The Strategy of Center for Computational Sciences

Masayuki Umemura
(Center for Computational Sciences, University of Tsukuba)

Mission of CCS

1. The mission of the CCS is to promote **“Multidisciplinary Computational Science (MCS)”** through the tight cooperation between computational and computer scientists by developing and operating leading-edge computing systems.

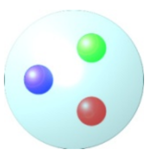
2. We strengthen **international collaborations** aiming at a world-wide COE which plays a key role to develop “Multidisciplinary Computational Science” for advances in science and technology.

Cooperation between Computational and Computer Science

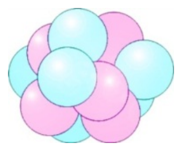
Project Office for Exascale Computational Sciences

Project Office for Exascale Computing System Development

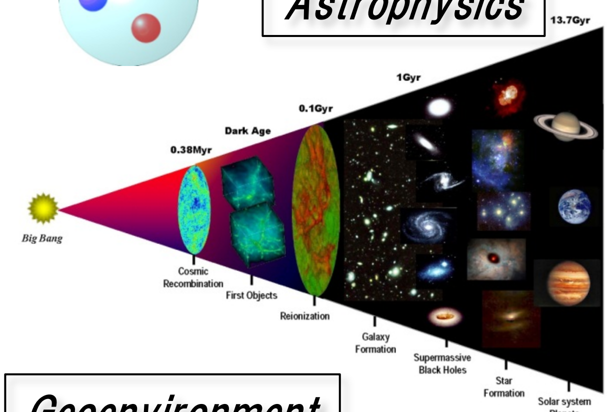
Particle Physics



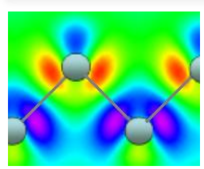
Nuclear Physics



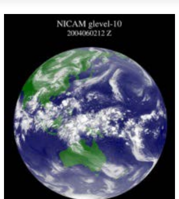
Astrophysics



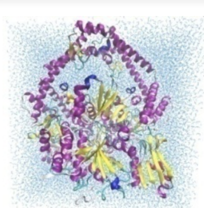
Materials Science



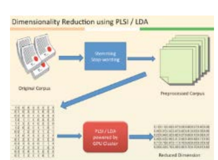
Geoenvironment

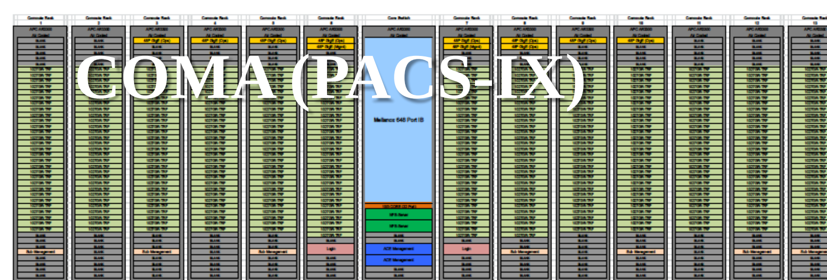


Bioscience

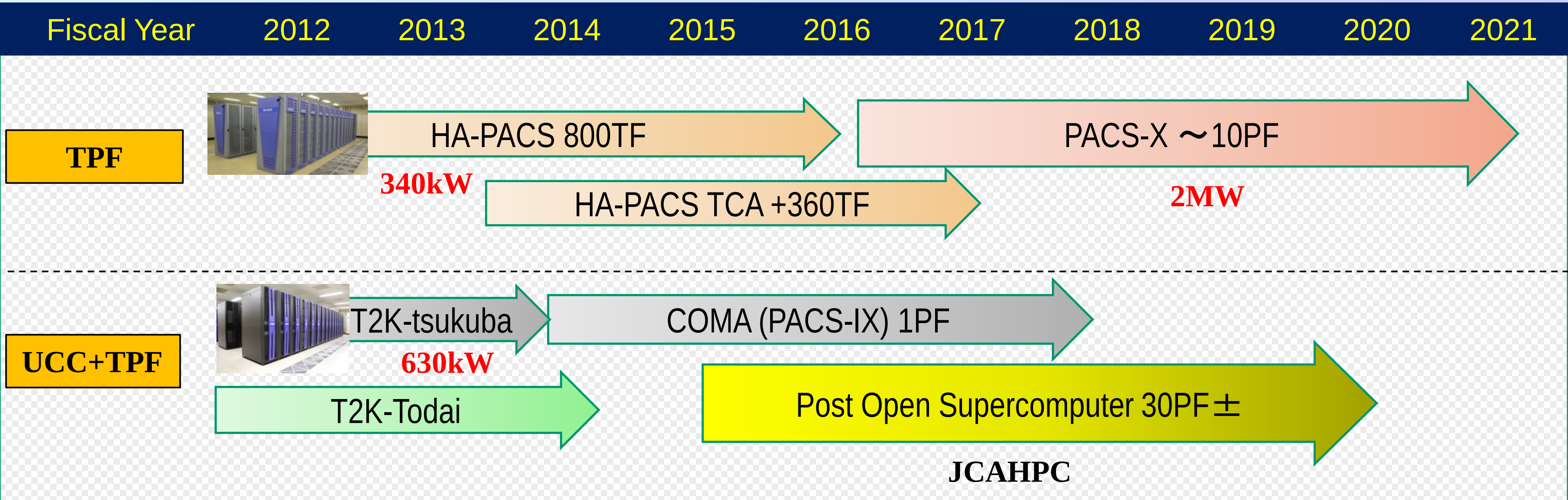


Database





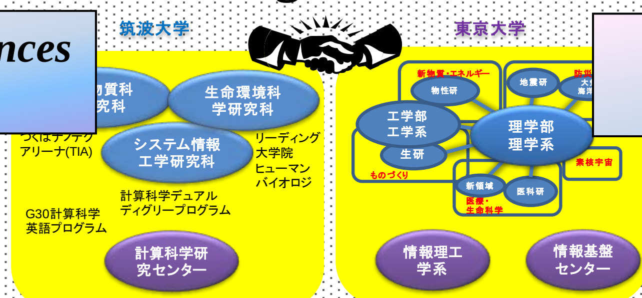
Future Plans of Computing System Development



TPF = Technology Path-Forward Machine
UCC = Upscale Commodity Cluster Machine

- **Joint Center for Advanced High Performance Computing (JCAHPC)**

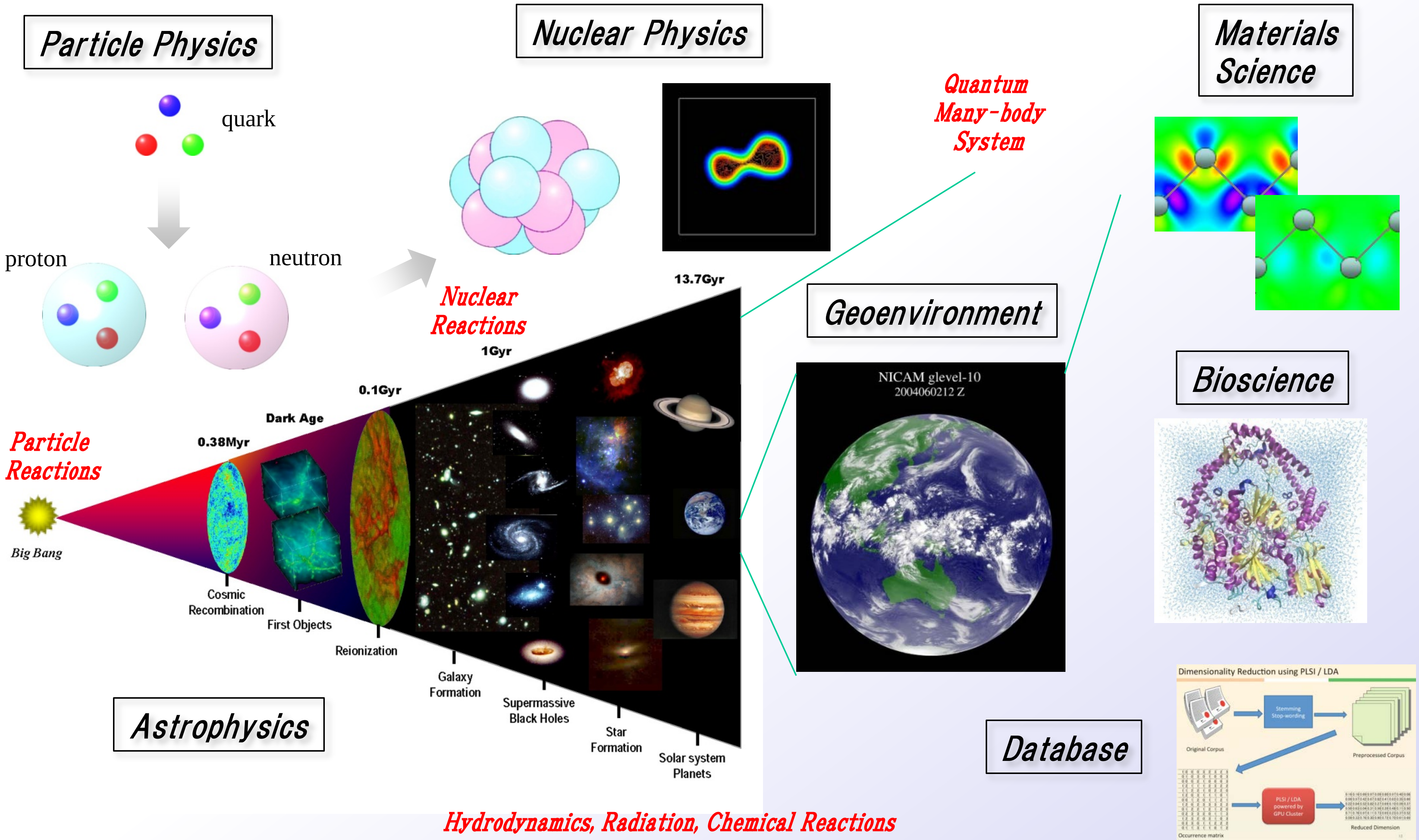
Center for Computational Sciences
U. Tsukuba



