HPC at CCS

University of Tsukuba

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

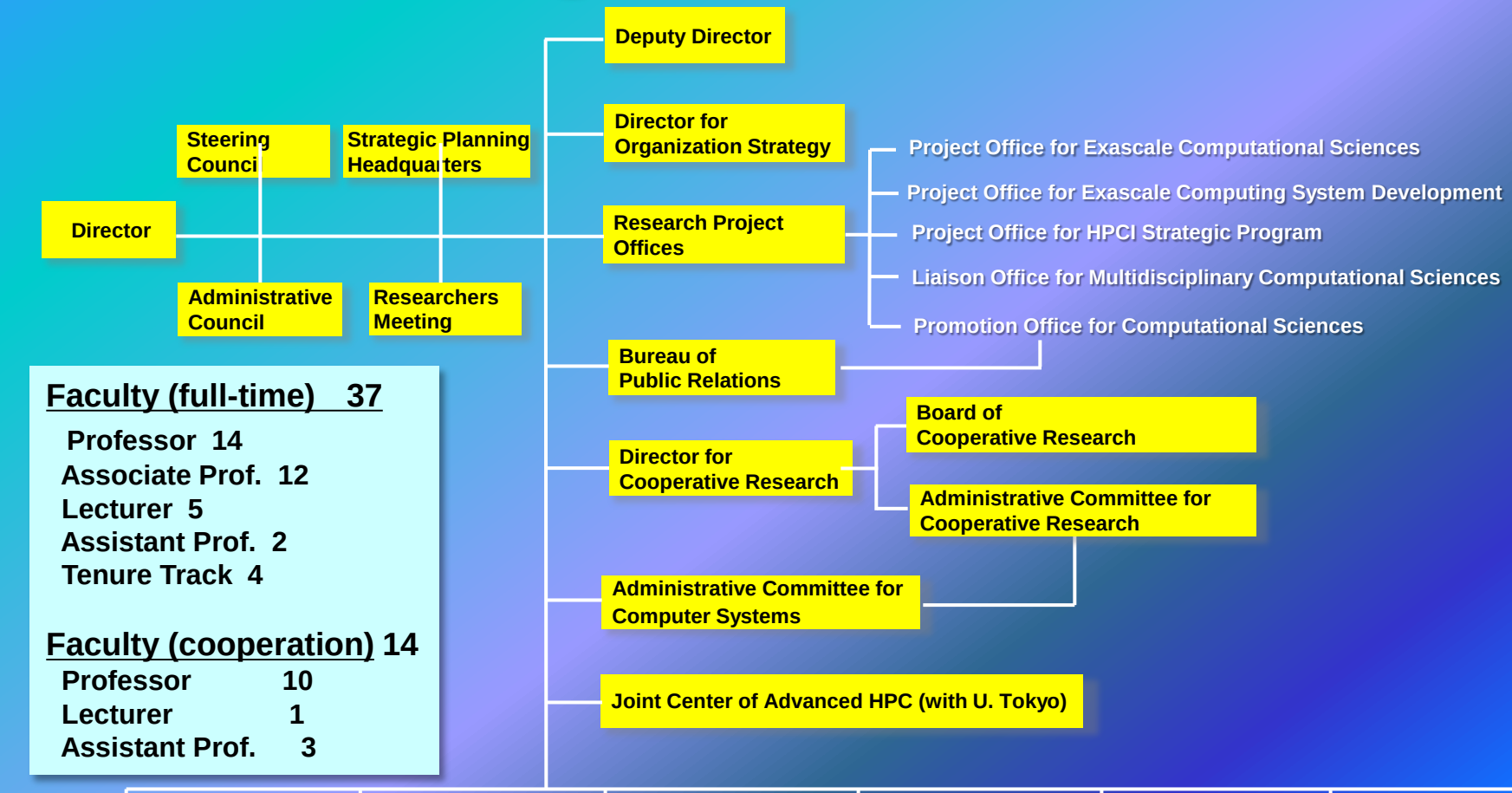
8 Positions Recruited in FY2013

"Organization for the Support and Development of Strategic Initiatives"

Particle Physics Group	Tenure Track*	
Astrophysics Group	Tenure Track*	
Nuclear Physics Group	Professor	Takashi NAKATSUKASA
	Tenure Track*	
Condensed Matter Group	Associate Prof.*	
Life Science Group	Professor	Yasuteru SHIGETA
Atmospheric Science Group	Tenure Track*	
Astrobiology	Professor*	

