread domain scientific applications on limited system resource under realistic condition, the co-designing concept among HPC system researchers and domain application researchers is necessary. It is the most fundamental concept of our CCS to carry out every research based on the tight collaboration among system scientists and application scientists. It means that our CCS is a kind of ideal research field for tight collaboration towards co-design manner of future HPC and computational sciences. Currently, all the projects based on accelerated computing devices, system design, algorithm, storage and networking in CCS have been performed under such collaboration, and we must proceed this traditional concept in CCS upon our success history.

8.5 Publications

8.5.1 Journal Papers

- Y. Kodama, S. Itoh, T. Shimizu, S. Sekiguchi, H. Nakamura, N. Mori: Imbalance of CPU temperatures in a blade system and its impact for power consumption of fans. Cluster Computing, 16(1): 27-37 (2013)
- Y. Miki, D. Takahashi, M. Mori: Highly scalable implementation of an N-body code on a GPU cluster, Computer Physics Communications, 184(9): 2159-2168 (2013)

- A. Imakura, L. Du, H. Tadano: A Weighted Block GMRES Method for Solving Linear Systems with Multiple Right-Hand Sides. JSIAM Letters, 5: 65-68 (2013)
- T. Sakurai, Y. Futamura, H. Tadano: Efficient Parameter Estimation and Implementation of a Contour Integral-Based Eigensolver. J. Alg. Comput. Tech., 7(3): 249-269 (2013)
- I. Yamazaki, H. Tadano, T. Sakurai, T. Ikegami: Performance Comparison of Parallel Eigensolvers Based on a Contour Integral Method and a Lanczos Method. Parallel Computing, 39(6-7): 280-290 (2013)
- Adnan, M. Sato: Dynamic Multiple Work Stealing Strategy for Flexible Load Balancing. IEICE Transactions 95-D(6): 1565-1576 (2012)
- A. Hori, J. Lee, M. Sato: Audit: A new synchronization API for the GET/PUT protocol. J. Parallel Distrib. Comput. 72(11): 1464-1470 (2012)
- M. Naito, H. Tadano, T. Sakurai: A Modified Block IDR(s) Method for Computing High Accuracy Solutions. JSIAM Letters, 4: 25-28 (2012)
- Y. Nakamura, K. Ishikawa, Y. Kuramashi, T. Sakurai, H. Tadano: Modified Block BiCGSTAB for Lattice QCD, Comput. Phys. Comm., 183: 34-37 (2012)
- R. Kanbayashi, M. Sato: A distributed architecture of Sensing Web for sharing open sensor nodes. Future Generation Comp. Syst. 27(5): 643-648 (2011)
- S. Otani, H. Kondo, I. Nonomura, T. Hanawa, S. Miura, T. Boku: Peach: A Multicore Communication System on Chip with PCI Express. IEEE Micro 31(6): 39-50 (2011)
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9 Division of Computational Informatics: *Database Group*

9.1 Research Activity

9.1.1 Information Integration Framework

(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))

(1-1) High-Availability Scheme for Distributed Stream Processing

Distributed stream processing engines (DSPEs) have recently been studied to meet the needs of continuous query processing. Because they are built on the cooperation of several stream processing engines (SPEs), node failures cause the whole system to fail. High-availability schemes such as Active Standby (AS), Upstream Backup, and Passive Standby have proposed to address this issue. Active Stanby is a processing-pairs model, and the secondary receives processing results from the upstream and processes them in parallel with the primary. If the primary is alive, the secondary does not send its processing results downstream; it logs them in the output queue. After the stop-failure of the primary, the secondary starts to send processing results from the head of the output queue downstream, and takes over the primary. In Upstream Backup (UB), the upstream primary acts as a backup SPE and each secondary is merely waiting while the primary is alive. If the primary stops, the upstream primary resends all processing results, and the secondary reprocesses them to take over the primary's state. In AS, the upstream must always send processing results to the primary and secondary in parallel. Therefore, AS's bandwidth overhead becomes the same as between primaries. However, the recovery time of AS is less than UB, because the secondary always updates its state just as the primary does. In UB, the upstream sends processing results to the secondary only if the primary has stopped. That means bandwidth overhead of UB becomes 0 before failures. However, the recovery time of UB is longer than for AS, because the secondary must recover the primary's state from the initial state.

We have proposed a new high-availability scheme Semi-Active Standby (SAS). SAS has a tunable parameter called the batch size. As the batch size changes, SAS

is able to adjust the trade-off between bandwidth overhead and recovery time. SAS behaves as UB until the size of the output queue achieves the batch size. After the output queue size reaches the batch size, all data in the queue is sent to the downstream secondary. If we set a smaller batch size, SAS shows larger bandwidth overhead and shorter recovery time. On the other hand, if SAS is set to a larger batch size, SAS shows smaller bandwidth overhead and a longer recovery time. In addition to SAS, we have proposed Adaptive Semi-Active Standby (A-SAS). A-SAS enables adaptive balancing of the bandwidth overhead and recovery time by the cost model-based automatic tuning of the batch size.

(1-2) R-Tree for Update-Intensive Applications

With the rapid advances in positioning systems - such as Global Positioning System (GPS) and Radio-Frequency Identification (RFID) - and mobile computing technologies, managing up-to-date information about the locations of massive moving objects has become a critical area of research.

In this work, we have proposed an R-tree-based index structure (called R^{sb}-tree, R-tree with semibulk loading) for efficiently managing frequent updates from massive moving objects. Basic concepts of R^{sb}-tree are threefold. 1) Update Buffering: Newly incoming updates will be buffered at in-memory buffer to reduce disk I/O. 2) Semi-bulkloading: Exploiting bulk-insertions of buffered updates into the disk-resident R-tree, total I/O cost will be reduced drastically. 3) Deferring I/O Intensive Operations: I/O intensive operations (split, removal, overflow treatment, and underflow treatment) are needed to maintain a proper R-tree structure. We defer these operations by exploiting the in-memory buffer as much as possible.

In-memory buffer structure consists of Object Registry, Histogram, and Destruction List. Object Registry is a set of object-tuple <oid, loc, cell_id, t> hashed based on oid. Histogram is a two-dimensional histogram, where each cell contains OID list of OR entries for spatial search over OR. Destruction List is a set of object-tuple <oid, t, count> hashed on oid to defer the deletion of obsolete entries. All kinds of I/O intensive operations such as insert, delete, split, and removal are buffered/deferred as much as possible. Insert/delete/update are fully operated in the memory buffer. Flush is invoked when it is necessary to make room for the newly incoming update. FlushAll writes every OR entry in OR into R-tree. FlushCell writes the maximum histogram cell. Overflow/underflow treatments are deferred by relaxing the minimum entry threshold of R-tree nodes. Garbage clean is performed once every K updates and visits every leaf node in a DFS manner.

With a reasonable memory overhead (typically only 1 percent of the whole data set), the proposed approach far outperforms the previous works in terms of update and query performance in a realistic environment. Extensive experimental evaluation reveals that the proposed approach is far more efficient than previous approaches for managing frequent updates under various settings.

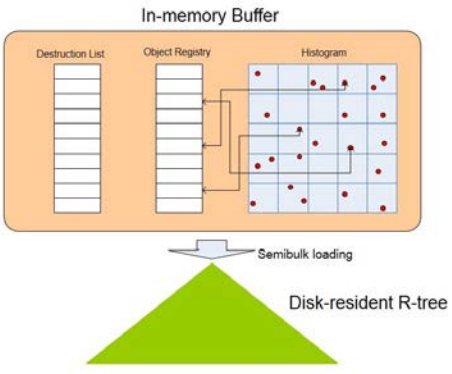


Fig. 1. Rsb-tree

(1-3) On Efficient Archiving of Stream Data

Stream data have become ubiquitous with the development of sensing devices, and therefore stream processing technology has also gained significance. A requirement of stream data processing is to provide persistence to stream data. This is not a trivial problem because to provide persistence to data, data should be written to a persistent device such as disk. Disk access cost is usually high due to random accesses, and multiple queries exacerbate the problem.

To deal with the problem, we proposed an efficient archiving method for data streams. The first technique is referred to as "operator merge." It merges multiple operators to a single operator. Since the number of operators accessing the disk is reduced from N to 1 for each stream, the number of disk accesses is reduced, thereby accelerating archiving. The second technique is referred to as "write control." It divides archiving procedures into three parts; it then assigns threads for each part so that the threads run simultaneously. The first thread conducts operators, the second writes tuples to a shared intermediate region on disk, and the third reads tuples from it and finalizes the writing of tuples. Controlling the threads so that they do not interfere with disk accesses accelerates archiving.

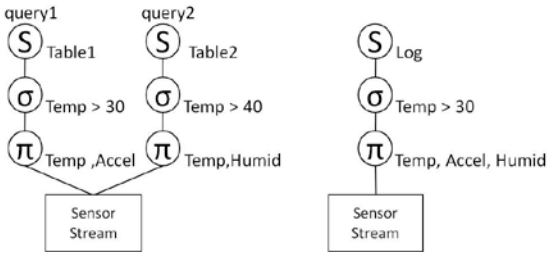


Fig. 2. Operator Merge

(1-4) Privacy Preserving Stream Data Processing

We have proposed a scheme of security aware stream processing, and then proposed two efficient techniques to reduce memory consumption to deal with encrypted data streams. Data streams are encrypted in trusted area, and they are processed in the public cloud located on untrusted area without decrypting to defend streams against malicious attacks there. The result of query evaluation is decrypted on another trusted area that user exists. Our contributions are summarized as follows.