Information Technology Center
U. Tokyo

- **Feasibility Study toward Exa-scale Computing (National Project)**

Computational Sciences



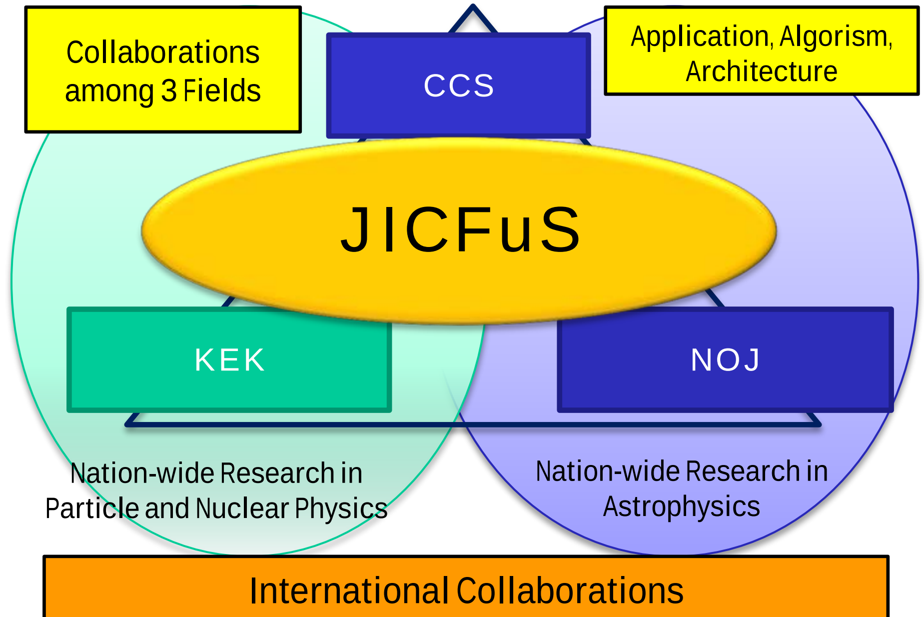
Inter-University Project 1

Joint Institute for Computational Fundamental Science

JICFuS

Collaboration among Particle, Astro, and Nuclear Physics

Strategic Programs for Innovative Research (SPIRE) Field 5
"The origin of matter and the universe"



New Positions

Particle Physics Group — **International Tenure Track***

Astrophysics Group — **International Tenure Track***

Nuclear Physics Group — **Professor Takashi NAKATSUKASA**

International Tenure Track*

February 1, 2009	Joint Institute for Computational Fundamental Science (JICFuS) established
September 27, 2010 – March 31, 2011	"Strategic Programs" Feasibility Study Field 5 "The origin of matter and the universe"
April 1, 2011	Strategic Programs for Innovative Research (SPIRE) Field 5 "**The origin of matter and the universe**" started
September 28, 2012	K computer for common use started

Inter-University Project 2

Organization for Collaborative Research on Computational Astrobiology (CAB)

Computational astrobiology is a new frontier, in which the synergy of astrophysics, planetary science, biology, and material science through first principle simulations.

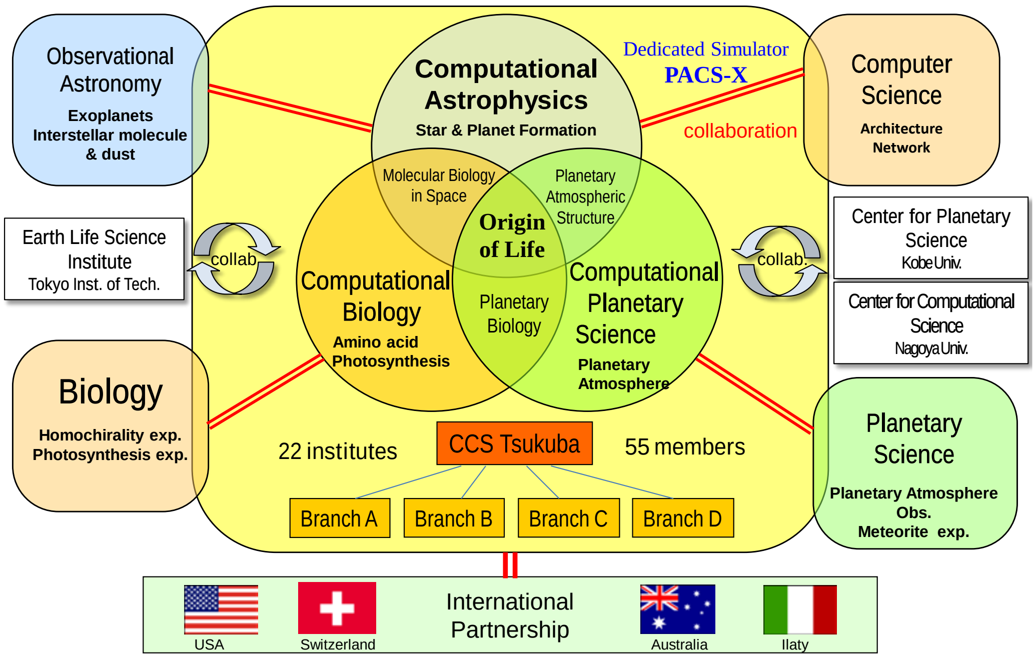
◆ Objective

Explore the basic physics and chemistry regarding the origin of life in the space, and establish Computational Astrobiology.