* new positions

Organization of CCS



Faculty (full-time) 37

Professor	14
Associate Prof.	12
Lecturer	5
Assistant Prof.	2
Tenure Track	4

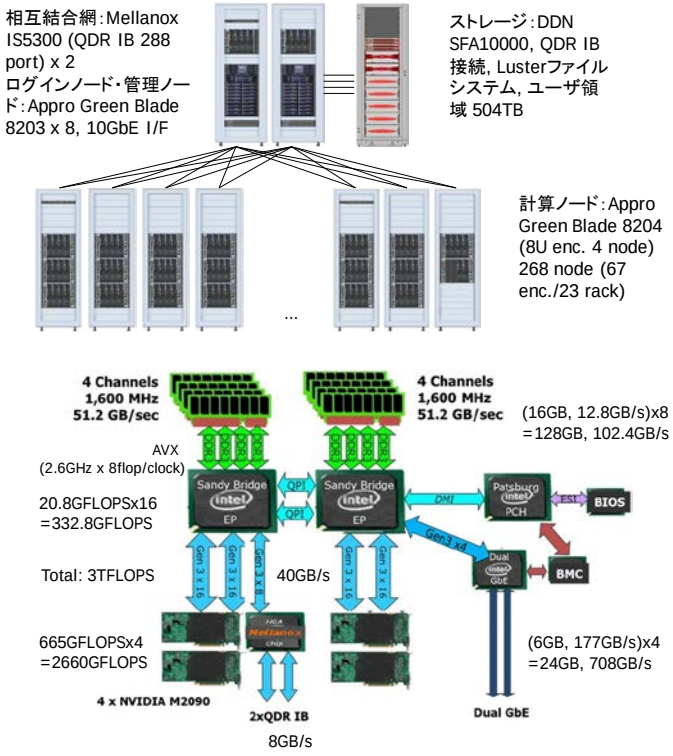
Faculty (cooperation) 14

Professor	10
Lecturer	1
Assistant Prof.	3

Division of Particle Physics	Division of Astrophysics & Nuclear Physics	Division of Quantum Condensed Matter Physics	Division of Life Science	Division of Global Environmental Science	Division of High Performance Computer Systems	Division of Computational Informatics
Particle Physics Group	Astrophysics Group Nuclear Physics Group	Material Science Group	Biological Function and Information Group Molecular Evolution Group	Atmospheric Science Group	High Performance Computing System Group	Database Group Computational Media Group

HA-PACS system (base-cluster)

- System spec.
  - 268 nodes
  - CPU 89TFLOPS + GPU 713TFLOPS = total 802TFLOPS
  - Memory 34TByte、memory bandwidth 26TByte/sec
  - Bi-section bandwidth 2.1TByte/秒
  - Storage 504TByte
  - Power 408kW
  - 26 ranks, Installed on Jan, 2012
  - Operation started from Feb, 2012



- Spec of compute nodes
  - CPU x2 + GPU x4/node

  （4 GPU: 2660 GFLOPS + 2 CPU: 332 GFLOPS~ 3 TFLOPS / node）
  - Advanced CPU：Intel SandyBridge： high-peak performance enhanded by 256bit AVX instruction, and high memory bandwidth by 1600MHz DDR3 (2.6GHz SandyBridge-EP (8 core) = 166.4 GFLOPS, 51.2GB/s memory bandwitdh, 128GB)
  - x40 lane for CPU direct I/O of PCIe Gen3
  - Advanced GPU：NVIDIA M2090: M2070 512core enhance version：peak performance 665GFLOPS
  - Interconnect network
    - Infiniband QDR x 2 rail (trunk)
    - Connected by PCIe Gen3 x8 lane

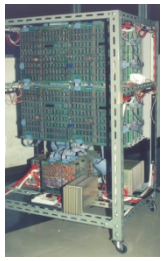
Development of Massively Parallel Computer Systems in CCS

- 1977 research begins (by Hoshino, Kawai)
- 1978 1st machine
- 1996 CP-PACS (top of Top500)
- 2006 7th machine PACS-CS
- 2012 8th machine HA-PACS