(Contribution 1) Data processing scheme over encrypted streams: our scheme encrypts data stream tuples and queries in trusted area by an encryption module. Therefore query evaluations are executed over encrypted data. Tuples obtained by query evaluations are still encrypted, and transferred to users in trusted area. Then a decryption module in the area decrypts them and it sends them to users. (Contribution 2) Efficient techniques to reduce memory size: obviously, the above scheme needs more memory size and network bandwidth because an encryption module

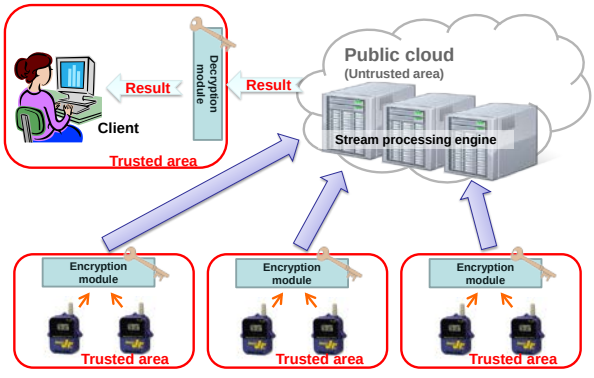


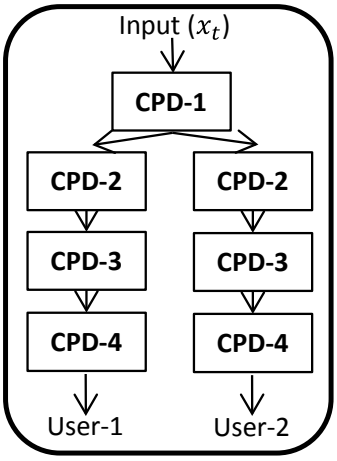
Fig. 3. Query Processing over Encrypted Data Streams

generates multiple encryption data (DET, OPE, HOM). We reduce it by analyzing continuous queries in two ways. First approach is to reduce the types of encryption by checking the types of operators in continuous queries. Second approach is to reduce the amount of synopses for window operators such as window aggregate or window join by inserting projection operator appropriately. We have also shown our approach reduces the size of memory through experiments on a prototype stream processing system which we implemented for the evaluation. To the best of our knowledge, this is the first proposal that realizes query processing over encrypted data streams.

(1-5) Outlier Detection over Packet Streams

Machine learning techniques or data mining techniques are sometimes adopted for malware detection. For example, an incident analysis system NICTER uses change point detection technique (CPD) to detect malware in real-time using its dark net traffic generated by more than 160,000 unused IP addresses. CPD is an outlier detection technique for time series data based on autoregressive model with the concept of discounting. CPD requires 6 parameters to be executed. The parameters are deeply related to detection accuracy as other machine learning techniques. Choosing a single parameter set that shows the best accuracy is desirable. Such a choice is impossible without predicting the future. Therefore, multiple parameter sets should be chosen and multiple CPD should run simultaneously to improve the accuracy of malware detection. We have been developing yet another DSMS which provides not only relational operators but also data mining operators including CPD.

On running the DSMS, we found a serious performance issue when running N processes. To accelerate simultaneous execution of multiple CPD procedures, this paper proposes a multiple query optimization scheme for CPD. For relational database system, a variety of multiple query optimization (MQO) techniques have been studied such as sharing common sub-expressions. On the other hand, our proposal is dedicated for CPD, and it shares internal steps in CPD, which is different from usual MQO. To the best of our knowledge, this is the first work that describes MQO for CPD.



Pattern 1: *Sharing* α_K, α_R

Fig. 4. Sharing CPD

(1-6) Transactional Stream Processing

A recent trend in data stream processing shows the use of advanced continuous queries (CQs) that reference non-streaming resources such as relational data in databases and machine learning models. Since non-streaming resources could be shared among multiple systems, resources may be updated by the systems during the CQ execution. As a consequence, CQs may reference resources inconsistently, and lead to a wide range of problems from inappropriate results to fatal system failures. We addressed this inconsistency problem by introducing the concept of

transaction processing into data stream processing. We introduce CQ-derived transaction, a concept that derives read-only transactions from CQs, and illustrate that the inconsistency problem is solved by ensuring serializability of derived transactions and resource updating transactions. To ensure serializability, we proposed three CQ-processing strategies based on concurrency control techniques: two-phase lock strategy, snapshot strategy, and optimistic strategy. Experimental study showed our CQ-processing strategies guarantee proper results, and their performances are comparable to the performance of conventional strategy that could produce improper results.

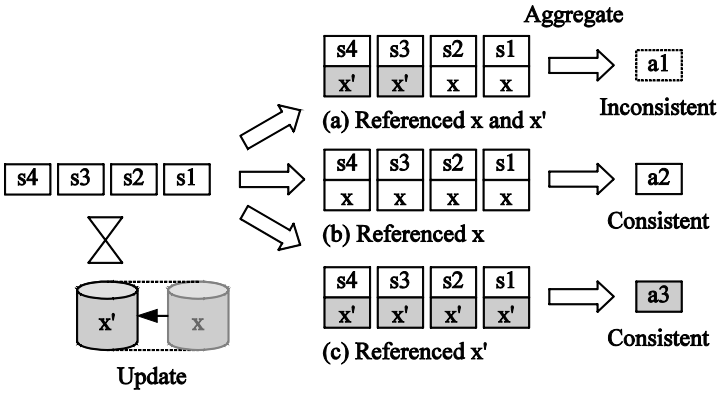


Fig. 5. Stream-relation Join and Database Update

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))

(2-1) Outlier Detection

In recent years many new techniques for collecting data have resulted in an increase in the availability of uncertain data. For example, many new hardware technologies such as sensors generate data which is imprecise, many scientific measurement techniques are inherently imprecise, and in many applications such as privacy-preserving data mining, the data is modified by adding perturbations to it.

In this work, we focus on outlier detection on uncertain data. We focus on distance-based approach because it is the simplest and the most basic one, and can be used as preprocessing before applying more sophisticated application dependent outlier detection techniques. We focus on uncertainty of attribute values and the uncertainty is modelled by the Gaussian probability density function. Specifically, the three problems are addressed: 1) Distance-based outlier detection on uncertain static data, 2) Top-k outlier detection on uncertain static data, 3) Continuous outlier detection on uncertain data streams.

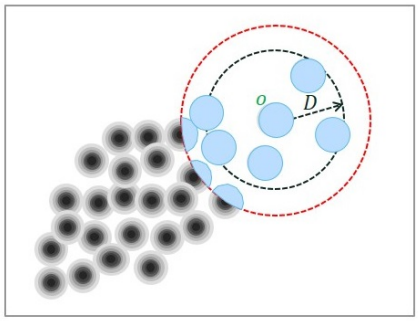


Fig. 6. Distance-based Outliers on an Uncertain Dataset

For the first problem, we gave a novel definition of distance-based outliers on uncertain data. Then, since the probability

computation is expensive, a cell-based approach was proposed to speed up the outlier detection process. The proposed approach identifies and prunes the cells containing only inliers based on its bounds on outlier score, and detects the cells containing only outliers. An approximate approach of outlier detection using the bounded Gaussian uncertainty was also proposed. The basic idea is that the bounded Gaussian distribution is a good approximation of the Gaussian distribution and can increase the outlier detection efficiency at a small loss of accuracy.

In addition, we presented an efficient top-k distance-based outlier detection approach for the second problem, and continuous outlier detection approach on uncertain time series data streams.

(2-2) Web Page Ranking Based on Social Bookmark Analysis

Web services called Social Bookmarks (SBMs) are attracting attention. A web page registered on SBM is refereed by user interests, preferences, convenience and a variety of individual review points. If a page is bookmarked by many users, it seems more informative, and also seems to have reliable content. So a bookmark from an SBM user to a web page is a vote, and the number of bookmarks to web pages in SBM is a barometer of web page values.

We proposed a ranking method called S-BITS using bookmark relationships between bookmarkers and web pages. S-BITS ranks web pages based on a bipartite graph between bookmarked web pages and bookmarking users like the HITS algorithm. It estimates a web page value based on who bookmarks the page, and also estimates a bookmarker value based on what pages that person bookmarks. When a bookmarker is knowledgeable and/or trustworthy, a page gets a high score if that person bookmarks the page. In the experiments, our method yielded better results than an existing web search engine and another bookmark-based page ranking method SBRank.

In SBM, there are many users who do not update or delete bookmark information pointing to obsolete web pages. Actually, there are many obsolete web pages: old news and press releases that are not worth a look. To judge the current value of a web page based on SBM, we should look at how the page has been bookmarked until now, and how frequently the page has been bookmarked. One way to observe the degree of obsolescence is to compare page bookmarking rates between the past and present. Based on this idea, we proposed S-BIT* improving S-BITS. We estimate the "Activation Level." of each page, which shows how attractive a page is on a particular date. Analyzing time-series variation of social bookmarking frequency, we can estimate the activation level of a web page the Hidden Markov Model (HMM). S-BITS* incorporates this activation level concept. Our experiments showed that S-BITS* yields better ranking. These experiments suggest that our estimation method of activation levels is effective and is similar to the human sense of worth.