◆ Dedicated Simulator PACS-X

Develop a supercomputer with state-of-the-art technology of accelerator for quantum mechanical, molecular dynamic, and hydrodynamic simulations.

Organization for Collaborative Research on Computational Astrobiology (CAB)



New Positions

Condensed Matter Group	**Associate Prof.***
Life Science Group	**Professor**
	Yasuteru SHIGETA
Atmospheric Science Group	**Tenure Track***
Planetary Science	**Professor***

Key Science Projects

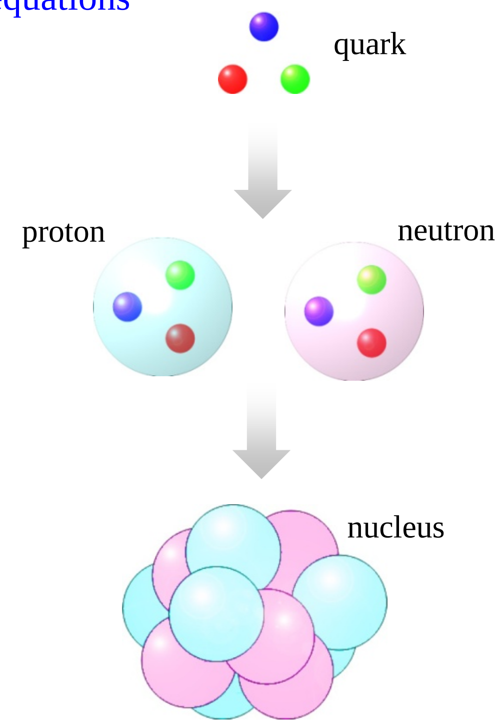
Project 1: Asymmetric Photoreaction of Amino Acids by Interstellar Circularly-polarized Light

Project 2: Turbulence-Particle Interaction, and Forward & Inverse Cascade

Particle Physics

Multi-scale physics

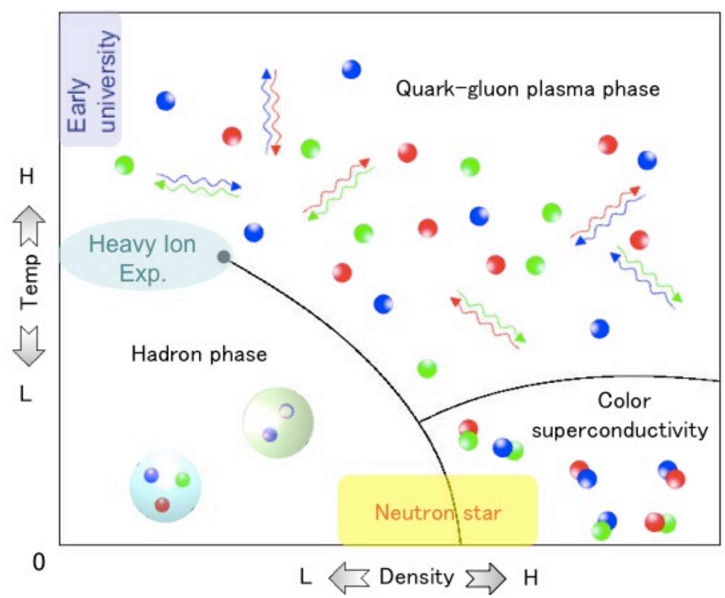
Investigate hierarchical properties via direct construction of nuclei in lattice QCD
GPU to solve large sparse linear systems of equations



Finite temperature and density

Phase analysis of QCD at finite temperature and density
GPU to perform matrix-matrix product of dense matrices