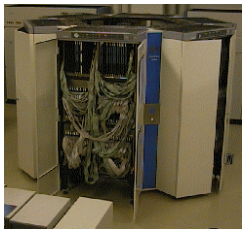
CP-PACS
- First large-scale general-purpose MPP system in Japan
  - Development supported by ``Research of Field Physics with Dedicated Parallel Computers'' funded by the Ministry of Education of the Japanese Government.
  - ranked as No. 1 system in the November 1996 Top 500 List.
- Collaboration by physicists and computer scientists
- Collaboration with industry, and released as Hitachi SR2201

1978
1st PACS-9

1980
2nd PAXS-32



1989
5th QCDPAX



1996
6th CP-PACS
(top of Top500 list in 1996)

2006
7th PACS-CS

2012
8th HA-PACS

Year	System	Performance
1978	PACS-9 (PACS I)	7 KFLOPS
1980	PACS-32 (PACS II)	500 KFLOPS
1983	PAX-128 (PACS III)	4 MFLOPS
1984	PAX-32J (PACS IV)	3 MFLOPS
1989	QCDPAX (PACS V)	14 GFLOPS
1996	CP-PACS (PACS VI)	614 GFLOPS
2006	PACS-CS (PACS VII)	14.3 TFLOPS
2012	HA-PACS (PACS VIII)	802 TFLOPS

COMA (PACS-IX) System

Computation node	CPU	Intel E5-2670v2 (Ivy Bridge-EP) 2.5GHz x2
	# of cores	20 (10 cores / CPU)
	MIC	Intel Xeon Phi 7110P 61 core x2
	Main memory	64 GB (DDR3 1866MHz x 8 channel, 119.4GB/s)
	MIC memory	16 GB (8GB/MIC, 352GB/sMIC)
	Peak performance	400 GFLOPS (CPU) + 2147 GFLOPS (MIC)
	Network HCA	InfiniBand FDR
	Peak network b/w	7 GB/s
Number of nodes		393
Interconnection configuration		Fat-Tree with full bisection b/w
Peak performance		1.001 PFLOPS (CPU: 157 TFLOPS, MIC:844 TFLOPS)
Network bisection b/w		2.75 TB/s
Shared file system		Lustre file system
File system capacity		1.5 PB (user space)

File server

Cooperation between Computational and Computer Science

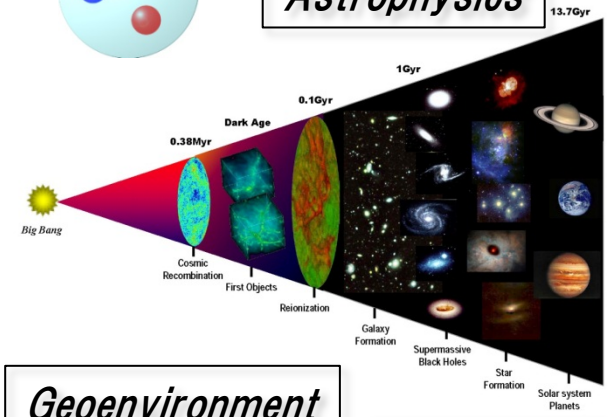
Project Office for Exascale Computational Sciences

Project Office for Exascale Computing System Development

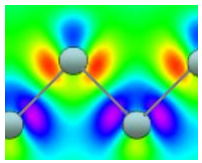
Particle Physics

Nuclear Physics

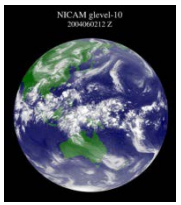
Astrophysics



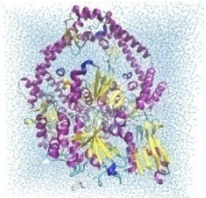
Materials Science



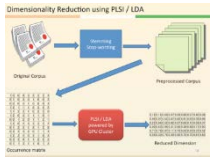
Geoenvironment



Bioscience



Database



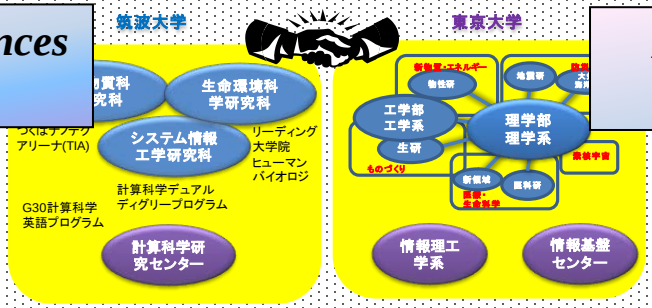
Future Plans of Computing System Development