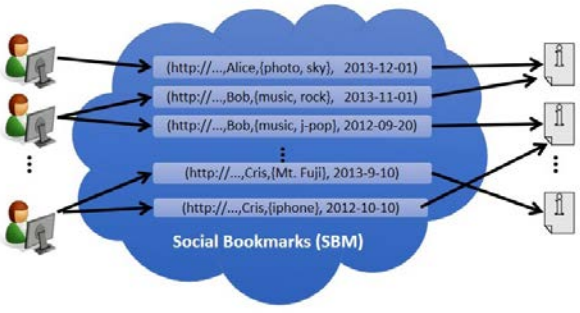


Fig. 7. Social Bookmarking

(2-3) Microblog Analysis

Recently, microblogs, such as Twitter and Sina Weibo, have been attracting considerable attentions as a new type of information in the Internet. They have some interesting characteristics that many users exchange short messages in a real-time manner, while presenting similar features as other (ordinary) social medias, like SNS. For this reason, it is becoming increasingly important to extract useful information from microblogs. To address this problem, we conducted several researches:

TURank: Twitter User Ranking Based on User-Tweet Graph Analysis

In Twitter, the number of users is usually quite large, and it is therefore hard for the users to find out useful users. There are some related works in that the number of followers or follow graph (Twitter social graph) is used to quantify the users' authority. However, they are not sufficient in the sense that they do not take into account the posts from the users, though content analysis over short messages often results in noisy and unreliable results.

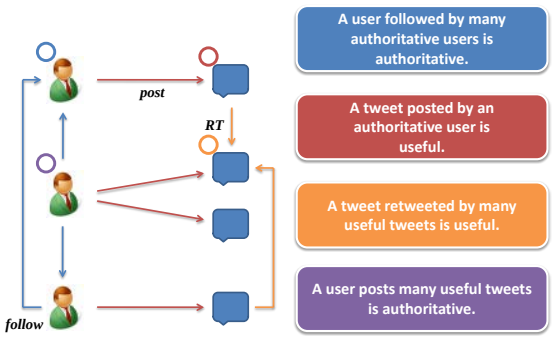


Fig. 8. Twitter Social Graph.

In this work, we proposed TURank (Twitter User Rank), which is an algorithm that measures the Twitter users' authority scores considering both a Twitter social graph and how tweets actually flow among users by taking into account Retweets. More precisely, we construct a graph consisting of 1) Twitter users, 2) posts, 3) follow/followed edges, 4) post/posted edges, and 5) Retweet/Retweeted edges (Figure 1: Twitter social graph.), and apply ObjectRank, a graph analysis method for graphs containing heterogeneous nodes and edges, to get Twitter user's ranking considering the above mentioned aspects. The experimental results showed that the proposed scheme can accurately rank the users than other competitive methods.

Tag-based User Topic Discovery using Twitter Lists

There are growing needs to find useful information from Twitter, because an enormous amount of information is transmitted in real time. Twitter users play an important role as information sources and transmit information based on their interests or preferences. Therefore, to identify useful information, it is important to know what topics users tend to transmit information about.

In this work, we proposed a method to estimate the user topics by tagging users using Twitter lists. Twitter lists are the official functionality to make a "user list" and share it. The list members (users

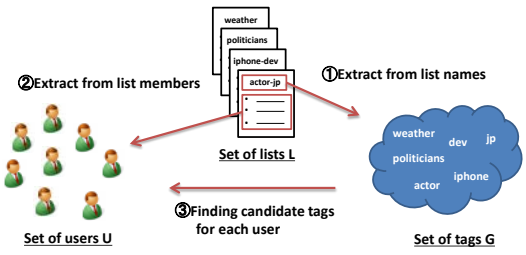


Fig. 9. Tag Generation from Twitter Lists.

included in the list) often relate to a certain topic described as the list name (Fig. 9). Experimental results show the effectiveness of the proposed method.

Recommending Fresh URLs using Twitter Lists

Recommender systems for social media have attracted considerable attentions due to its inherent features, such as a huge amount of information, social networks, and real-time features. In microblogs, which have been recognized as one of the most popular social media, most of URLs posted by users are considered to be fresh (i.e., shortly after creation). Hence, it is important to recommend URLs in microblogs for appropriate users because users become able to obtain such fresh URLs immediately.

In this work, we proposed a URL recommender system using Twitter user lists. Twitter user list is the official functionality to group users into a list along with the name of it. Since it is expected that the members of a list (i.e., users included in the list) have similar characteristics, we utilize this feature to capture the user interests. Experimental results showed that our proposed method achieves higher effectiveness than other methods based on the follow-followed network which does not offer user interests explicitly.

Landmark-Based User Location Inference in Social Media

Location profiles of user accounts in social media can be utilized for various applications, such as disaster warnings and location-aware recommendations. In this work, we proposed a scheme to infer users' home locations in social media. A large portion of existing studies assume that connected users (i.e., friends) in social graphs are located in close proximity. Although this assumption holds for some fraction of connected pairs, sometimes connected pairs live far from each other.

To address this issue, we introduced a novel concept of local landmarks, which are defined as users with a lot of friends who live in a small region. Local landmarks have desirable features to infer users' home locations such as providing strong clues and allowing the locations of numerous users to be inferred using a small number of landmarks. Based on this concept, we proposed a landmark mixture model (LMM) to infer users' location. The experimental results using a large-scale Twitter dataset showed that our method improves the accuracy of the state-of-the-art method by about 27%.

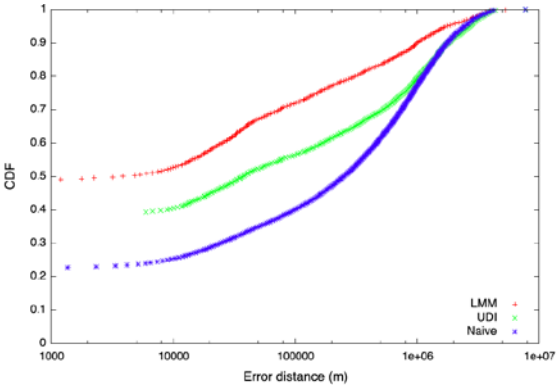


Fig. 10. Performance of the Proposed Scheme

(2-4) GPU-based Acceleration of Data Mining

GPGPU (General-purpose computing on graphic processing unit) has been gaining much public attention as a new computational platform. The idea is to exploit GPUs for not only graphical processing, but also general-purpose computation. GPGPU now covers diverse range of applications, such as physical simulation,

audio processing, video processing, and cryptography processing, etc. In work group, we have exploited GPU to accelerate various data mining tasks.

Efficient Probabilistic Latent Semantic Indexing using Graphics Processing Unit

In this work, we proposed a scheme to accelerate the Probabilistic Latent Semantic Indexing (PLSI), which is an automated document indexing method based on a statistical latent semantic model, exploiting the high parallelism of Graphics Processing Unit (GPU). Our proposal is composed of three techniques: the first one is to accelerate the Expectation-Maximization (EM) computation by applying GPU matrix-vector multiplication; the second one uses the same principles as the first method, but deals with the sparseness of co-occurrence of words and documents; and the third one is to use the concurrent kernel execution, which is available on NVIDIA Fermi architecture, in order to speed up the process. We compared the performance of the proposed scheme with the non-parallelized implementation. The results showed that our method could be more than 100 times faster than the CPU-based implementation in our environment. By dealing with the sparseness of the data, we could not only process more documents and words using GPU, but we could also keep more data on the device memory so that we can avoid massive data copy transfer between the host and the device susceptible to reduce the execution performance.

GPU Acceleration of Probabilistic Frequent Itemset Mining from Uncertain Databases

Uncertain databases have been widely developed to deal with the vast amount of data that contain uncertainty. To extract valuable information from the uncertain databases, several methods of frequent itemset mining, one of the major data mining techniques, have been proposed. However, their performance is not satisfactory because handling uncertainty incurs high processing cost. In order to address this problem, we utilized GPGPU.

In this work, we proposed a method for frequent itemset mining from uncertain databases using GPU. The main idea is to speed up probability computations by making the best use of GPU's high parallelism and low-latency memory (Fig. 11). We also employed an algorithm to manipulate a bitstring and data-parallel primitives to improve performance in other parts of the method. Extensive experiments showed that our proposed method is up to two orders of magnitude faster than existing methods.

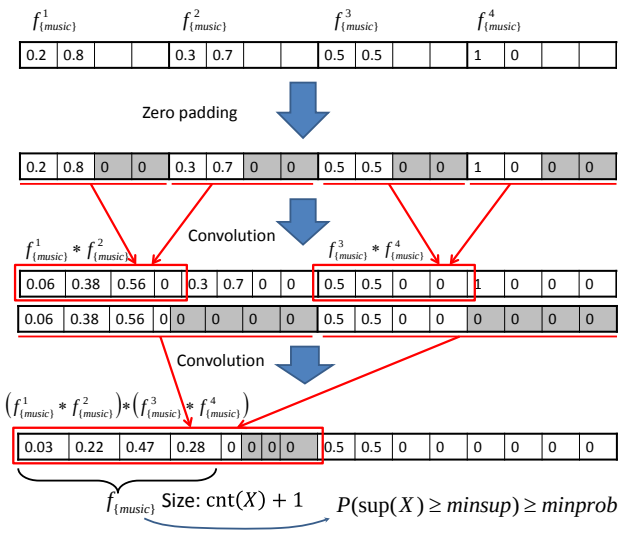


Fig. 11.Computing SPMF on GPU.