Expected QCD phase diagram



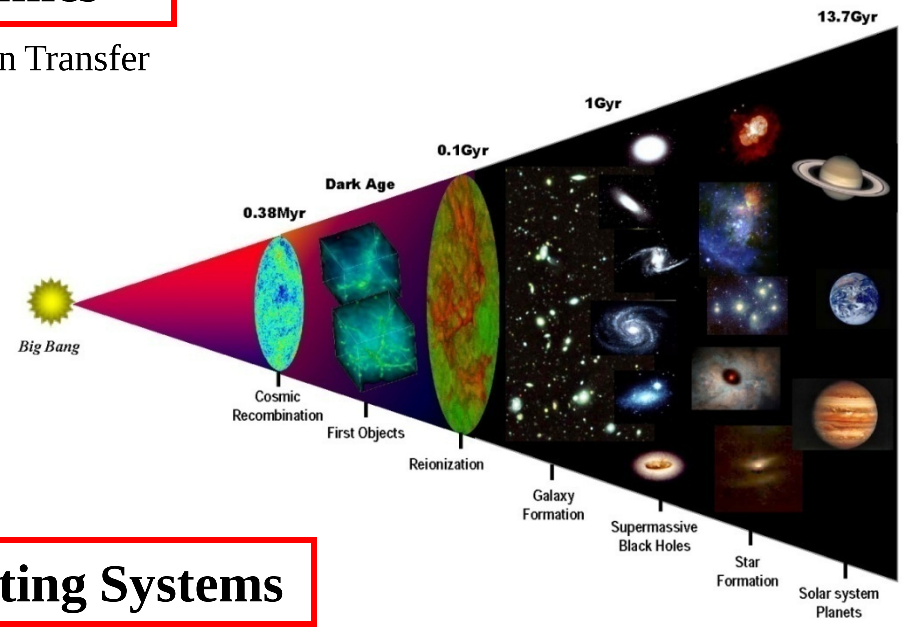
Astrophysics

(A) 6-Dimensional Radiation Hydrodynamics

3-Dimenasional Hydrodynamics + 6-Dimensional Radiation Transfer

<u>Goals</u> Galaxy Formation
Cosmic Reionization
Formation of Supermassive Black Hole

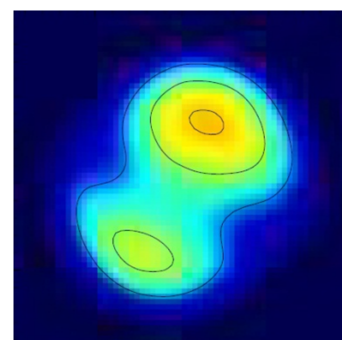
- Acceleration by GPU/TCA of ray tracing and chemical reactions, which are of strong scaling.
- Realization of radiation hydrodynamics

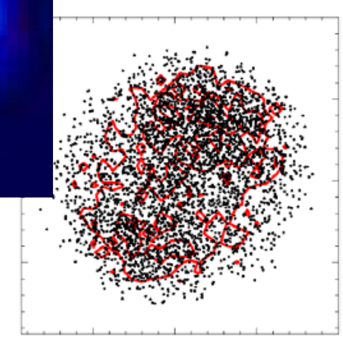


(B) 6D Vlasov Simulation of Self-Gravitating Systems

<u>Goals</u> Dark Matter Dynamics
Collisionless plasma

- A direct integration of collisionless Boltzmann equation
- Not suffer from two-body relaxation which is inevitable in N-body simulation





Nuclear Physics

Simulation with real-time and real-space method for many-fermion systems

Nuclear response and reaction dynamics relevant to nucleosynthesis

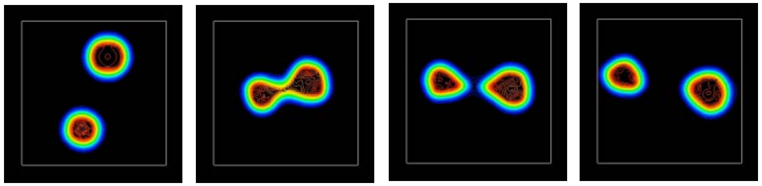
- Nuclear transfer reaction to produce r-process nuclei experimentally
- Fusion reaction of light nuclei
- Systematic investigation of nuclear response function

Application of nuclear methods to other fields

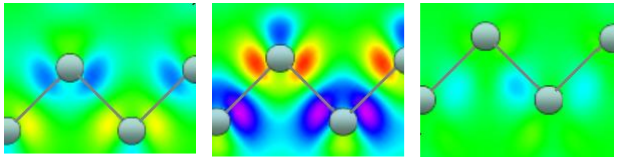
- First-principles calculation for light-matter interaction
- Propagation of ultra-intense laser pulse
- Simulation for atto-second electron dynamics

Methodology : Time-dependent mean-field theory (TDDFT, TDHF, TDHFB) with real-time and 3D real-space method

Merit of GPU calculation : High performance calculation for the operation of Hamiltonian on orbital wave functions



TDHF simulation to produce neutron-rich nuclei by multi-nucleon transfer reaction



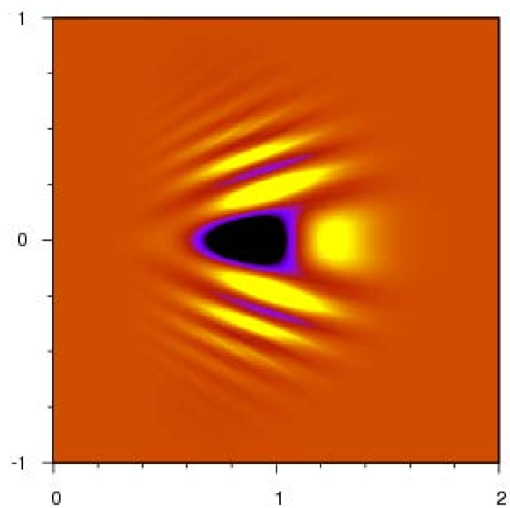
Atto-second electron dynamics in solid induced by ultrashort laser pulse