Fiscal Year	2012	2013	2014	2015	2016	2017	2018	2019	2020	2021
TPF		HA-PACS 800TF **340kW**			HA-PACS TCA +360TF		PACS-X ～10PF **2MW**			
UCC+TPF		T2K-tsukuba **630kW**			COMA (PACS-IX) 1PF					
		T2K-Todai					Post Open Supercomputer 30PF±			
							JCAHPC			

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

Particle Physics

quark

proton

neutron

Nuclear Physics

Quantum Many-body System

Materials Science

Nuclear Reactions

Geoenvironment

Particle Reactions

13.7Gyr
1Gyr
0.1Gyr
Dark Age
0.38Myr
Big Bang
Cosmic Recombination
First Objects
Reionization
Galaxy Formation
Supermassive Black Holes
Star Formation
Solar system Planets

NICAM glevel-10
2004060212 Z

Bioscience

Astrophysics

Database

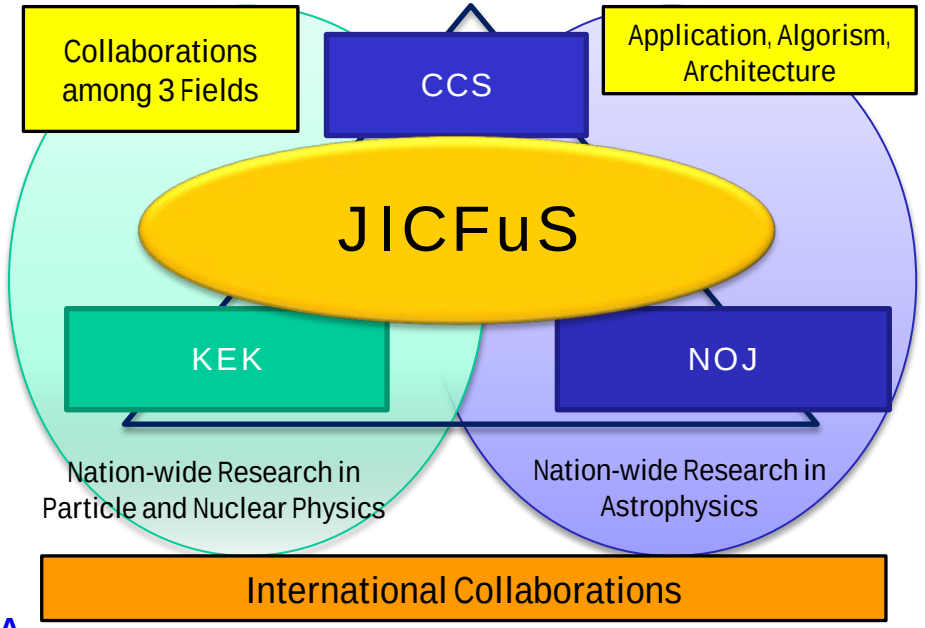
Dimensionality Reduction using PLSI / LDA

Hydrodynamics, Radiation, Chemical Reactions

Joint Institute for Computational Fundamental Science

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

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.