Moreover, we proposed multi-GPU methods for GPU-based clusters. First, we developed methods on a single node with multiple GPUs, and then we extended the methods to use a GPU cluster. The proposed methods reduce data dependencies by distributing candidates of probabilistic frequent itemsets among GPUs. In addition, the methods consider load balancing, which is also an important issue to achieve scalability. Experiments showed that the single-node methods realize near-linear speedups, and the methods on a GPU cluster of eight nodes achieve up to a 7.1 times speedup.

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))

XML (Extensible Markup Language) is a standardized data format for semi-structured data and documents, and growing amount of information is being accumulated in the form of XML in various application domains. Besides, RDF (Resource Description Framework) is gaining its popularity due to the emergence of LOD (Linked Open Data). With the aim of investigating techniques for managing massive XML/RDF resources, we have conducted the following researches.

(3-1) Online Analytical Processing of XML Data

Given a set of XML data, it is desirable if it is possible to extract valuable information from them by analytical processing, rather than by simple query retrieval. For this purpose, in this work we developed a technique called XML-OLAP (Online Analytical Processing), which enables us to perform multidimensional analytical processing over XML data. More precisely, we proposed a novel (formal) definition 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.

(3-2) Parallel Processing of XML Data using PC-Clusters/Multi-core Processors

For a large collection of XML data, it is highly required to process queries over them as fast as possible. In the meantime, due to the commoditization of PCs and multi-core CPUs, it is becoming increasingly important to develop parallel processing methods for database systems, including XML databases, for achieving better query

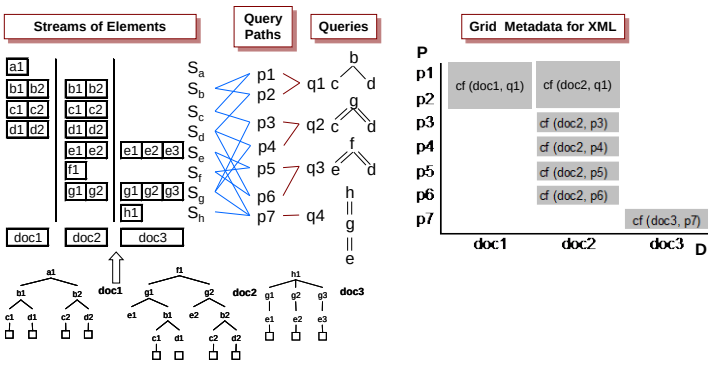


Fig. 12.XML Data Partitioning in GMX.

performance. In this work, we addressed the problem of parallel XML query processing using PC-clusters/multi-core CPUs.

First, we proposed a scheme of data partitioning scheme for XML data based on a grid metadata model for XML data that gives a conceptual view to partition XML data, specifically for holistic twig joins processing (Fig. 12). The proposed model adopts a cost-based model and facilitates a set of partition refinement methods for workload balancing purpose. The model has features of reducing the workload variance significantly on the cluster system; duplicating XML data necessarily to avoid data dependency among cluster nodes, and exploiting inter query parallelism and intra query parallelism. We evaluated the effectiveness of our proposed model in the experiment that our data partitioning method has better workload balance and has an impact on better parallel speed up performance as well.

Second, we proposed a parallel TwigStack algorithm executed on a shared-memory multi-core system for achieving scalable query performance against large XML data. Our proposed scheme explores the following features. Firstly, we perform on-the-fly partitioning on input streams of XML nodes for subsequent parallel execution and, thereby, ensure that query solutions in a partition can be obtained by the TwigStack algorithm without being dependent on other partitions. Secondly, we propose a scheme for estimating the optimal partition size for a given system configuration by taking L2-cache size into account. Finally, we introduce a partition prefetching technique to alleviate the overheads of performing the on-the-fly partitions. The experimental results demonstrated that our proposed parallel algorithm works effectively and efficiently. The parallel speedup scales up to the number of available CPU-cores.

(3-3) A Framework for Faceted-navigation of XML Data

With the growth of XML data, it is required to provide a quick solution to search for desired information out of massive XML data. However, conventional query languages for XML data, such as XPath and XQuery require a user to be familiar with both the languages and the structure of XML data, which becomes a barrier for many (non-expert) users.

In this paper, we proposed a framework of faceted navigation over XML data, in which users can navigate a collection of XML data using a simple query interface without issuing complicated queries. General faceted navigation schemes are used to browse objects (or records) containing multiple properties. However, because XML is semi-structured in nature, it is not straightforward to apply faceted navigation to XML data. More precisely, we formulate faceted navigation over XML data by

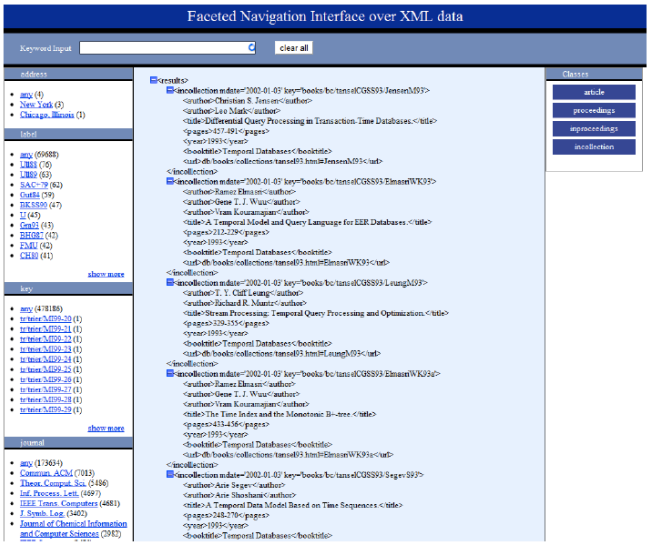


Fig. 13.Faceted-navigation over XML Data.

giving dentitions of class, property, object, and facet in XML data. We then formulate typical user interactions in faceted navigation as operations over aforementioned concepts (class, object, and facet). We also proposed a system based on the proposed framework. Finally, we showed experimental evaluations using the prototype system to show the effectiveness of our proposed scheme.

(3-4) Energy-efficient XML Stream Processing

The rapid growth of energy consumption by computer systems has drawn a considerable public attention in relation to the emerging global/environmental phenomena, such as global warming, carbon dioxide emission, etc. Consequently, there have strong demands for computer systems to reduce energy consumption, while maintaining high computational power. In this work, we proposed a scheme of energy-efficient XML stream processing through element-skipping parsing. Although parsing is one of the most computationally heavy part in the process of XML stream processing, existing techniques do not focus on the efficiency of XML parsing. To this problem, in our scheme, we proposed element-skipping parsing where the parsing of such XML elements that do not contribute to the final query result is skipped with the coordination of XML parser and query processor. We showed that the scheme is effective in reducing the execution time as well as energy consumption of stream-based XML query processor.

(3-5) RDF/LOD Data Processing

LOD (Linked Open Data) has rapidly been diffusing in accordance with the Open Data movement. Consequently, there is a global trend for governments, industries, and institutes to publish their data in the form of RDF (Resource Description Framework) using SPARQL endpoints. To better manage such massive information resource in RDF format, we conducted the following researches.

Efficient Reasoning and Querying over Large-Scale RDF Data

When querying RDF and RDF Schema (RDFS) data, for improving the performance, it is common to derive all triples according to RDFS entailment rules before query processing. An undesirable drawback of this approach is that a large number of triples are generated by the RDFS reasoning, and hence considerable amount of storage space is required if we materialize the RDFS closure. In this work, we proposed RDF packages, which is a time and space efficient format for RDF data. In an RDF package, a set of triples of the same class or triples having the same predicate are grouped into a dedicated node named Package. Using Packages, we can represent any metadata that can be expressed by RDF. An important feature of the RDF packages is that, when performing RDFS reasoning, the same rules can be applied without any modification, thereby

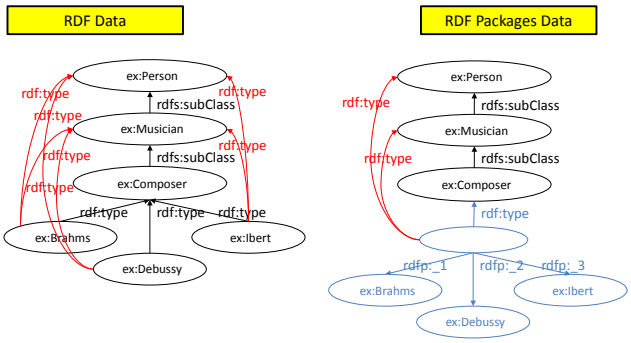


Fig. 14. Space-efficient Representation of RDF Data using RDFPackages.

allowing us to use existing RDFS reasoners. In this work, we discussed the model of RDF packages and its rules, followed by the transformation between RDF and RDF packages. We also discussed the implementation RDF packages using an existing RDF framework. Finally, we demonstrated the performance of the proposed scheme in triple size, reasoning speed, and querying speed.