Materials Science

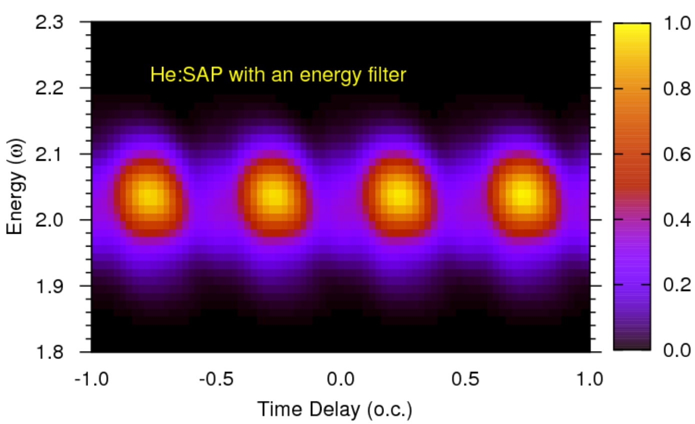
Develop a general numerical method to solve the time-dependent Schrödinger equation for many-electron quantum systems and use it to

$$i\frac{\partial}{\partial t}\Psi = H\Psi$$

- ***understand*** atomic, molecular and materials structures and their dynamics
- ***search*** a way to ***control*** the structures and dynamics in femtosecond (10^{-15} s) or even attosecond (10^{-18} s) time scales.



Holographic image of an electron wavepacket colliding with ionic core.



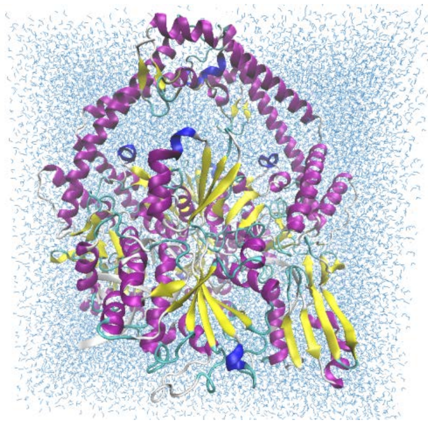
Controlling the XUV transparency by IR laser in attosecond time scale

Bioscience

New developments in computational biosciences

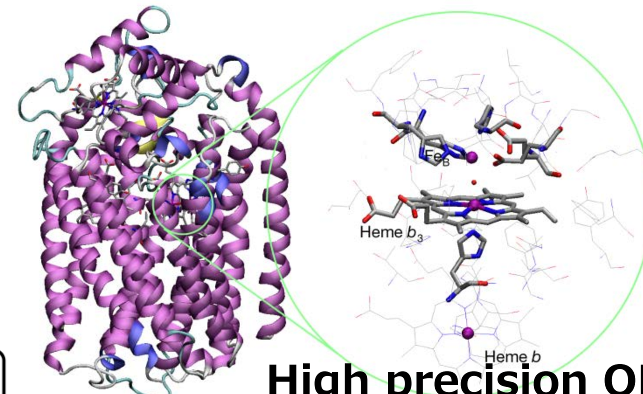
GPU acceleration
- **Molecular Dynamics (MD)**
- **Quantum Mechanics (QM)**

①



Macroscale MD
DNA-protein complexes)

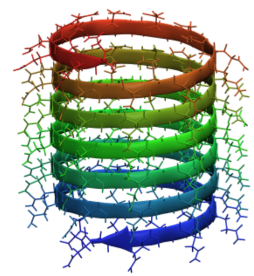
②



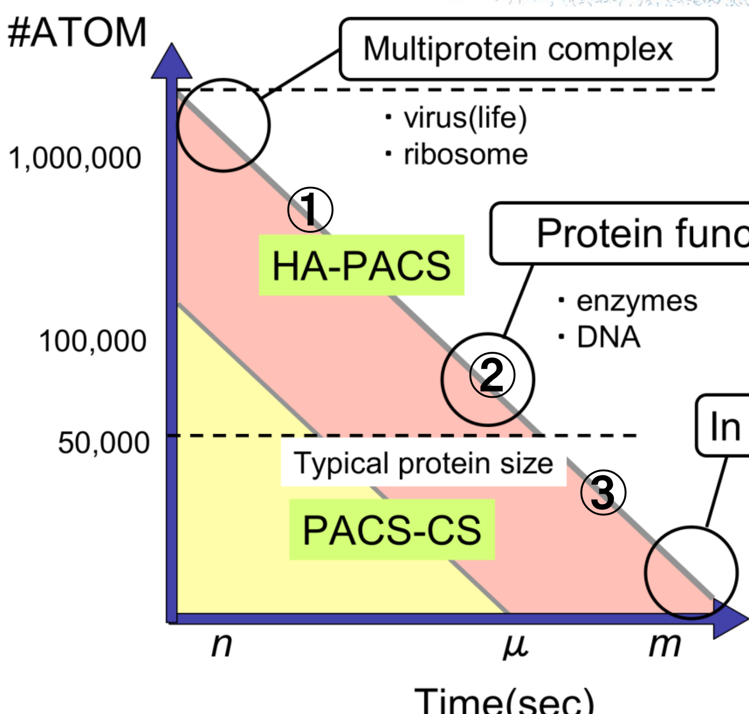
Large QM region
> 100 atoms

High precision QM calculations for reaction mechanisms
(QM/MM-MD, RSDFT-CPMD, PW-CPMD)