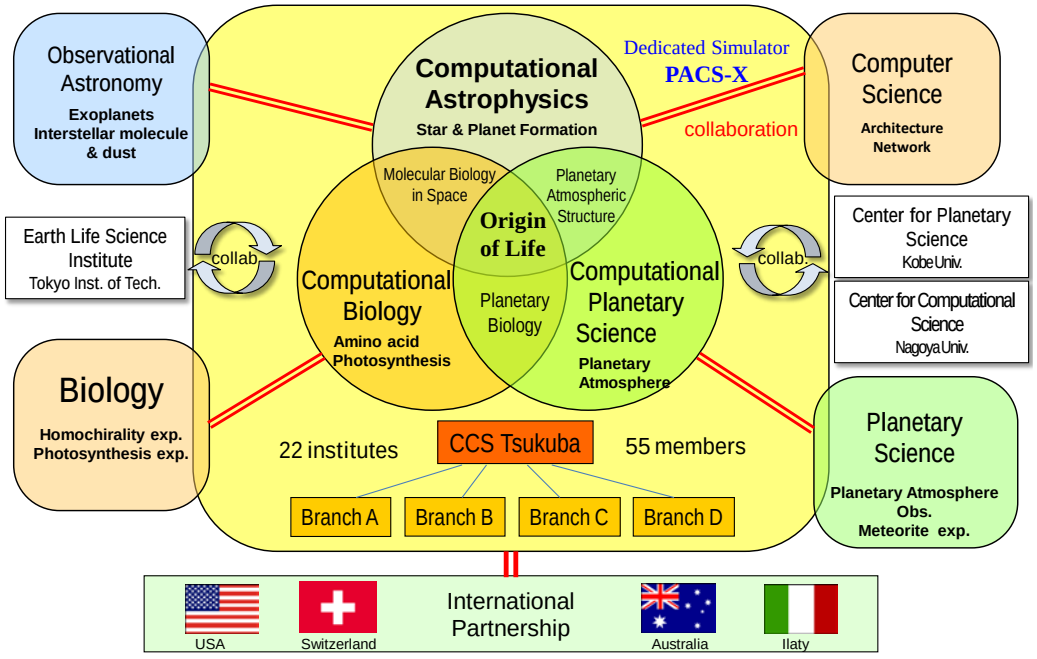
◆ Objective

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

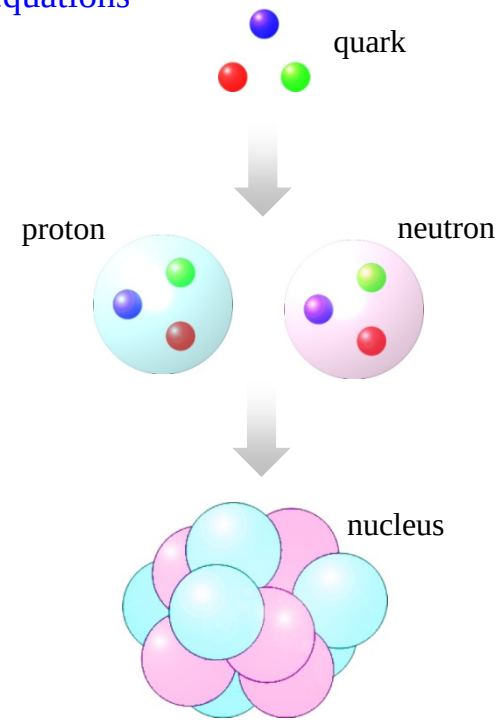
Project 1: Asymmetric Photoreaction of Amino Acids by Interstellar Circularly-polarized Light

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

Particle Physics

Multi-scale physics

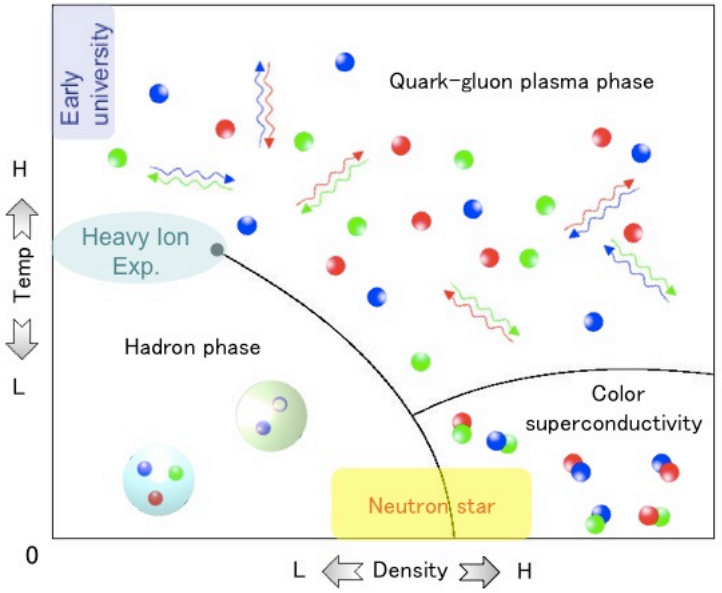
Investigate hierarchical properties via direct construction of nuclei in lattice QCD
GPU to solve large sparse linear systems of equations