An ETL Framework for Online Analytical Processing of Linked Data

In this work we proposed an ETL framework for the online analytical processing of linked data. More and more data are published online in machine-readable formats, and linked data is one of the major ways to do it. Such data often contain numerical data, as well as text, and there is a strong demand to perform analytical processing over them using existing OLAP systems. Our proposed framework is to streamline the ETL process from Lined Data to multidimensional data models for OLAP. Unlike other related approaches, our framework does not require any dedicated RDF vocabularies for multidimensional analysis. Instead, we exploit the relationships among entities, inherent hierarchical structures, and external references to derive multidimensional schema and semantic hierarchies. This allows us to perform OLAP analysis over general Lined Data even if they are not based on RDF vocabularies for OLAP. In the experiments, we demonstrated that our scheme can be applied to existing datasets.

(3-6) Privacy-preserving Database Querying

Privacy-preservation techniques are gaining considerable attentions from public due to the global diffusion of the Internet and various services in it, such as SNS. In particular, in the cloud-computing environment where computational resources, including database contents, are hosted at the cloud-service provider, it is crucial to protect the data privacy.

Encryption can provide strong security for sensitive data against inside and outside attacks. This is especially true in the "Database as Service" model, where confidentiality and privacy are important issues for the client. In fact, existing encryption approaches are vulnerable to a statistical attack because each value is encrypted to another fixed value. We presented a novel database encryption scheme called MV-OPES (Multivalued-Order Preserving Encryption Scheme), which allows privacy-preserving queries over encrypted databases with an improved security level. Our idea is to encrypt a value to different multiple values to prevent statistical attacks. At the same time, MV-OPES preserves the order of the integer values to allow comparison operations to be directly applied on encrypted data (Fig. 15). Using calculated distance (range), we proposed a novel method that allows a join query between relations based on inequality over encrypted values. We also presented techniques to offload query execution load to a database server as much as possible, thereby making a better use of server resources in a database

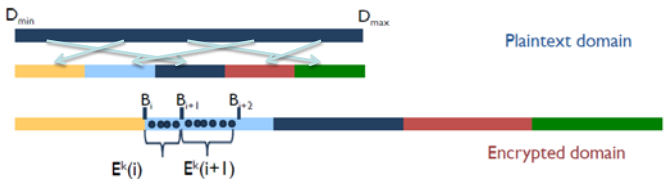


Fig. 15. Multi-valued Order-preserving Encryption.

outsourcing environment. Our scheme can easily be integrated with current database systems as it is designed to work with existing indexing structures. It is robust against statistical attack and the estimation of true values. MV-OPES experiments showed that security for sensitive data can be achieved with reasonable overhead, establishing the practicability of the scheme.

9.1.4 Database Applications in Science Domains

(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))

As a group in the Center for Computational Sciences (CCS), we actively collaborate with other research divisions/groups in CCS, as well as with those in other research institutes, such as AIST and ISAS/JAXA.

(4-1) Faceted-Navigation System for QCDml Ensemble XML Data

The International Lattice Data Grid (ILDG) is a data grid for sharing and exchanging lattice QCD gauge configurations among researchers in particle physics. To facilitate the domain researchers to find desired data, we have developed a faceted navigation system for QCDml ensemble XML data, which is an XML-based metadata format for the dataset. A faceted navigation system allows a user to search for one's desired information in an exploratory way, thereby enabling the user to browse a set of XML data without using specialized query languages such as XPath and XQuery. However, designing a faceted navigation interface for XML data is not straightforward due to the tree and flexible, tree-like nature of XML.

In this work, we attempted to design and implement a dedicated faceted navigation system for QCDml on top of an XML database. The interface is designed by taking the domain experts' usability into account. We also care about the system's performance. In general, the process of faceted navigation is computationally expensive because of the need for aggregate computation of each available facets. In order to alleviate this, we make use of a relational database system as the engine to speed up the aggregate computation. We finally demonstrate the implemented faceted navigation system, which has been made available on the Web.

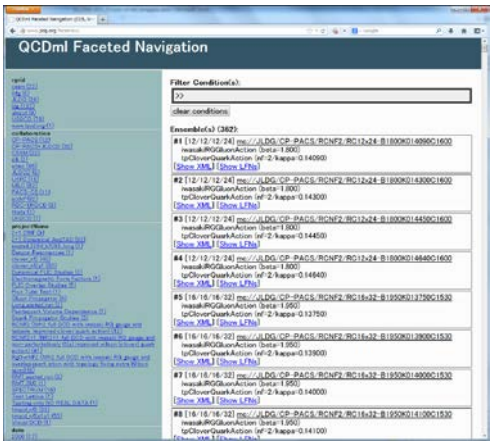


Fig. 16.
http://www.jldg.org/facetnavi/

(4-2) Event Detection from Large Scale Satellite Sensor Data

With the advances of sensing technologies, massive amount of scientific data have been collected and analyzed in these days. LSST generates 20 TB per night,

LHC generates 15 PB per year, and an earth observation satellite sensor data related to GEO-Grid has generated more than 170 TB so far. ASTER sensor data are high resolution image data provided GEO-Grid. ASTER data provides three kinds of data. One of them is thermal infrared radiometer, which is shortly denoted as TIR. Originally, TIR data are utilized to discover mineral resources and to observe status of atmosphere and the surface of ground and sea.

Unlike the above cases, we believe that TIR can be used to detect hot spots all over the world. The meaning of "hot spots" is places that generate thermals which include steel plants or fires. This work proposed a threshold based method and a statistics based method to discover hot spots from TIR data. We implemented our methods with SciDB. All of procedures in our methods are implemented by array manipulation operators which are natively supported by SciDB and UDFs. The result of experiments which detect steel plants showed that statistics based method outperforms threshold based method as for recall.

Steel Plants	# data	Duration
Kashima	9	2002—2011
Sumitomo Yahata	9	2000—2011
Sumitomo Metal Engineering (Wakayama)	7	2002—2011
Nippon Steel Corporation (Nagoya)	9	2000—2011
Kobe Steel Group	8	2002—2011
JFE East Japan	14	2000—2011
JFE West Japan	12	2001—2009
Nisshin Steel (Kure)	9	2002—2011

Fig. 17. Detected Hot Spots

(4-3) X-ray Outburst Detection from X-ray Astronomy Data

X-ray outburst is a phenomenon that an X-ray object emits strong X-ray in a short period of time. Prof. Ebisawa (ISAS/JAXA) and his group have found that some X-ray objects happen to present similar light-curves in shape. To exhaustively survey such similar light-curves out of massive X-ray astronomy data, we applied similarity search techniques for time-series data.

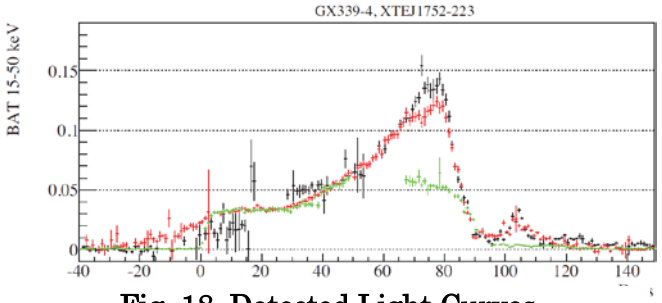


Fig. 18. Detected Light Curves.

9.2 Research Results

Information Integration Framework

(1-1) High-Availability Scheme for Distributed Stream Processing

We have developed a new high-availability scheme Semi-Active Standby (SAS), which can adjust the trade-off between bandwidth overhead and recovery time. Extending SAS, we have developed Adaptive Semi-Active Standby (A-SAS), which enables adaptive tuning under a given constraint.

(1-2) R-Tree for Update-Intensive Applications

We have developed an R-tree-based index structure (called R^{sb}-tree, R-tree with semibulk loading) for efficiently managing frequent updates from massive moving objects. With a reasonable memory overhead (typically only 1 percent of the whole

data set), the proposed approach far outperforms the previous works in terms of update and query performance in a realistic environment.

(1-3) On Efficient Archiving of Stream Data

To provide persistence to stream data is an important issue. We proposed an efficient archiving method for data streams. Our proposed system did not violate any deadline misses until the input rate reached 100 tuples /s.

(1-4) Privacy Preserving Stream Data Processing

We have proposed a scheme that evaluates queries over encrypted data streams, CryptStream. The result of experiments showed that our first technique reduced 90 % size of memory space.

(1-5) Outlier Detection over Packet Streams

To accelerate simultaneous execution of multiple change point detection (CPD) queries, we applied multiple query optimization scheme. The result of experiments showed that proposed method achieved by a factor of 5 performance improvement.

(1-6) Transactional Stream Processing

Advanced continuous queries (CQs) reference non-streaming resources such as databases and machine learning models. When non-streaming resources are updated, CQs may reference resources inconsistently. To address this issue, we have proposed a new concept of transactional stream processing, and developed some execution schemes to realize it.

Data Mining and Knowledge Discovery

(2-1) Outlier Detection

We have developed novel outlier detection schemes for uncertain datasets, where the uncertainty of attribute values is modelled by the Gaussian probability density function. We invented three schemes: 1) Distance-based outlier detection on uncertain static data, 2) Top-k outlier detection on uncertain static data, 3) Continuous outlier detection on uncertain data streams.