③



Long time MD
(Prion Proteins)



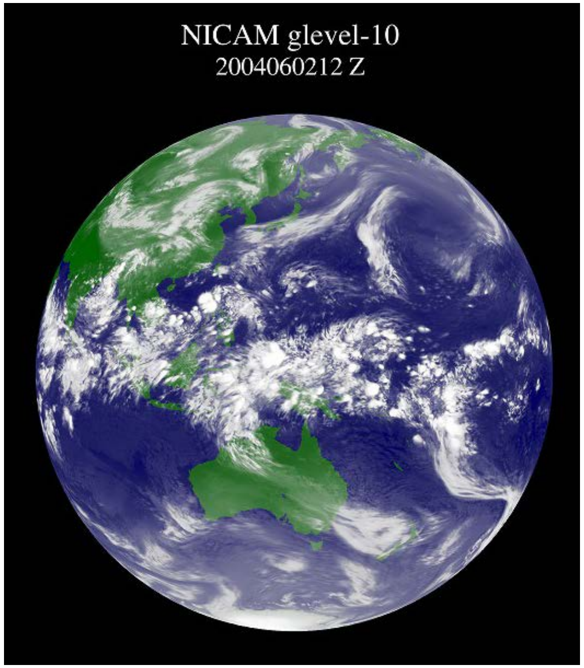
Geoenvironment

Objectives

✓GPU application to the Next-Generation Atmospheric General Circulation Modell NICAM
✓GPU application to the Large Eddy Simulation (LES)
✓GPU application to the 3D Normal Mode Expansion of the atmospheric state variables

New Position

International Tenure Track

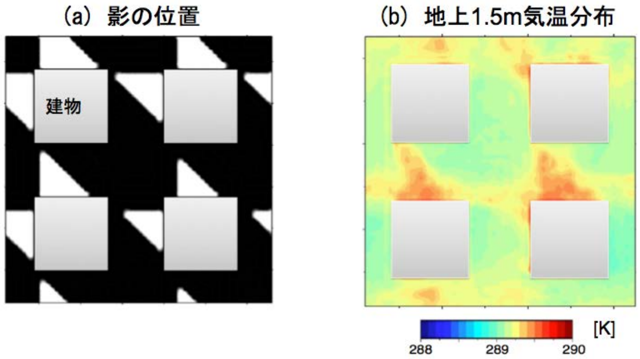


Expected Products

- LES model with 10 m spatial resolution is developed by the GPU application
- NICAM physical processes is efficiently calculated by the GPU application
- Energetics analysis of the high-resolution atmospheric GCM is possible by the GPU application

Merit of the GPU/TCA application

Weather forecasting model by a grid discretization is a type of stencil computation. The memory access is therefore simple, and the computational acceleration up to 10 times speed is possible by the GPU/TCA application.

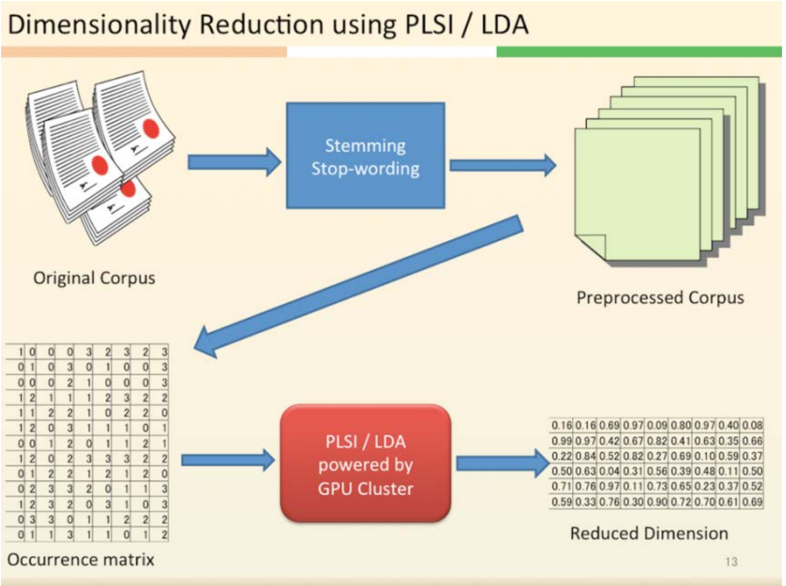


Data Mining of Big Data based on GPGPU

- Research objective and plan
  - **Accelerating data mining** from big data using **GPU**
  - Target mining algorithms
    - Document clustering
      - PLSI (Probabilistic Latent Semantic Indexing)
      - LDA (Latent Dirichret Allocation)
    - Probabilistic association-rule mining
  - Developed algorithms for single-GPU.
  - Develop multi-GPU versions for GPU-cluster environment based on the current algorithms.

