Center for Computational Sciences
University of Tsukuba

筑波大学計算科学研究センター

Foundation of the Center

Center for Computational Sciences was founded on April 2004 as an inter-university research facility for computational sciences, reorganizing and expanding Center for Computational Physics (April 1992-March 2004). In addition to the Divisions of Particle and Astrophysics and High Performance Computing Systems, new Divisions were created on Material and Life Sciences, Geoenvironmental and Biological Sciences, and Computational Informatics.

Objectives

The Center aims to carry out research on critical issues of fundamental science, material science, life science and environmental science through large-scale simulations and large-scale data analyses. To realize this goal, the Center performs research and development of high performance computing systems and networks, and advanced study in computer and information sciences. The Center is an inter-university facility, thus offering functions as an international as well as a national center for computational sciences.

Organization

The Center has 6 research divisions as shown right. The faculty consists of 34 regular positions and 3 visiting professor positions. Researchers outside the Center who are closely involved in the activities of the Center are appointed as associated research fellows.

Large-scale numerical simulation project

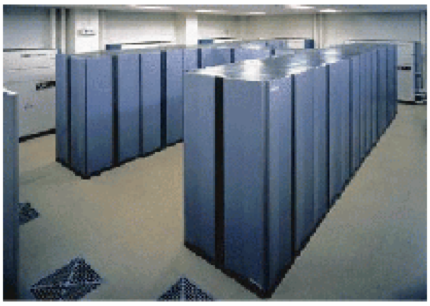
The Center is an inter-university facility, open to researchers of universities and other research institutions in Japan. Since 1998, the Center has been inviting proposals, twice per year, for large-scale numerical research with CP-PACS, making the computational power of the CP-PACS accessible to researchers throughout Japan.

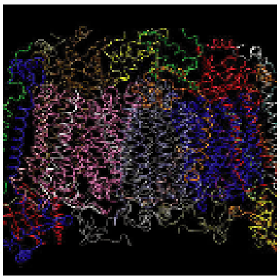
International activities

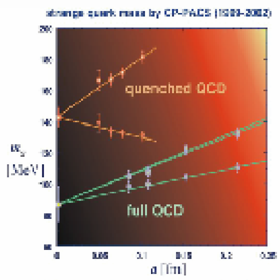
The Center organizes international symposia, and invites visitors from abroad in order to promote international exchange and collaboration of scholars in computational sciences.

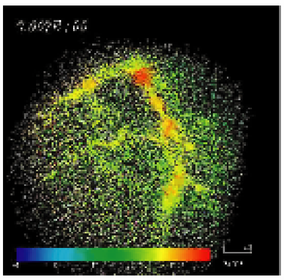
Chronology

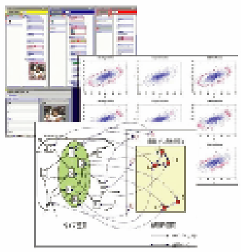
1992	April 1	CP-PACS Project begins (five-year project)
	April 10	Center for Computational Physics founded (10 year term)
	July 3	Opening ceremony of the Center held
1993	August 26	Computer building completed
1994	March 1	Front Computer System (phase I) starts operation
1995	March 1	Front Computer System (phase II) starts operation
	March 30	Research building completed
	April 1	Designated as COE
1996	March 25	CP-PACS (1024PU) completed and installed
	September 18	CP-PACS (2048PU) completed and installed
1997	March 31	CP-PACS Project ends
	April 1	Research for the Future Program "Development of Next-Generation Massively Parallel Computers" begins (five-year project)
1998	March 1	Front Computer System (phase III) starts operation
	March 1	Large-scale Simulation Project with open use of CP-PACS begins
2002	March 31	Research for the Future Program "Development of Next-Generation Massively Parallel Computers" ends
2002	April 1	second 10 year term of Center for Computational Physics begins
2004	April 1	Center for Computational Physics is reorganized and expanded to Center for Computational Sciences
	June 10	Opening Ceremony of the Center held

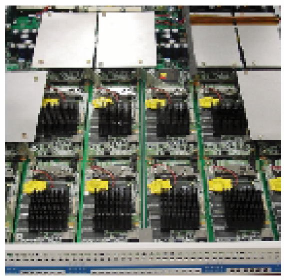












Access to the Center

Bus

JR Tokyo station

Take the Tsukuba Express Bus bound for Tsukuba Center from the Yaesu South Exit of Tokyo Station, and get off at Tsukuba Center terminal. At the Tsukuba Center, take a bus for "Tsukuba-daigaku-chuo" and get off at "Dai-ichi gakugun-tou-mae".

Narita International Airport

Take the Narita-Tsukuba-Tsuchiura Shuttle Bus outside the terminal building, and get off at Tsukuba Center. At the Tsukuba Center, take a bus for "Tsukuba-daigaku-chuo" and get off at "Dai-ichi gakugun-tou-mae".

JR Tsuchiura station, JR Arakawa-oki station, JR Hitachino-ushiku station

Take a bus for "Tsukuba-daigaku-chuo" at Tsuchiura, Arakawa-oki, and Hitachino-ushiku stations on JR Jobane line, and get off at "Dai-ichi gakugun-tou-mae".

Car

Expressway

Exit Sakura-Tsuchiura interchange on the Joban Expressway, and go north on Higashi-odori Ave. for about 6km.

Open Load

At the Gakuen-higashi-odori-iriguchi on Route 6, go north on Higashi-odori Ave. for about 10km.