(2-2) Web Page Ranking Based on Social Bookmark Analysis

We have developed a ranking method called S-BITS using bookmark relationships between bookmarkers and web pages. We have also developed S-BIT* improving S-BITS by incorporating the “Activation Level.” of each page. The experiments suggested advantages of the proposals.

(2-3) Microblog Analysis

We have developed the following methods for Twitter: 1) a user ranking and a user-topic detection scheme, 2) URL recommendation method, and 3) a user-location estimation method.

(2-4) GPU-based Acceleration of Data Mining

We have developed methods to accelerate probabilistic latent semantic indexing (PLSI) and probabilistic frequent-itemset mining.

XML and Web Programming

(3-1) Online Analytical Processing of XML Data

We have developed online analytical processing (OLAP) for XML data.

(3-2) Parallel Processing of XML Data using PC-Clusters/Multi-core Processors

We have developed parallel query processing methods for XML data using PC-clusters/multi-core CPUs.

(3-3) A Framework for Faceted-navigation of XML Data
We have developed a framework for faceted-navigation over XML data
(3-4) Energy-efficient XML Stream Processing
We have developed an energy-efficient query processing over XML streams.
(3-5) RDF/LOD Data Processing
We have developed methods for RDF and LOD data: 1) a space-efficient representation of RDF/RDFS data for efficient query and reasoning and 2) an ETL-framework for OLAP over LOD data.
(3-6) Privacy-preserving Database Querying
We have developed a novel privacy-preserving query processing scheme for numerical data in cloud environment.

Database Applications in Science Domains
(4-1) Faceted-Navigation System for QCDml Ensemble XML Data
We have developed a faceted-navigation system for QCDml ensemble XML data for International Lattice Data Grid (ILDG).
(4-2) Event Detection from Large Scale Satellite Sensor Data
We implemented hot spot detection methods with SciDB. The result of experiments showed that proposed method successfully detected hot spots including steel plants.
(4-3) X-ray Outburst Detection from X-ray Astronomy Data
We have investigated techniques for similarity search over X-ray astronomy data to detect similar X-ray outburst light curves.

9.3 Collaboration

9.3.1 Division of Global Environmental Science

GPV/JMA Archive

As a collaborative work with the Division of Global Environmental Science and the Division of High Performance Computing Systems in CCS, we have been developing, maintaining, and managing GPV/JMA Archive. Its objective is to archive 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.

Fig. 19.
http://gpvjma.ccs.hpcc.jp/~gpvjma/

Automatic Classification of Pressure Patterns

In climate research, pressure patterns are often very important. When a climatologist needs to know the days of a specific pressure pattern, for example "low pressure in West area of Japan and high pressure in East area of Japan (Japanese winter type)," they have to check a huge number of surface weather charts in a visual manner. To overcome this problem, we have proposed an automatic classification using support vector machine (SVM), which is a machine learning method. We tried to classify pressure patterns into two classes: "winter type class" and "non-winter type class." For both training dataset and test dataset, we used the JRA-25 dataset from 1981 to 2000. Experiments showed that our method obtained a greater than 0.8 F-measure. Beyond that, we found that the differing results are based on differences in training dataset.

9.3.2 Division of Particle Physics

As a part of our collaboration, we take part in the ILDG (International Lattice Data Grid) and JLDG (Japan Lattice Data Grid). ILDG was initiated in 2002 to provides standards, services, and tools to facilitate sharing and exchange of lattice QCD gauge configurations among organizations in collaboration using a grid infrastructure across five regional grids: CSSM (Australia), JLDG (Japan), LDG (Europe), UKQCD (UK), and USQCD (USA).

9.3.3 National Institute of Advanced Industrial Science and Technology (AIST)

We collaborate with the database group in the Advanced Industrial Science and Technology (AIST) in the area of scientific data management. In particular, we have collaborated in the GEO Grid (http://www.geogrid.org) to develop applications of massive satellite sensor images.

9.3.4 Japan Aerospace Exploration Agency (JAXA)

We collaborate with Institute of Space and Astronautical Science (ISAS) in the Japan Aerospace Exploration Agency (JAXA). More precisely, we have been investigating X-ray astronomy data to detect X-ray outbursts. In addition, we attempt to analyze bibliographic data in the area of astrophysics stored in the SAO/NASA Astrophysics Data System (ADS) to extract useful information regarding researchers and research papers.

9.4 Future Plan

1) Research and Development for Data Engineering Challenges

In recent years, "Big Data" has become a new ubiquitous term. Big Data has started to give huge impacts on many aspects of human life and our society. To address technical issues and challenges involved in Big Data, data engineering is one of key principles and we have to continue our activities to advance the technologies. We have studied a wide variety of topics in data engineering. Especially, we have conducted our research from the viewpoints of information integration framework, data mining & knowledge discovery, and XML & Web programming. We will continue to intensively perform research and development in those areas. We also try to make our research activities practical as much as possible in cooperation with other groups in CCS.

As well as Volume, Big Data involves Variety, Velocity, and Veracity. As for the topic of information integration framework, we attempt to address all these issues. Especially, we will have a more and more variety of data and data sources. Realtime processing and analysis of such heterogeneous big data is a strong demand from the society. Development of a data integration framework which can really accommodate Big Data is a key technical challenge. We need to develop novel schemes to address new issues as well as combining and integrating existing technologies for data acquisition, data cleaning, data management, data mediation, data analysis, stream processing, and so on. We will make the best of powerful computing facilities in CCS to tackle Big Data challenges. As for data mining and knowledge processing techniques, we will have to enable more deep analysis of large-scale real datasets. Integration, mining, and analysis of heterogeneous datasets involve many interesting research issues. Recent evolution of new social media and social information services will provide many new research opportunities. In social media analysis, privacy-related issues are also important. As for techniques related to XML and Web programming, we will address new emerging issues such as e-book contents management and social readings. The movement toward LOD (Linked Open Data) also provides new technical challenges. We will continue our research activities to challenge all these issues.

2) Scientific Data Management

We have been collaborating with Division of Global Environmental Science in development and maintenance of GPV/JMA Archive. We will continue the development, and try to improve the usability of the system. We will also continue our collaboration with Division of Particle Physics in the ILDG (International Lattice Data Grid) and JLDG (Japan Lattice Data Grid) projects. We do not limit the research domain to data management in meteorology and particle physics, and try to address data engineering problems in other scientific domains. Actually, in 2013, we started a collaboration with the Biological Science Group to develop a system for managing biological sequence alignment data with the aim of supporting the research activities of the domain researchers.

3) Reinforcement of Cooperation with Other Divisions and Organizations

In addition to the collaboration with Division of Global Environmental Science and Division of Particle Physics, we will continue and expand collaborations with National Institute of Advanced Industrial Science and Technology (AIST) and Japan Aerospace Exploration Agency (JAXA). We will strengthen collaboration

with the computational media group within our division in research on realtime sensing, data mining, and media processing. We are also collaborating with a number of industrial partners in research on stream processing and data mining. We will continue our endeavor to return our research contributions to society.

9.5 Publications

9.5.1 Journal Papers

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10 Division of Computational Informatics: *Computational Media Group*

10.1 Research Activity

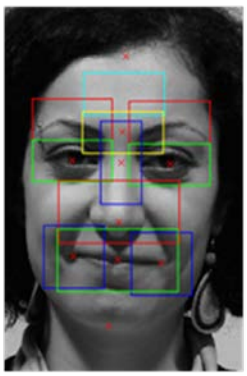
The Computational Informatics Research Division is founded in 2004 and the medium-term/long-term mission of this division is to investigate novel methods at the frontier of computational informatics through computational media, which will be a key technology to unite human beings and vast data / high performance computation world.
Since computational media should be used as a tool to promote collaboration between people and data/process at computer side, real-time processing and instant reaction are essential. We call this research framework as "Real-World Computational Informatics".
As for the computer-side resources, sensors, database, grid/cloud computing, and computer network should be integrated gracefully. They should be served in a fashion of fusion of data and process to users as a form of computational media. Cameras and their videos are the main resource in our group because we think visional communication is the most promising path to let people understand digital world intuitively and deeply. We utilize Mixed Reality and Augmented Reality technology for this purpose.
Our research achievements have been published to flagship international journals in the areas of computer vision and virtual reality. As for outreach activities, we set up our booth at Innovation Japan for 2008, 2009, 2010, and 2011.
Our research activities have been supported partially from the research funds listed here. We appreciate their support.

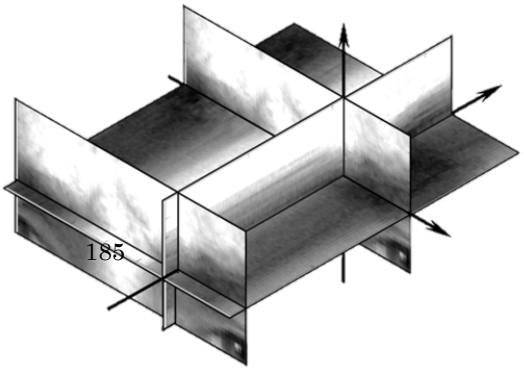
- "HD Quality Improvement of Free Viewpoint Video Browsing by Human Billboard for Large-Scale Space," by Grant-in-Aid for Scientific Research (B), Japan Society for the Promotion of Science, 2013-2016.
- "Spatio-Temporal Analysis and Mixed-Reality-Based Visualization of Video Images of Environmental Cameras toward Safe and Efficient Viewing," by Grant-in-Aid for Scientific Research (B), Japan Society for the Promotion of Science, 2011-2014.