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



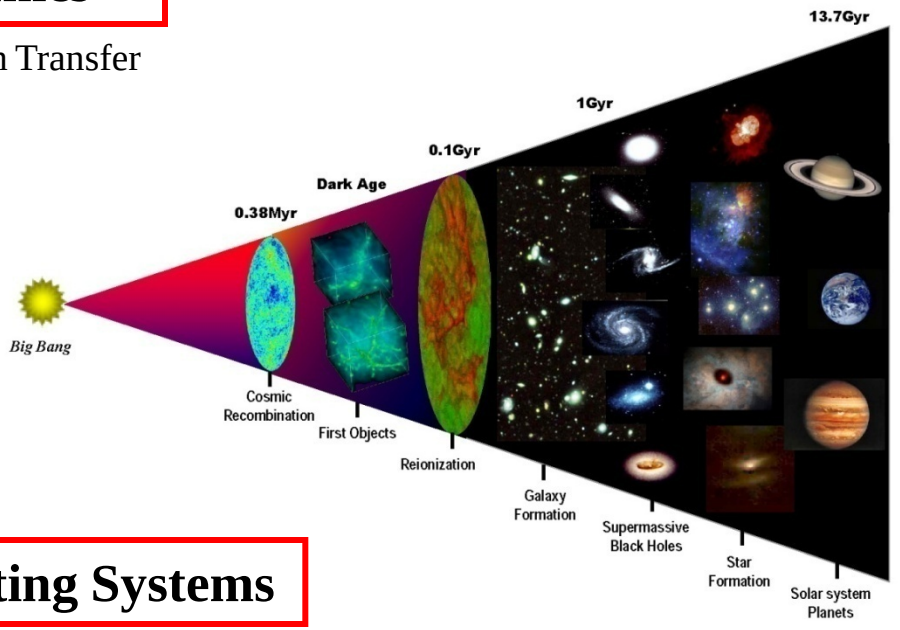
Astrophysics

(A) 6-Dimensional Radiation Hydrodynamics

3-Dimenasional Hydrodynamics + 6-Dimensional Radiation Transfer

Goals Galaxy Formation
Cosmic Reionization
Formation of Supermassive Black Hole

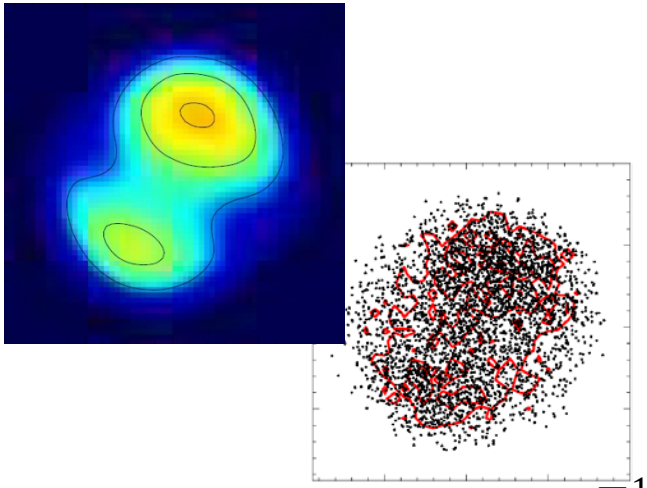
- Acceleration by GPU/TCA of ray tracing and chemical reactions, which are of strong scaling.
- Realization of radiation hydrodynamics



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

Goals 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

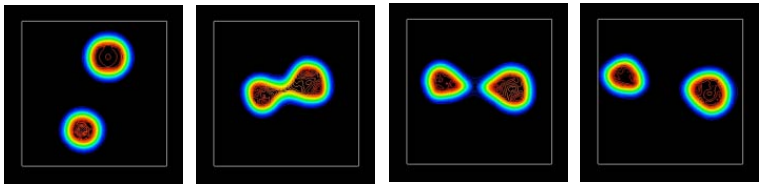
- Nuclear transfer reaction to produce r-process nuclei experimentally
- Fusion reaction of light nuclei
- Systematic investigation of nuclear response function

Application of nuclear methods to other fields

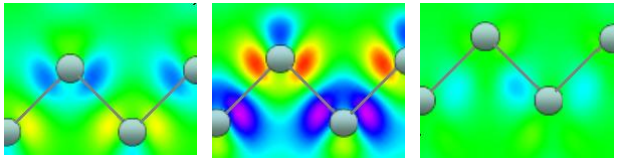
- First-principles calculation for light-matter interaction
- Propagation of ultra-intense laser pulse
- Simulation for atto-second electron dynamics