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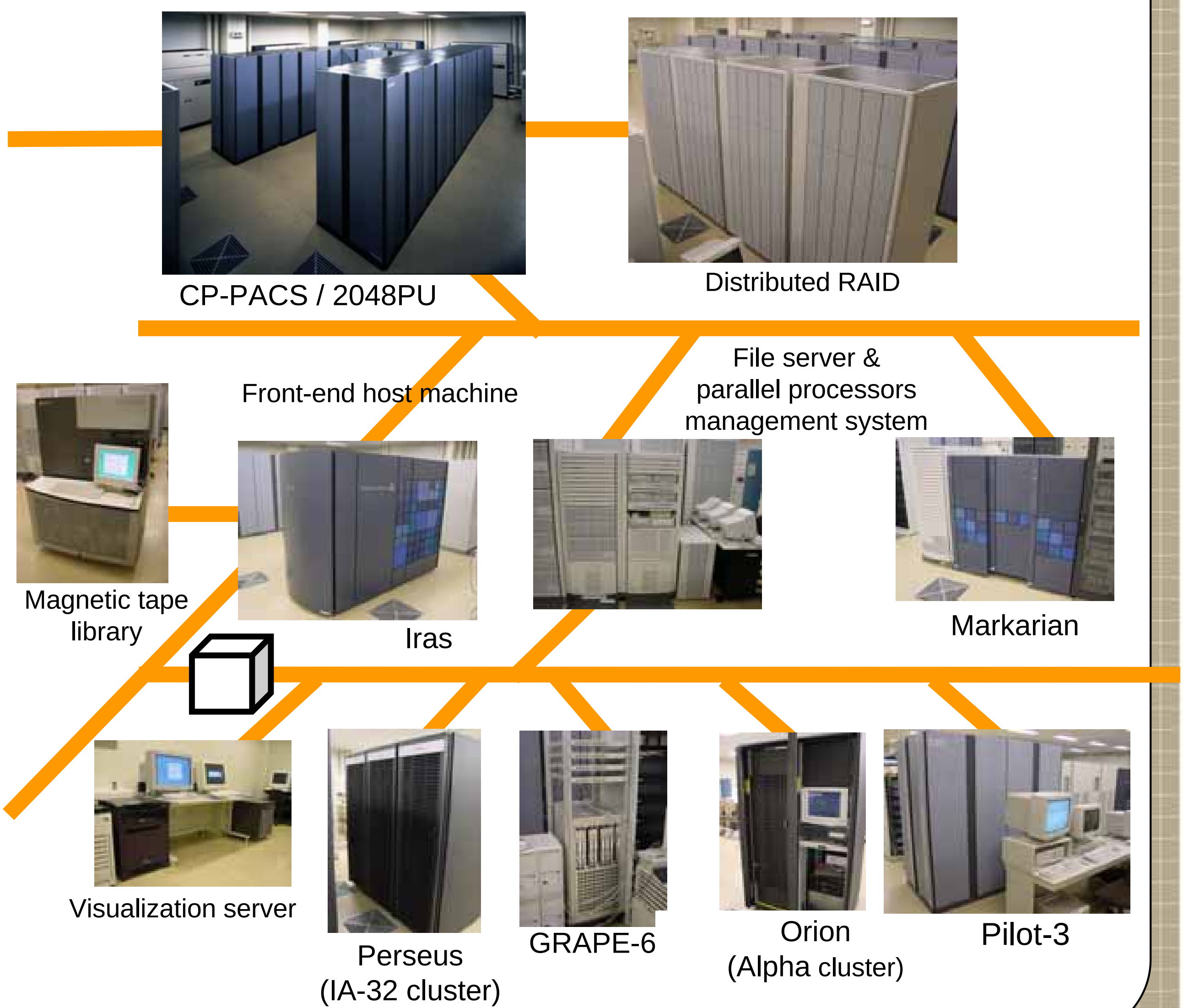
Computational Resources of the Center

The computational facilities consist of **CP-PACS**,a massively parallel processor, and surrounding front-end computer systems.

The front-end computer system includes Pilot-3 which is a small-sized CP-PACS, data analysis servers and file servers to analyze and save data produced by CP-PACS, a 2 TByte disk system and a 16TByte magnetic tape library. A parallelized visualization system, a special-purpose GRAPE-6 parallel system for gravity calculation used for **HMCS** (Heterogeneous Multi-Computer System), and several PC-based cluster systems are also available. For data sharing based on Grid technology, 12 TByte of NAS RAID system is provided.

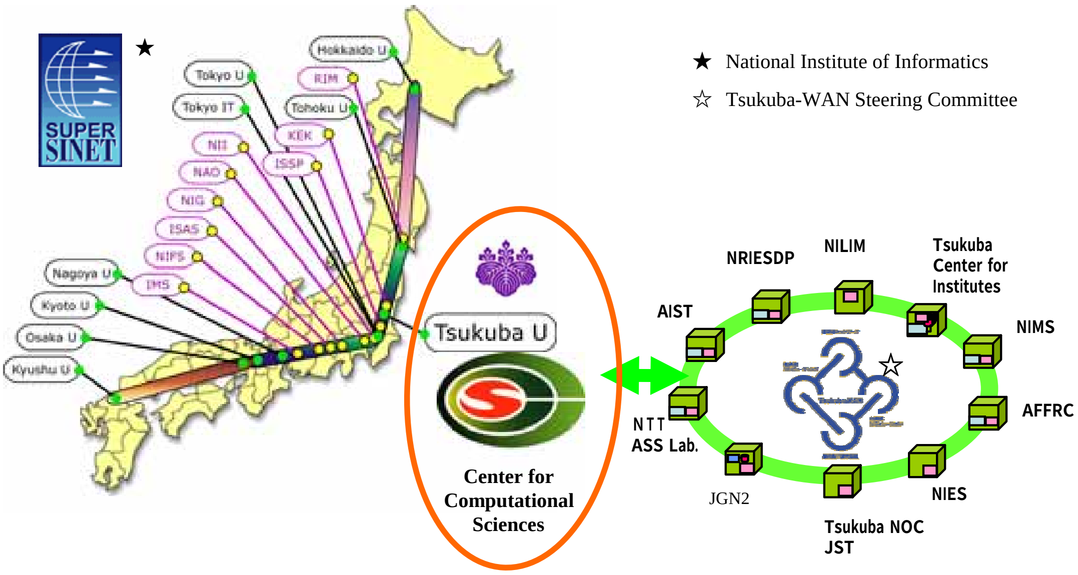
These facilities are connected with dual Gigabit Ethernet LAN for high speed data exchange among them. Using these facilities, a wide variety of research is being pursued in computational sciences using not only traditional vector processing schemes but also new scheme for clusters and special purpose machines .



Network and Clusters

External network environment

University of Tsukuba is connected to Super-SINET, a 10Gbps nation-wide network which connects universities and research institutes under MEXT in Japan. It is also connected to Tsukuba-WAN which connects major research institutes under various ministries in Tsukuba Science City. The center has three dedicated links to Super-SINET for various experiments, and one dedicated link to Tsukuba-WAN for Grid research. As the junction point of these network links, we carry out wide variety of research based on Grid technology to share valuable data and computational resources. An important application is the archive of data produced by CP-PACS, the gravity special-purpose machine GRAPE-6 and other resources.



Computational sciences by PC clusters

Recent remarkable progress of microprocessors used in PCs and workstations motivates high performance computing using clusters made of commodity microprocessors. As the performance of microprocessors becomes comparable to that of supercomputers a decade ago, the cluster of PC's connected by a commodity network can achieve similar or even higher, performance than traditional MPP systems.

PC-based cluster systems

While using these cluster systems to solve real computational physics problems, we also study performance of clusters as the high performance computing platform of next generation, and pursue new technologies on software and networking for them.