- “Information Compression for Displaying Immersive Perception by Boundary Search of a Feeling of Strangeness in Mixed Reality Space”, by Grand-in-Aid for 萌芽, Japan Society for the Promotion of Science, 2011-2014.
- “An Observer Oriented Free-Viewpoint Video Generation,“ by Grand-in-Aid for Young Scientists (A), Japan Society for the Promotion of Science, 2009-2011.
- “A Development of Walking-Out Support System Development of Visually Impaired Person in Indoor and Outdoor Daily Scene by Sensor Integration of Imaging and GPS,” grant of MHLW, 2009.
- “See-through Vision : Visual Augmentation for Pedestrians by Using Surveillance Cameras,“ by Grand-in-Aid for Scientific Research (A), Japan Society for the Promotion of Science, 2006-2009.
- “A Video Surveillance Method by Using Environmental and Mobile Cameras with Considering Privacy Issue,” by Grand-in-Aid for Young Scientists (A), Japan Society for the Promotion of Science, 2006-2009.

1.1.1 Massive Sensing and Sensor Fusion for Human Mind Analysis

Since the estimation of human mind is a key technology of HCI, we have invented a new computer vision based method which is effective on interview scenario. Facial micro-expressions are fast and subtle facial motions that are considered as one of the most useful external signs for detecting hidden emotional changes in a person. However, they are not easy to be detected and measured as they appear only for a short time under 1 second, with small muscle contraction in the facial areas where salient features are not available.
We propose a new computer vision method for detecting and measuring timing characteristics of facial micro-expressions. The core of this method is based on a descriptor that combines pre-processing masks, histograms and concatenation of spatial-temporal gradient vectors. The figure on left shows the masks where muscle under skin should make changes visually. The figure right shows a micro-expression can be found by temporal analysis. Our proposed 3D gradient histogram descriptor is able to detect and measure the timing characteristics of the fast and subtle changes of the facial skin surface. This method is specifically designed for analysis of videos recorded using a hi-speed 200fps camera. Final classification of micro expressions is done by using a k-mean classifier and a voting procedure. The Facial Action Coding System was utilized to annotate the appearance and dynamics of the expressions in our new hi-speed micro-expressions video database.
We have established a novel facial video database that gives a basis of facial motion analysis. The advantages of our new open database include the support of high speed video, thermal imaging, motion captured data under strict experiment procedure with subjects of wide variety of cultural difference. This database is available at our web site, and we have been talking with foreign research institutes for further expansion of this research.

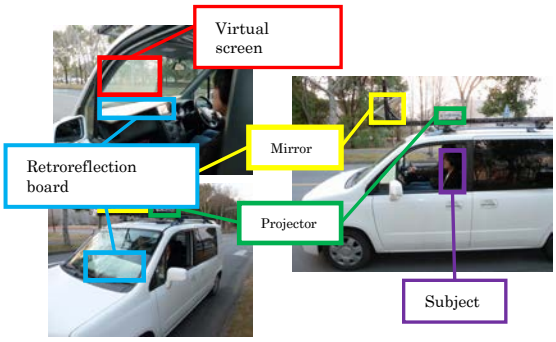




(Left) Masks on a face.
(Right) Spatio-temporal change at forehead.

1.1.2 Driver support by Augmented Reality technology

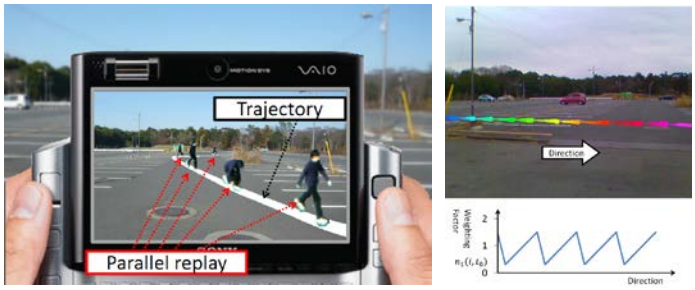
One of the most critical applications of computational media is to support a driving task in a vehicle on road. Since we think AR display on windshield called "windshield display" is a promising device, we have been working on developing novel technologies on windshield display.
One of our achievements is explained here in this report. We have proposed a new road map visualization method at windshield display (Figure left). Road structure ahead of a vehicle is shown by CG line segments at the upper area of driver view in augmented reality fashion (Figure right). Road line segments are virtually placed as if they are lifted up in the sky. By our new visualization method, the rendered CG does not occlude roads and objects on the roads that are crucial for drivers. Yet the drivers can easily understand the road map because the road line segments in the sky has vertical correspondence with the road on the ground. We have implemented a prototype of window shield display and realized our new visualization method on a vehicle. We also conducted a preliminary experiment for evaluation.



(Left) Windshield display
(Right) Lifted road map at windshield

1.1.3 Compact Video Expression of Moving Objects at Outdoor Scene

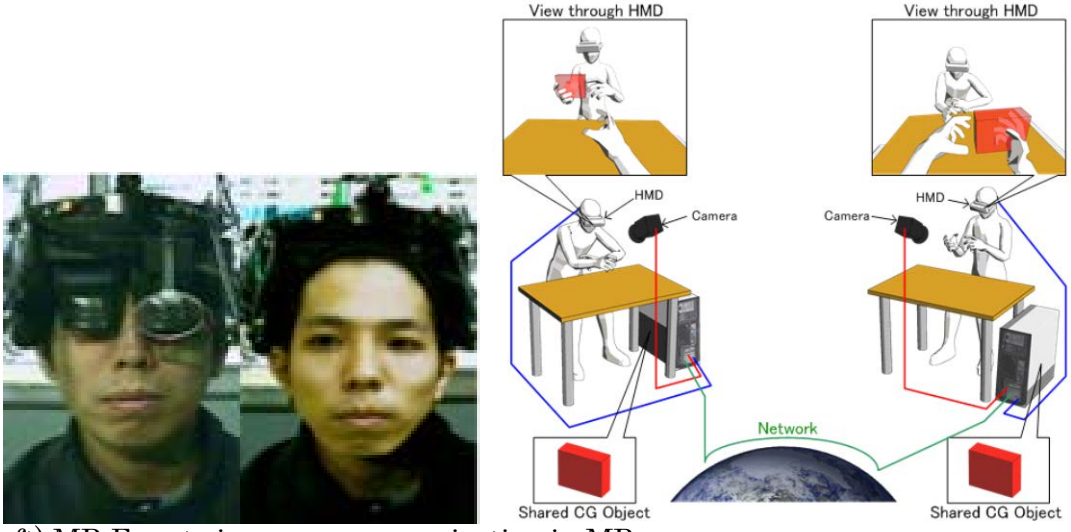
Effective browsing of video recorded by surveillance cameras is one of the most challenging missions because it is a typical problem of high-level mixture of data mining, data browsing, and computer network.
One of our research works achieved in past few years is the proposal of a new Mixed-Reality presentation of spatio-temporal behaviour of a moving object in a reviewer's view. The behaviour of the moving object was recorded in advance as a sequence of pairs of spatial position and its texture by environmental camera. A reviewer can see parallel replays (Figure) of the moving object so that he/she can shorten the time to browse the behaviour. Since large number of simultaneous replays increases the chance of overlapping textures, we propose the method to determine the best number of replays. We also propose an enriched visualization of trajectory of the moving object so that the reviewer can recognize the moving direction of the object easily. We have conducted subject tests on our proposed trajectory visibility and simultaneous replays of the moving object and show the results.



Parallel replay of moving objects and visual aid

1.1.4 Shared Mixed-Reality

The project aims to realize an advanced communication media using Mixed-Reality technique. One of the crucial problems to realize such communication media is that some facial appearances are lost by wearing HMD (Head Mounted Display). We develop an MR face that is effective for improving communication in Mixed-Reality space by restoring the lost eye expression. In order to realize collaborative workspace, we developed a remote face-to-face Mixed Reality (MR) system that enables two people in distant places to share MR space. Challenging issues to realize such an MR system include capturing, sending, and rendering each user's appearance in real time. We developed a method to represent user's upper body and hands on the table as a single deformed-billboard.

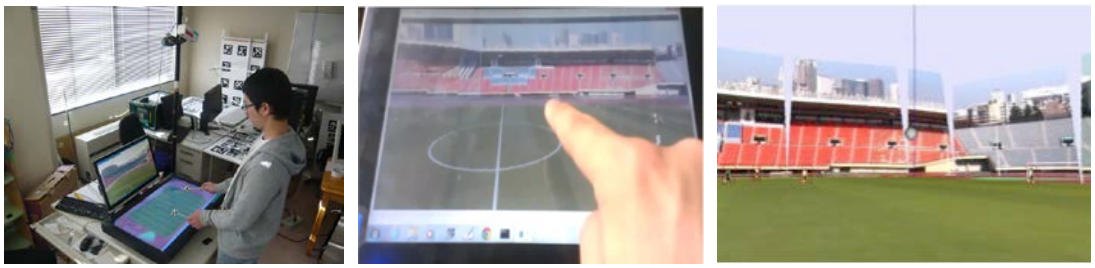


(Left) MR Face to improve communication in MR space.
(Right) Face-to-face tabletop remote collaboration in Mixed Reality.