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



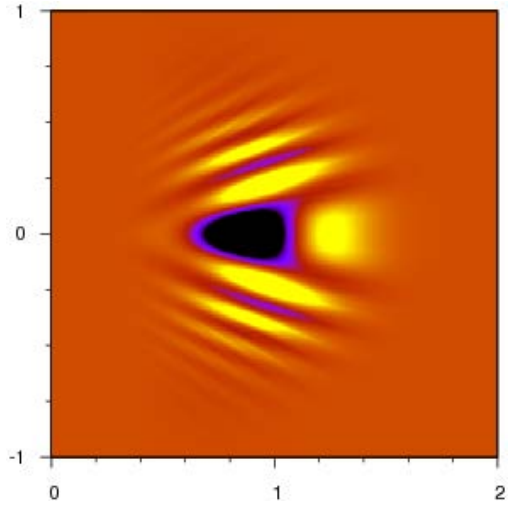
Atto-second electron dynamics in solid induced by ultrashort laser pulse

Materials Science

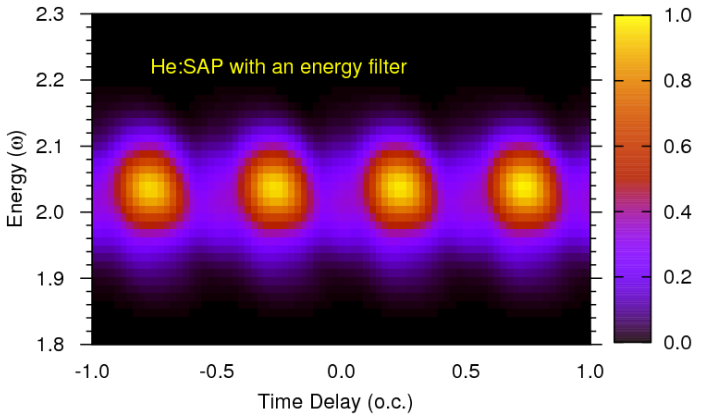
Develop a general numerical method to solve the time-dependent Schrödinger equation for many-electron quantum systems and use it to

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

- ***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.



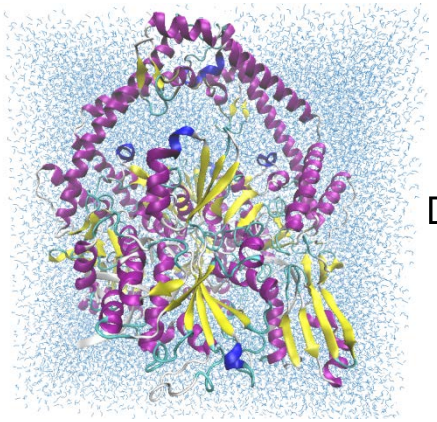
Controlling the XUV transparency by IR laser in attosecond time scale

Bioscience

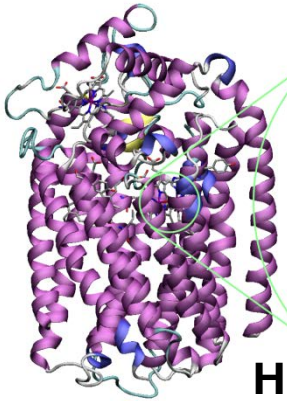
New developments in computational biosciences

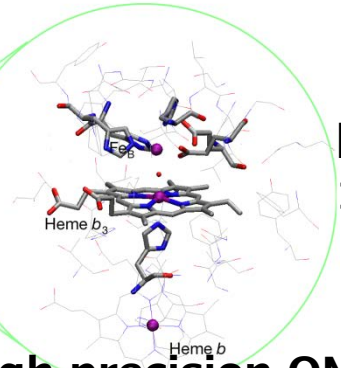
GPU acceleration
・Molecular Dynamics (MD)
・Quantum Mechanics (QM)

①



Macroscale MD
DNA-protein complexes)