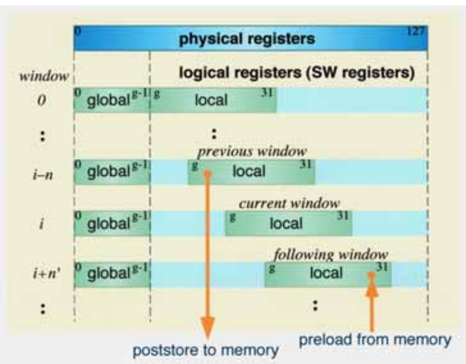
Massively parallel processor CP-PACS : Overview and processor architecture

Overview of CP-PACS

The CP-PACS is an MIMD (Multiple Instruction Multiple Data) parallel computer with a theoretical peak speed of 614 GFLOPS and a distributed memory of 128GByte. The system consists of 2048 processing units (PU's) for parallel floating point processing and 128 I/O units (IOU's) for distributed input/output processing. These units are connected together in an 8✕17✕16 three-dimensional array by a Hyper- Crossbar network. The well-balanced performance of the CPU, network and I/O devices supports the high capability of the CP-PACS for parallel processing.

Global view of CP-PACS

Node processor module



Pseudo-vector processing by sliding window

Node processor for high-speed vector processing

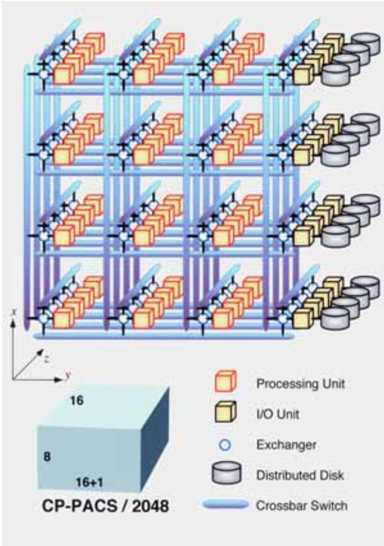
Each PU of the CP-PACS has a custom-made superscalar RISC processor with an architecture based on the PA-RISC 1.1. In large-scale computations in scientific and engineering applications on a RISC processor, the performance degradation occurring when the data size exceeds the cache memory capacity is a serious problem. For the processor of the CP-PACS, an upward compatible enhancement of the architecture, called the **PVP-SW** (Pseudo Vector Processor based on Slide-Window) has been developed.

In PVP-SW, it is available to utilize a large number of physical registers by sliding the logical register window. The access latency to a pseudo pipelined memory is hidden by continuously issued Preload/Poststore special instructions which can specify all physical registers as the target directly. With these features, an efficient vector processing is realized on its basic scalar architecture.

Massively parallel processor CP-PACS:
Interconnection network and overall performance

Hyper-crossbar network for high-speed data exchange

The Hyper-Crossbar network of the CP-PACS is made of crossbar switches in the x-, y-, and z-directions connected together by an Exchanger at each of the three-dimensional crossing points of the crossbar array. Each Exchanger has a PU or IOU attached to it so that data transfer of any pattern is possible by stepping through a maximum of three crossbar switches. Data transfer through the network is made through **Remote DMA** (Direct Memory Access), in which data are sent or received directly between the user memory space of the processors with a minimum of intervention from the Operating System. This leads to a significant reduction in the start-up overhead and high effective throughput.

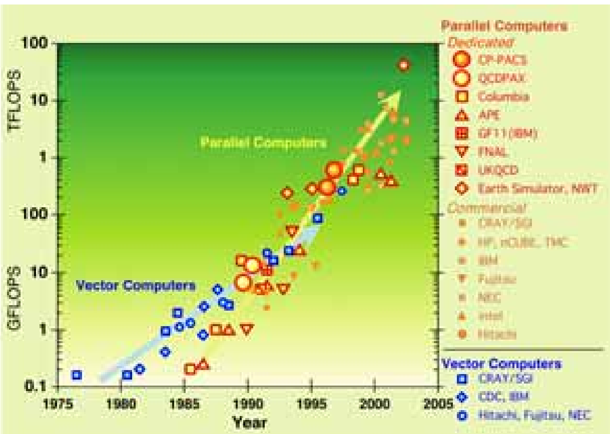


Network and disk I/O

Distributed disk system and external I/O

The distributed disk system of the CP-PACS is connected to 128 IOU's on the 8×16 plane at the end of the y-direction of the Hyper-Crossbar network by a SCSI-2 bus. RAID-5 disks are used for fault tolerance. The IOU's handle file I/O requests issued by the PU's in an efficient and distributed way using Remote DMA through the Hyper-Crossbar network.

For external I/O, one of the IOU's is connected to the front-end host by HIPPI. An Ethernet connection is also provided for system control without interrupting data transfer on HIPPI. In addition, 16 IOU's are connected to the disk and visualization servers through parallel 100 base-TX Ethernet.



Performance of supercomputers

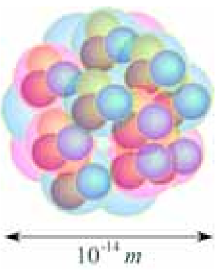
Development of parallel computers and CP-PACS

Parallel computers have been the world's fastest computers since 1992, taking the title from vector supercomputers. Dedicated parallel computers developed for particle physics and other physics applications (red symbols) have played a significant role in this trend. The QCDPAX, which achieved 14GFLOPS in 1990, contributed much to particle physics, and paved the way toward the CP-PACS Project.

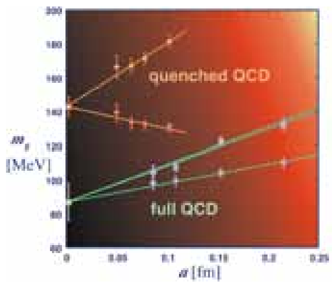
The CP-PACS computer started operation in March 1996 with 1024 processors (307GFLOPS). An upgrade to the final 2048 processor system, which achieved a peak speed of 614GFLOPS, was completed in September 1996. In November 1996, the CP-PACS was ranked No. 1 in the TOP 500 List of Supercomputers. The CP-PACS has been developed in collaboration with Hitachi Ltd.

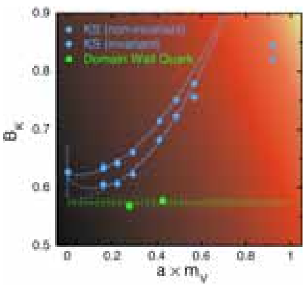
Division of Particle Physics and Astrophysics
Computational Particle Physics

Ab initio calculation of hadrons from quarks:
Determination of fundamental parameters in Nature



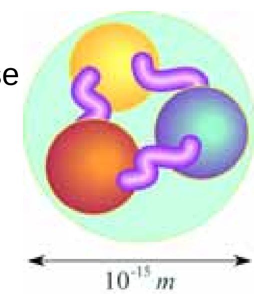
Numerical simulation of Quantum Chromodynamics (QCD) formulated on a space-time lattice is the only way to extract various properties of hadrons directly from the fundamental theory of quarks. Although a vast amount of computation is required, this provides us not only with a stringent test of the fundamental theory of Nature, but also with a direct determination of fundamental parameters in QCD, such as the quark mass and strong coupling constant, which cannot be measured by experiment because quarks are confined within hadrons. CCS has been one of the core institutes in computational particle physics through development of the dedicated parallel computer CP-PACS and its application to QCD. The right figure shows our result for the *s* quark mass, which implies a much lower value than previous estimates in the quenched approximation.