1.1.5 Free Viewpoint Video Browsing

The project had researched 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, and developed the world first 3D live free-viewpoint display system. In order to realize an advanced contents technology by using the free-viewpoint video technology, we are continuously researching about interactive browsing methods for 3D free-viewpoint video display, which enables an ordinary person, without any special knowledge about video capturing and editing, to enjoy the video.

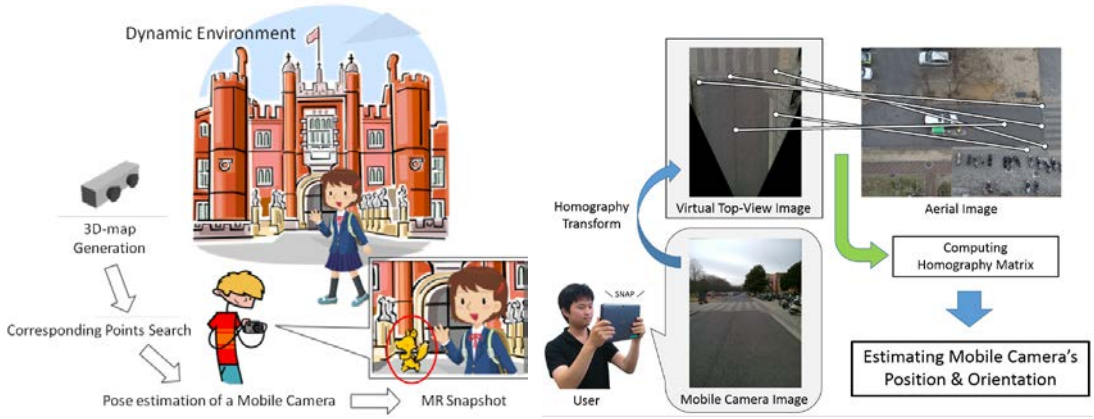
The outcomes are two types of 3D free-viewpoint browser. One of them enables a user can intuitively control the virtual camera in 3D space by moving 3D position trackers with bi-manual operation. The other browser can be realized much easier by utilizing popular device such as smart-phone and tablet-PC. We also developed an automated video browsing method without any user interaction. In the method, a user can enjoy the soccer game video captured at a player's viewpoint.



(Left) Free-viewpoint browser using 3D interface with bi-manual operation.
(Center) Virtual camera controlling method using multi-touch gestures.
(Right) Automatic player's view generation of real soccer scenes.

1.1.6 Mobile Camera Localization Using Environmental Cameras

This project aims to research an advanced system that visually supports users by combining the advantages of mobile and environmental cameras. Since the positional information is useful for supporting user, we develop a mobile camera calibration method by using visual information captured by mobile and multiple environment cameras. A method for estimating the pose of a mobile camera in a dynamic scene by using an environmental stereo camera is an example of the outcomes. By utilizing the dynamic objects' 3D point as landmarks for camera calibration, a robust pose estimation method can be realized. In the outdoor scene, we proposed a method for estimating the position and orientation of a mobile camera by referring corresponding points between a mobile camera image and an aerial image. Experimentally, we confirmed that the accuracy of the proposed method is better than that of a GPS.



(Left) A mobile camera calibration method using an environmental stereo camera. (Right) A mobile camera localization method using aerial-view images.

10.2 Collaboration

As for our outreach activities, we have presented our cutting-edge technologies at Innovation Japan which is intended to promote nationwide collaboration between Japanese universities and industries. We set our booth at 2008, 2009, 2010, and 2011, and got a number of guests and their positive comments. The titles of the technologies given at Innovation Japan were:

2008 Navigation technology within Multi-video space
(Japanese title: 多重映像空間のナビゲーション技術)

2009 Visualization technology of surveillance camera videos
(Japanese title: 監視カメラ映像を「見える化」する技術)

2010 3D free-viewpoint video browser for intuitive and direct user control
(Japanese title: 直感的閲覧が可能な 3 次元自由視点映像ブラウザ)

2011 High precision/multi-modal database establishment for hostile intent detection
(Japanese title: 害意検出のための高精度マルチモーダル DB 構築)

Our exhibition results in having our collaborative research works, one with NEC Yahoo, and Hitachi by their financial support.

10.3 Future Plan

Computational Media and Mixed Reality are cutting-edge technology to present a novel visual world to our eyes, and they are regarded as a promising next-generation human-interface technology. The Computational Media Group will continue the researches on the state-of-the-art technologies on this research literature.
Special topics we will focus on as our next challenges are listed below.

(1) Spatio-temporal video analysis and its utilization for data navigation
(2) Advanced RGB-D data analysis and visualization
(3) Vehicle localization by road monitoring camera
(4) Visual Support for Drivers by Mixed Reality
(5) Novel Cubic Display with Diorama and Projection AR
(6) Realizing corroborative work environment in where multiple remote-users can virtually share real objects in each site.
(7) Developing a facial expression enhancement of MR face to realize smoother video communication.
(8) Improving the resolution of generated video (e.g., 4K) with keeping real-time processing.
(9) Developing a contents management system that enables video creators generate attractive movies using free-viewpoint movie technologies.
(10) Developing a navigation system for a pedestrian who uses a mobile device (e.g., a smart phone, a tablet-PC etc.,) by the developed mobile camera localization method.
(11) Developing a data managing/mining method for visual information given by the massive number of users.

10.4 Publications

10.4.1 Journal Papers

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11 Bureau of Public Relations

11.1 Activity

In fiscal year 2010, the bureau initiated activities aimed at improving relations with society in order to advance the mission of the Center for Computational Sciences (CCS) and to promote the computational sciences themselves. To that end, three public relations concepts underlying the purposes behind the establishment of the Center have been set forth for use in guiding daily operations.

Public Relations Concepts

- We will conduct bilateral public relations to foster enhanced relations between the Center and society.
- We will aim at increasing the visibility of the Center and the computational sciences.
- We will enhance the level of understanding of the fundamental policies of the Center, and work to improve public confidence in its actions.

Activity Policy for the Bureau of Public Relations

- We will support public relations and public hearings for researchers associated with the center.
- We will create content, including websites, in order to provide information to stakeholders.
- We will actively gather information and create feedback mechanisms for researchers within the center.
- We will create a risk management organization.
- We will examine and implement methods to measure visibility, levels of understanding, and degrees of confidence.

11.2 Activity Results

Website: http://www.ccs.tsukuba.ac.jp/

The website of CCS provides up to date information on researchers, projects, computer basics, database disclosures, symposiums/seminars, disaster preparedness and response, etc. The website has by 3560 page views per month in Japanese, and 460 page views in English per month in average, since October 2010.

Brochures

We prepare three types of brochures based on the intended readership: "Computational Sciences and Supercomputers" for the general public (this is aimed at high school readers and older); a Japanese text for professionals (aimed at graduate students and older); and an English text for professionals (for use by international graduate students and others).

Movies

Productions of 12 movies (Japanese and English), including an introduction to the Center, the computing facility, and 10 research fields, have been produced to date.

Tour and Open House

The number of visitors was 351 in fiscal year 2010, 1,056 in fiscal year 2011, and 844 in fiscal year 2012, 1315 in fiscal year 2013. We created a FAQ section on Center's website.

Media Promotions

Seven press releases were disseminated to the mass media in fiscal year 2011, and five were released in fiscal year 2012, and six were released in fiscal year 2013. Bureau of Public Relations prepared the manual for communication with mass media. (CCS メンバーのためのメディア対応について). The Center is also active on the social media Twitter (@CCS_PR), where it has gathered 3,290 submissions and 865 followers (as of December 2013).

Renovation of the Entrance Lobby

The bureau carried out the renovation of the lobby and set up the display such as old supercomputers, calculation nodes, and certificates of awards.

Risk Management

The bureau created the webpage about the Disaster Contingency Plan.

Research of Public Relations

The members of the bureau made two conference presentations. In 2013, the intensive public lectures about public relations for universities and research institutes was planned and managed by the bureau.

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- 矢部あずさ，吉戸智明，入江敦子，科学広報におけるトレーディングカードゲームの活用　日本天文学会 2012 秋
- 筑波大学重点公開講座「大学・研究機関のパブリックリレーションズー科学技術の PR 戦略」Jan 12 - 14, 2013

11.3 Collaboration

In order to facilitate the public relations for Strategic Programs for Innovative Research (SPIRE) Field 5 "The origin of matter and the universe" , strengthen the cooperation with High Energy Accelerator Research Organization (KEK) and National Astronomical Observatory of Japan, the member of Joint Institute for Computational Fundamental Science (JICFuS).

11.4 Future Plan

The bureau continues the activities of public relations based on the concept. Create a mechanism to collect up-to-date research results efficiently and publish to the public. In addition, collect the information from public, and introduce to the researchers in CCS.

Following are the new activities in the future plan:

Visualization of the Research Results

Using the technology of 4D2U (Four-Dimensional Digital Universe Project, NAOJ), examine the visualization in the field of particle physics, nuclear physics, and other fields of science. With examination, utilize the 3D theater at the annex of the CCS, introduced in FY 2011.

Study on the Evaluation Method about Public Relations

Make a study on the evaluation method for measuring popularity (awareness), understanding, reliability of the institute and sciences. In addition, we are planning to consider the qualitative and quantitative evaluation of science public relations and spokesman, with researchers of social sciences.