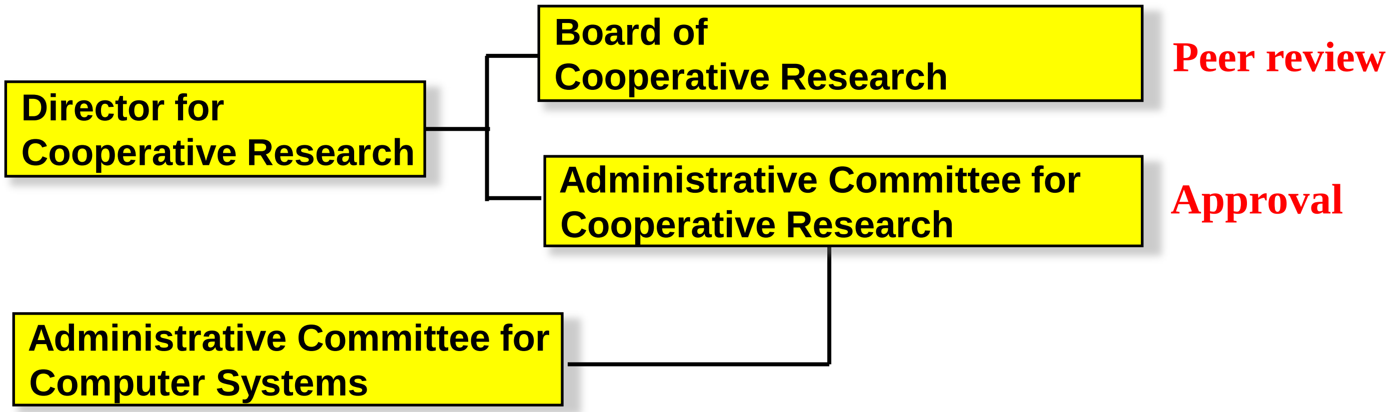
- Expected results and breakthrough
  - Application of GPU-cluster to problems other than numerical analysis or simulation.
  - Few existing works have applied GPU-cluster to data mining problems so far.
  - Promote the use of GPU-cluster as a platform for big data analysis.

- Applicability of GPU
  - Some data mining algorithms are suitable for GPU, but others may not.
  - A technical challenge is to combine CPU- and GPU-based computation taking account of the algorithmic characteristics.
- Scale of computation
  - Under consideration
  - Aiming at processing big datasets such that GPU-cluster is necessary.



Multidisciplinary Cooperative Research
- Joint-use Program of Supercomputers -

Continue "**Multidisciplinary Cooperative Research**" through the joint-use of computational facilities which are developed in CCS.



Since 2010, the CCS has been approved as a "national core-center" under the Advanced Interdisciplinary Computational Science Collaboration Initiative (**AISCI**) launched by the Ministry of Education, Culture, Sports, Science and Technology (MEXT) of Japan, and has provided the use of its computational facilities to researchers nationwide as part of the Multidisciplinary Joint-use Program.

MCS Programs

(Multidisciplinary Computational Science Programs)

- **MCS Symposia:** Call for proposals every year
  Several domestic symposia
  One or two international symposium
- **Travel support for Meetings**
  Financial Support for travel expenses to attend scientific meetings
- **International Schools of MCS**
  International expansion of “Computational Science Literacy”
- **Long-term visitors**
  Those who stay from a few weeks to a few months are encouraged to carry out MCS

Educational Activities in CCS

- **HPC Seminar**
  - This seminar presents knowledge, methods and techniques for programming modern high performance computer systems, including recent microprocessors, and its performance turning, parallel programming.
  - Participants: researchers and users of computational science (including researchers in companies)
  - Periods: 2 or 3 days in summer season
    - Held in July 2007(more than 80 participants)
  - Also broadcasted via internet

- Campus-wide courses on “computational sciences” for graduate students
  - Faculty members of CCS give lectures
  - Accredited as “unit” in graduate courses.
  - Courses
    - Computational Science Literacy
    - High Performance Parallel Computing Technology for Computational Sciences (overlapped with HPC Seminar)
  - Start from 2008

- Computational Science **Dual Degree (double major) Program**
  - Enables a graduate student in a doctoral program to simultaneously belong to a masters program of a different Graduate School, and receive both a doctoral degree in science and a masters degree in computer science, or *vice versa,* upon graduation*.*
  - Design of curriculum and courses for advanced computational science
  - Educate researchers who can push forward new Multidisciplinary computational science from global viewpoints
  - Plan: will be started in 2008 (Physics in Doctor course and Computer sciences in Master course)

- Education in each graduate school
  - CCS allocates space for some of students, and create environment to enable interactions to other fields.

Summary

1. “**Multidisciplinary Computational Science (MCS)**” is the central vision of the CCS, which is expanded by two pillar offices: "**Project Office for Exascale Computational Sciences**" and "**Project Office for Exascale Computing System Development**".

2. As for the development of computers, the succession of the **PACS-series** projects, the progress of Joint Center for Advanced High Performance Computing (**JCAHPC**), and the success of the Exa-scale Computing Feasibility Study should be key projects in the Center.

3. The two inter-university projects, Joint Institute for Computational Fundamental Science (**JICFuS**) and Organization for Collaborative Research on Computational Astrobiology (**CAB**), can be prime movers to make the CCS a world-wide core center for multidisciplinary computational science.

4. Continue Multidisciplinary Cooperative Research, MCS, and Educational programs.