On the CP-PACS, we further investigated hadronic quantities which are difficult to evaluate in other methods. The left figure shows our result on the *B*-parameter for *K* meson mixing, which is relevant for the asymmetry between matter and anti-matter in the universe. We also promote studies on quark-gluon plasma and chiral fermions on the lattice.

Toward a full simulation of quarks



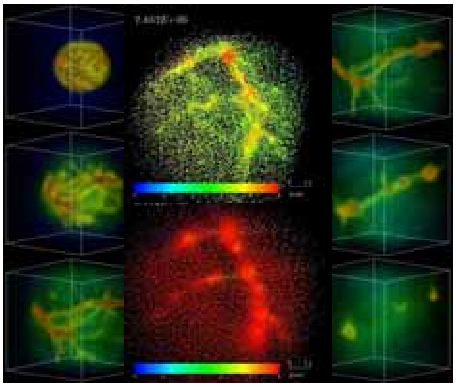
In most large-scale simulations in lattice QCD, only the lightest *u* and *d* quarks were included dynamically, because computation of dynamical quarks is demanding. On the other hand, the next lightest *s* quark is also expected to affect low energy physics since the *s* quark mass is comparable with the energy scales of QCD. We have started a grand challenge project to carry out simulations including all *u*, *d* and *s* quarks correctly by concentrating accessible supercomputers including the CP-PACS at CCS, VPP-5000 at ACCC Tsukuba, SR-8000 at KEK, and the Earth Simulator at JAMSTEC.

Division of Particle Physics and Astrophysics
Computational Astrophysics

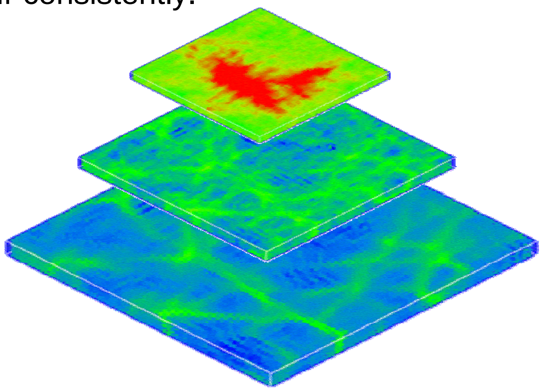
Evolution of the Universe and Formation of Astronomical Objects

A wide variety of astronomical objects in the universe are formed under a highly non-linear environment where gravitational, hydrodynamic, and radiative processes play significant roles in a complicate fashion. To analyze such a complex system numerical simulations by high-performance computers are quite effective.

We study the formation of cosmic structure, galaxies and stellar/planetary systems, using radiation hydrodynamics (RHD) which includes gravitational, hydrodynamic, and radiative processes self-consistently.



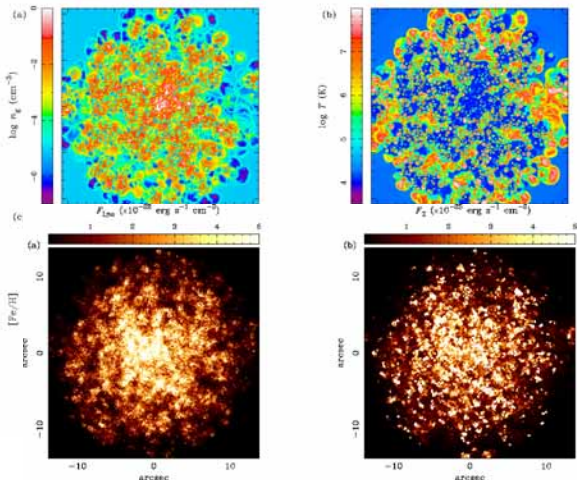
3D RHD simulation on the galaxy formation by HMCS (CP-PACS+GRAPE).



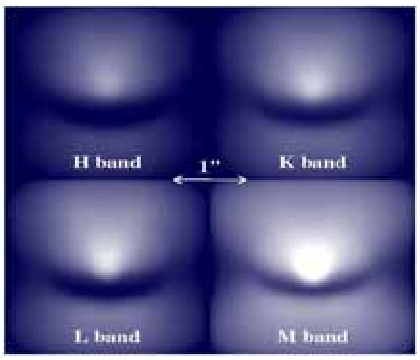
3D radiative transfer calculation on the cosmic reionization by CP-PACS

"Computational Observatory"

To make a giant advance in astrophysics supported by theory and observation by state-of-the-art facilities, we advocate a plan of "Computational Observatory" in which theory is directly confronted with observations through extensive numerical simulations.



Ultra-high resolution hydrodynamic simulation by CP-PACS on a galaxy at formation stage and observable images.

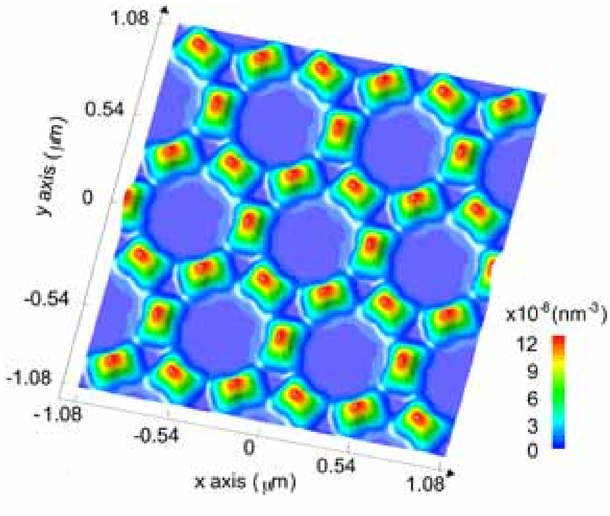


Observable images of a protostar by radiation transfer calculations by CP-PACS.

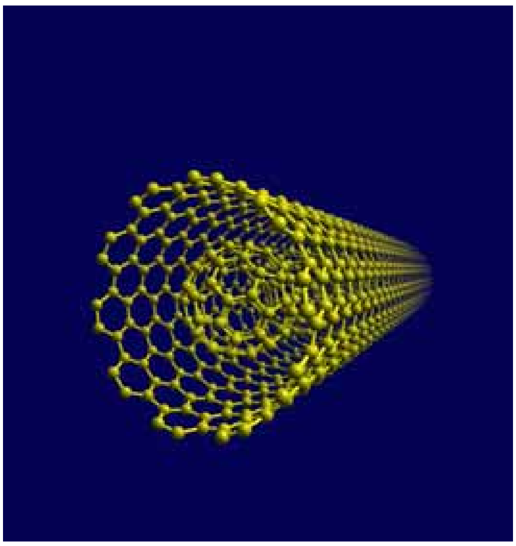
Division of Materials and Life Sciences
Computational Material Sciences

Design of artificial magnet based on semiconductor quantum wire networks

Physical properties and functions of nanostructures can be substantially controlled by their shapes as well as their constituent elements. We have succeeded to design the artificial ferromagnet fabricated only by non-magnetic InAs semiconductor quantum wires. Moreover, we have found that our designed ferromagnetism can easily be controlled by only applying electric and magnetic field.



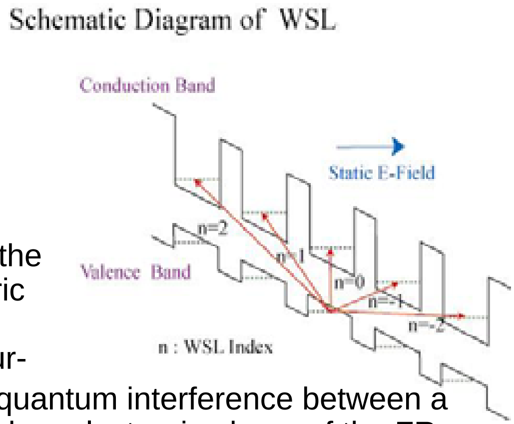
Electronic properties of Nano-Carbon Materials



Recently, an interesting complex consisting of fullerenes and nanotubes is synthesized. The material consists of a 1D array of fullerenes which are encapsulated by a carbon nanotube (occasionally called ``peapod"). Our first-principle calculations reveals that the space between the nanotube and the encapsulated fullerenes is a decisive factor to determine the energetics for the encapsulation process of the fullerenes in the nanotubes and the stability of resultant structures. It is also clarified that the electronic structures of peapods depend on the space and that they reflect electron states of the encapsulated fullerenes.

Division of Materials and Life Sciences
Computational Material Sciences

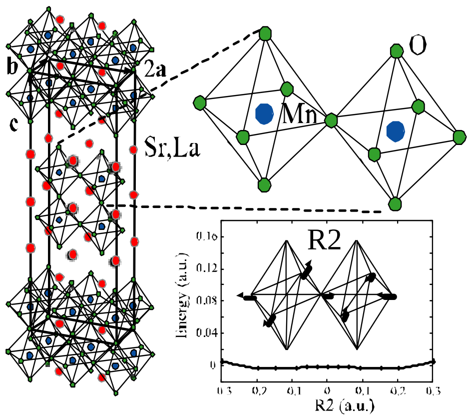
Nonlinear Optical Responses of Semiconductor Wannier-Stark Ladder



Superlattices where a static electric field is applied in the crystal growth direction are termed Wannier-Stark ladder (WSL), as is depicted in the figure. An exciton formed by photoabsorption is exclusively in a Fano-resonance (FR) state, not in a bound state. Nonlinear optical phenomena ascribable to the WSL exciton are investigated. An asymmetric Autler-Townes doublet, characteristic of excitonic FR, manifests itself in transient four-wave mixing (FWM) spectra. This is due to quantum interference between a microscopic polarization of FWM signals and an electronic phase of the FR state. Moreover, an optically coherent control of electronic states of WSL in terms of a combination of laser parameters with strength of the bias allows one to be accessible to the novel effect of the dynamic charge localization and delocalization, which is found further enriched by the Zener resonance of WSL.

Mechanism of Colossal Magnetoresistance in Manganite

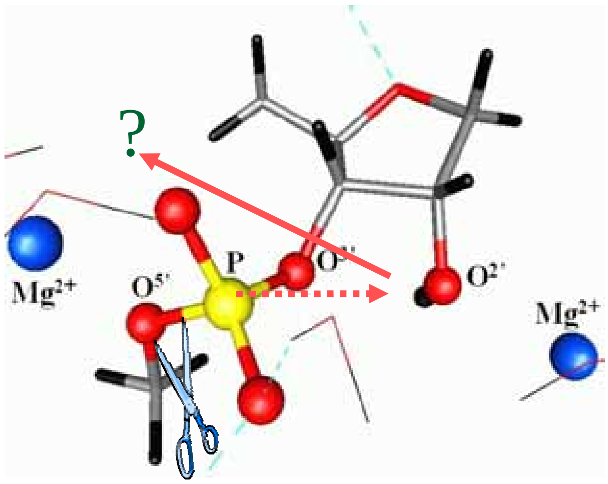
Some manganites show a remarkable reduction of resistance in a magnetic field called, “colossal magnetoresistance (CMR) effct”. The detailed mechanism of the CMR is still not known, but strong electron correlations and strong electron-lattice interaction are crucially important. In order to treat the strong electron correlations we have performed the complete active space self-consistent calculations on the manganite cluster Mn_2O_{11}. It has been found that the cluster is unstable with respect to symmetry breaking deformations (Polaron formation). We have obtained the stabilization energy that is close to the experimentally estimated value.



Division of Materials and Life Sciences
Computational Life Science

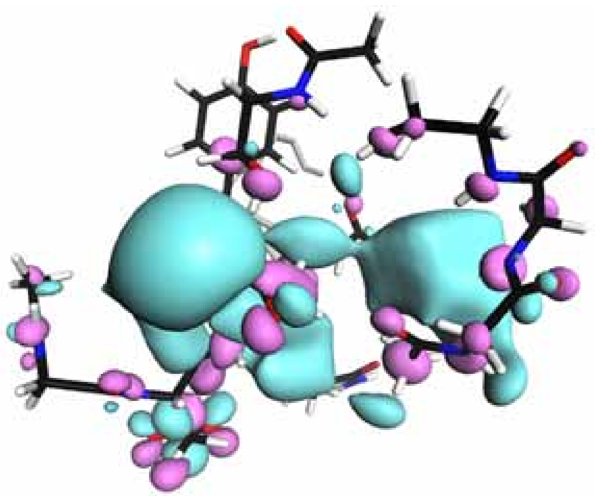
Mechanisms of Self-Cleavage of Ribozymes

RNA that is responsible for trans-fer of genetic information occa-sionally works as an enzyme (ribo-zyme). [The right is a reaction scheme of the self-cleavage of a ribozyme.]. Clarification of the ribozyme function is important in both science and medical applica-tion: The ribozyme is a possible tool for gene therapy. Our group has performed the first-principle quantum-theoretical molecular-dynamics calculations for the ribozyme for the first time and identified the reaction pathways and obtained the corresponding free-energy barriers.



Atoms and Electrons in Cytochrome *c* Oxidase

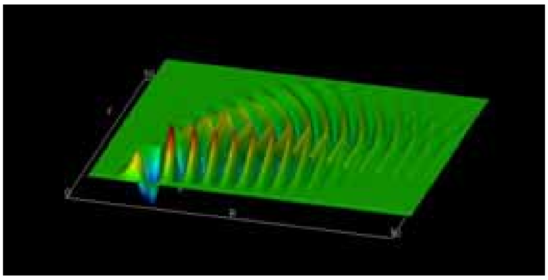
At the final stage of the respi-ration, a protein named cytochrome c oxidase shows structural change triggered by electron transfer, then exhibits a physiological functions, and eventually assists in the for-mation of ATP. Our group has explored the origin of the functions based on the quant-um-mechanical calculations. The right is distribution of a wavefunction of a nearly-free-electron state that we have found is closely related to atom-scale-mechanisms of the respiration processes.



Division of Materials and Life Sciences
Computational Nuclear Physics

Physics of Finite Quantum Many-Body Systems

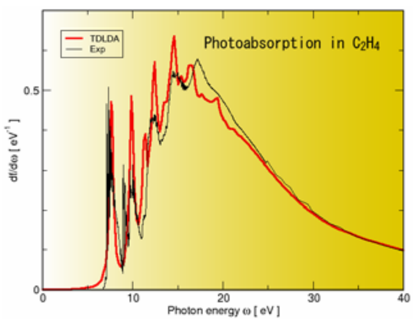
Quantum systems such as nuclei, atoms, and molecules, form a group of isolated finite matter in nature, having a number of common characteristic features. Moreover, recent developments in the nano-science technique enable production of new artificial elements in these finite quantum systems. Approaches of the computational science are very useful in studying these systems composed of a few to a few-hundreds of particles. Our current research includes nuclear structure and reaction; especially, microscopic theories of collective motion and prediction of novel structures in unstable nuclei. We also study dynamics of electrons in finite systems (atoms, molecules, clusters, etc.), including electronic excitations, optical response under weak and intense laser field.



Real-space calculation of deuteron breakup reaction

Quantum Simulation in Real-Time and Real-Space

Every matter in nature is a many-body system made of electrons and nuclei. The nucleus itself is a many-body system of nucleons as well. We are developing methods of quantum simulation to study dynamics of these fermionic many-body systems. The time-dependent density-functional theory is of current interest for the first-principle calculation of fermionic dynamics. Real-time and real-space technique has been developed to investigate dynamical properties of nuclei, atoms, molecules, and clusters. In addition, we develop a wave-packet method with the absorbing boundary condition for quantum scattering problems, applied to the linear response in the continuum, the few-body reaction models, etc.

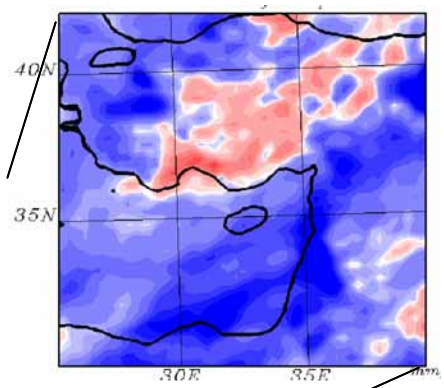


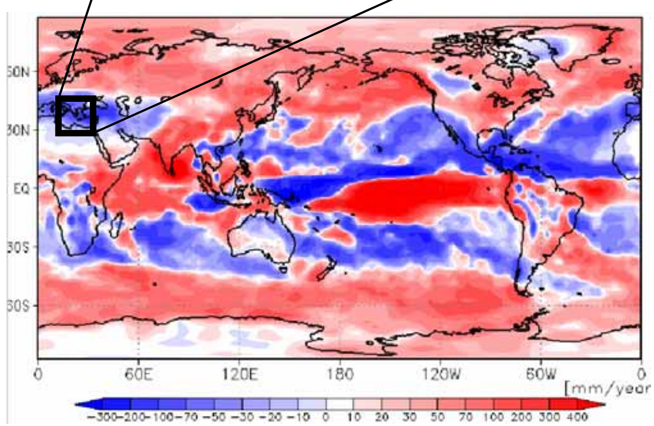
First-principle calculation of photoabsorption in ethylene

Division of Global Environment and Biological Sciences
Global Environmental Science

Prediction of Global Change

In recent years, reliable predictions are provided for global warming caused by the increasing anthropogenic greenhouse gases. More precise regional climate prediction is demanded, however, for mitigation on human impact especially for agriculture in each country or region. Numerous technical problems then arise, and computation becomes enormous when the model resolution is increased for regional climate prediction. In our group, the prediction of global change is performed by a combination of the regional climate model nested in the global climate model. The figures illustrate the precipitation change (blue for decrease) between 1990s and 2070s over the world predicted by the general circulation model at the Meteorological Research Institute (lower) and over the east Mediterranean where severe drought is anticipated, predicted by the regional climate model at the University of Tsukuba (upper).



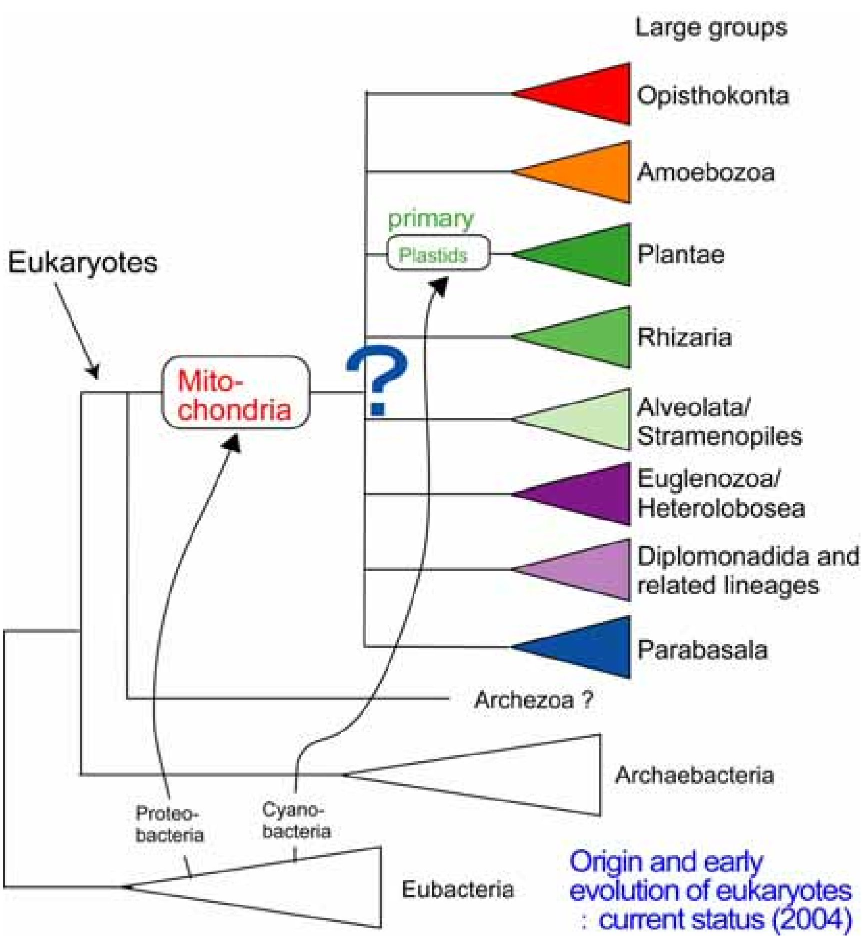


Data Assimilation for Meteorological Observations

Model atmosphere would approach the real atmosphere and eventually become identical if observed data are assimilated into the model atmosphere for infinite time interval. The technique is called 4 dimensional data assimilation. By this technique, we can infer the global feature of the atmosphere even if the meteorological observations are available sparsely only on the land. In our group, comparative experiments are conducted for the products of 4 dimensional data assimilation by many operational meteorological centers over the world. A new assimilation technique is developed by the application of Kalman Filter in the ensemble forecasts

Phylogenetic Inference on the Universal Tree of Life

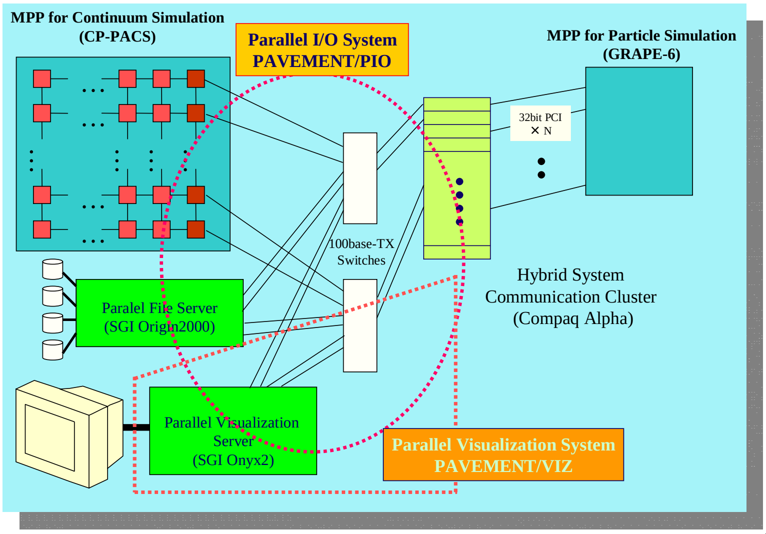
The central focus of our research is to gain insight into origin and early evolution of eukaryotes, the most important open problem in evolutionary biology.One of the goal of this research is to reconstruct the Universal Tree of Life including diverse organisms on the earth, based on molecular phylogenetic approach. Since a reliable phylogenetic inference simultaneously requires numerous genes and species, a large scale data analysis using high performance computers plays a key role in our study.



Division of High Performance Computing Systems
System Architecture

Heterogeneous Multi-Computer System (HMCS)

In the next generation computational physics, it is necessary to realize hybrid computations and simulations based on complex physical models containing various types of fundamental processes. In such a computational model, conventional computers built with a uniform architecture are not suitable for realizing efficient calculations. We propose a new platform named **HMCS** for these next generation computational physics simulations. HMCS is a conceptual framework to build systems combining vector machines, MPPs, clusters and special purpose machines, which have been used as stand-alone systems so far. We have constructed a prototype system based on a general purpose MPP CP-PACS and a special purpose system for gravity calculation GRAPE-6 connecting them with parallel network channels (see the figure on right), to realize a very high speed computational astrophysics simulation. In this system, two computational facilities are connected with a high bandwidth parallel I/O system PAVEMENT/PIO, and all particle data are transferred at every simulation time step. Using this system, the hydrodynamics incorporating with radiative transfer and self-gravity can be performed.



Research on High Performance Cluster Computing

Recent remarkable progress in microprocessors used in PCs and workstations motivates high performance computing using clusters out of commodity microprocessors. As the performance of the microprocessor becomes comparable to that of supercomputers a decade ago, the cluster of PC connected by commodity network can achieve the same, or even higher, performance than traditional MPP systems. The PC cluster is a promising high performance computing platform to exploit the computing power of modern microprocessors for several scientific applications. While using these cluster systems to solve real computational science problems, we also study performance of clusters as the high performance computing platform of next generation, and pursue new technologies on software and networking in the following topics.

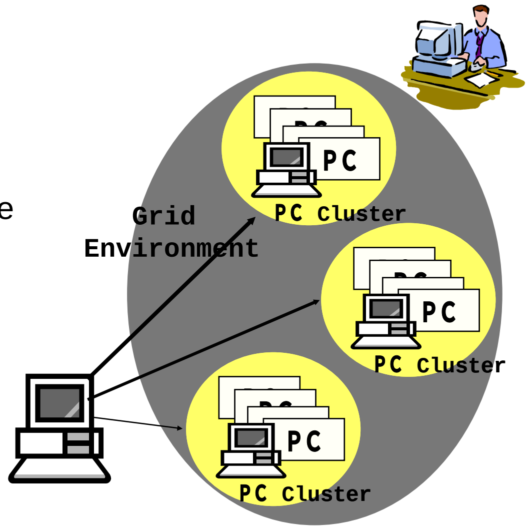
- **OpenMP programming system using software distributed shared memory for clusters**
- **The next generation of cluster networks using commodity network**
- **High-density low-power cluster technology**
- **High performance numerical libraries**

Division of High Performance Computing Systems
Grid and Networks

Grid Computing Research

The platforms for computational sciences make rapid progress every year. Recently, research and development of Grid, which is a network infrastructure to utilize on-line computational facilities on wide area network, has been gathering much interest in high performance network computing. Seamlessly connecting a large number and wide range of computers from super-computers to PCs all over the world may provide enormous amount of computational power. They cover not only computationally intensive applications but also large-scale storage system, data intensive applications and software for collaborative work among researchers. As the inter-connection point of the two high-speed networks, the Super-SINET and Tsukuba-WAN, we are promoting research and development of Grid technology as a new paradigm of computational physics based on various resource sharing, for example data sharing of QCD configurations produced by CP-PACS or computing facility sharing of the special-purpose computer GRAPE.

OmniRPC: a Grid RPC system for Grid Parallel Programming



OmniRPC is a Grid RPC system which enables seamless parallel programming in from Cluster to Grid Environment. To support typical master/worker grid applications such as a parametric execution, the OmniRPC provides “automatic-initializable remote module” to send and store data in the remote host. Since it may accept several requests for the subsequent calls by keeping the connection alive, the data set by the initialization is re-used, resulting in efficient execution by reducing the amount of communication. We assume that a typical grid resource is a cluster of clusters geographically distributed in several sites. For a cluster with private network, an agent process running the server host works as a proxy which relays the communications between the client and the remote executables. The OmniRPC system supports a local environment with “rsh”, a grid environment with Globus, and remote hosts with “ssh”.

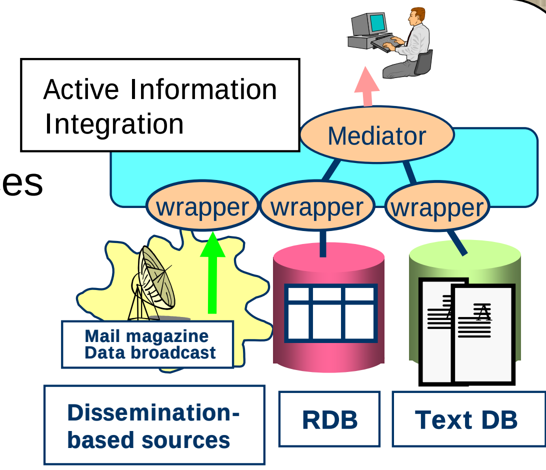
Grid Applications

- HMCS-G (Grid-enabled Heterogeneous Multi-computer System) : A system to access a special-purpose supercomputer GRAPE-6 for gravity calculation over Grid using the OmniRPC interface.
- CONFLEX-G(Grid-enabled Molecular Conformational Space Search Program): An exhaustive molecular conformational search program CONFLEX (developed by Dr. Goto, Toyohashi University of Technology) parallelized using OmniRPC for a grid environment. (supported by JST-ACT program of Japan)
- Parallel eigenvalue solver using Grid distributed resources: A generalized eigenvalue problem in a given domain by solving linear equations in parallel using OmniRPC.

Division of Computational Informatics
Computational Intelligence

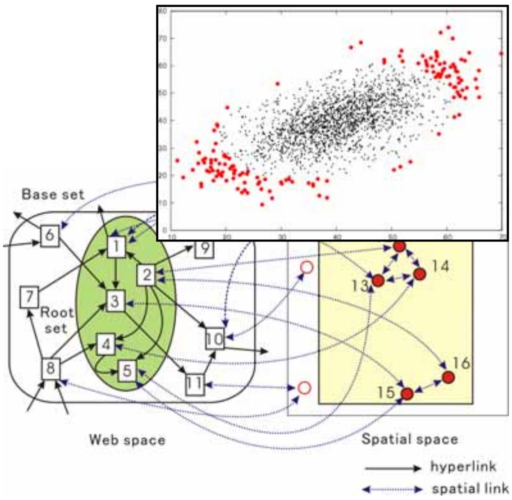
Information Integration

- Integration of distributed and heterogeneous information sources
- Integration of stream-oriented information sources
- Taxonomy-based Web search
- User interface for information integration



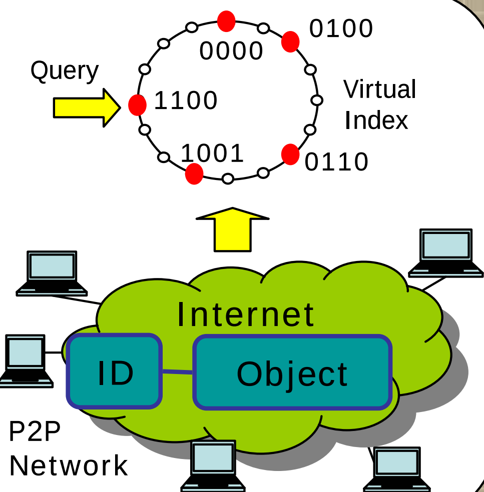
Data Mining and Knowledge Discovery

- Topic detection and tracking for text streams
- Web mining for spatio-temporal information discovery
- Outlier detection based on user intention



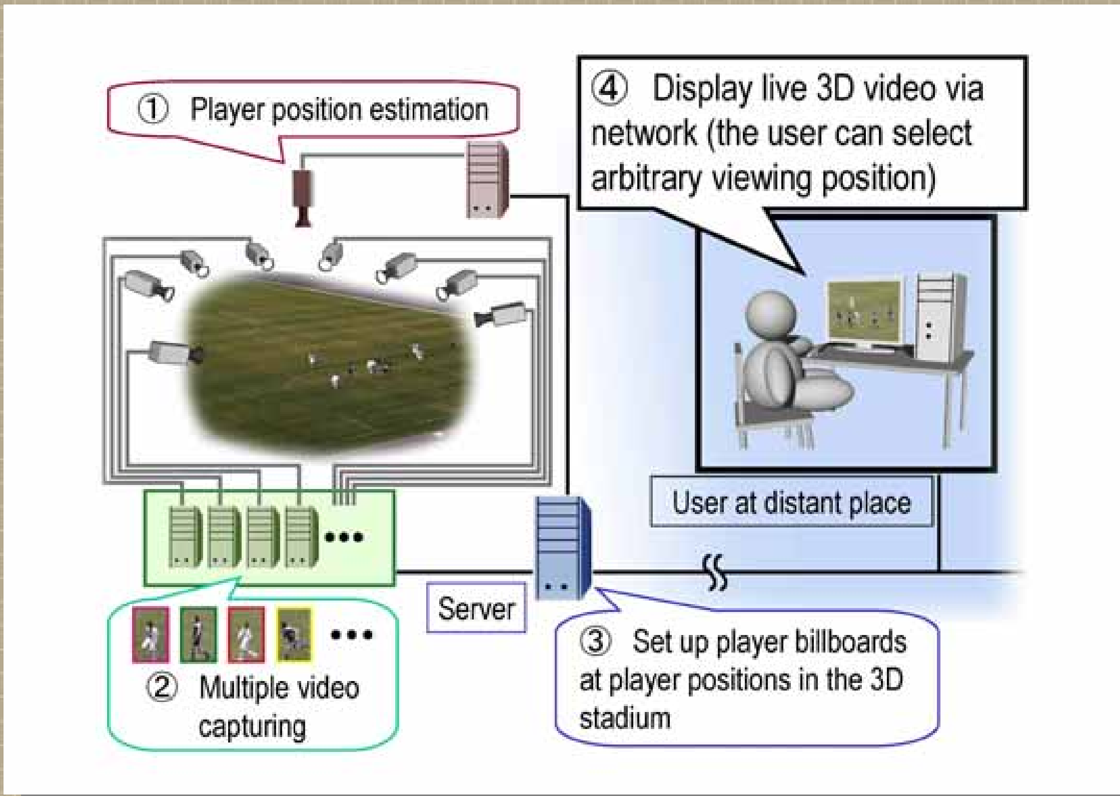
Web Computing

- Information search in P2P environments
- Example-based query processing on XML databases
- Efficient delivery and updates of XML data
- XML views over binary data



Division of Computational Informatics
Computational Media

Live 3D Video Transmission and Presentation



Outdoor Mixed-Reality for Pedestrians