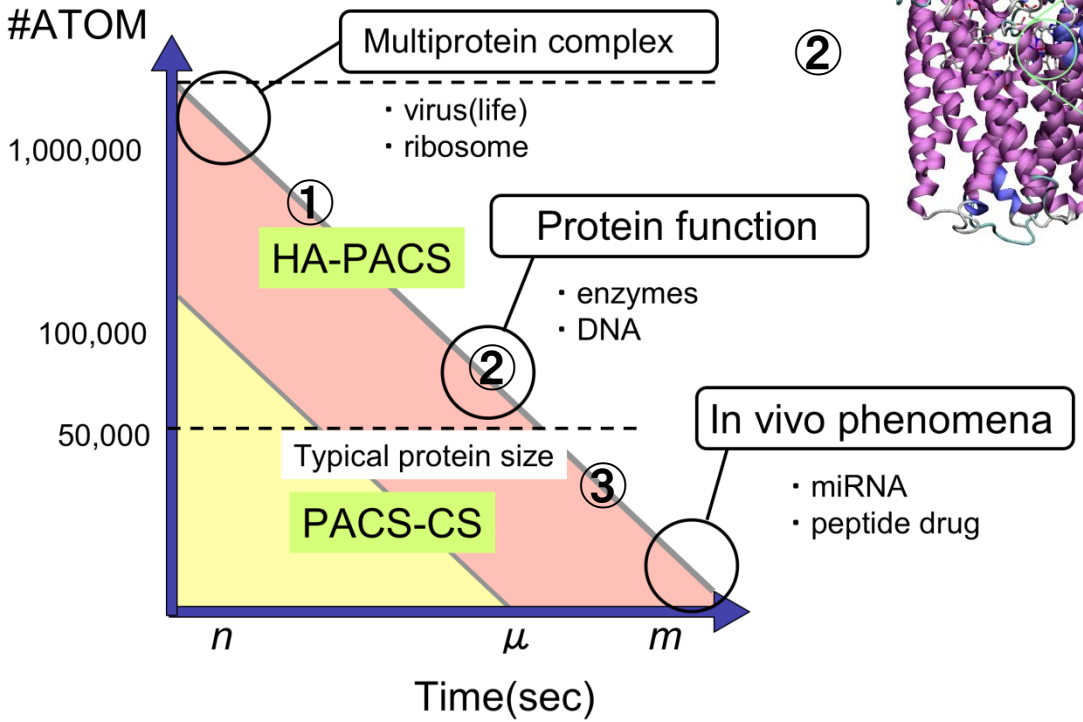




②

Large QM region
> 100 atoms

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



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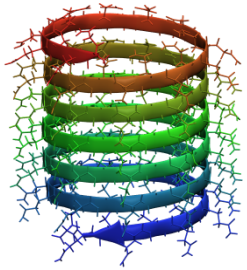


Long time MD
(Prion Proteins)

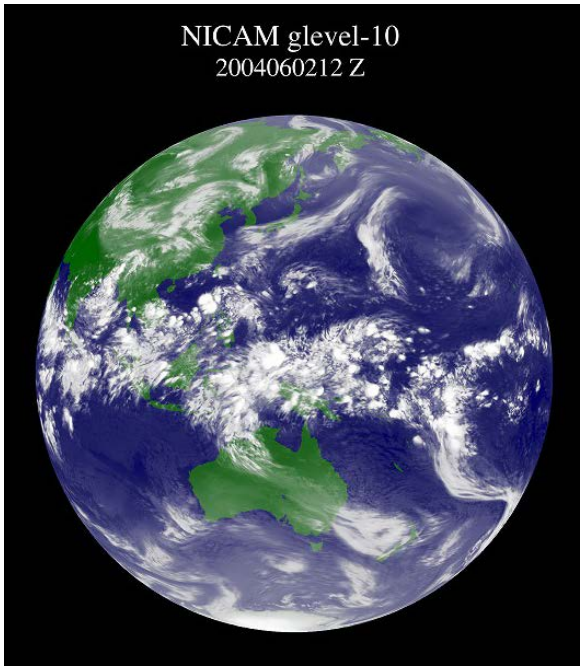
Geoenvironment

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

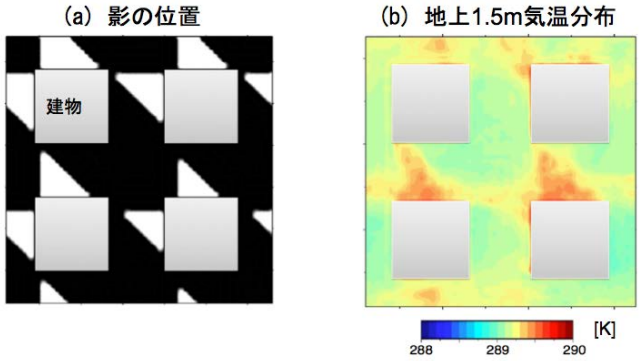
New Position

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

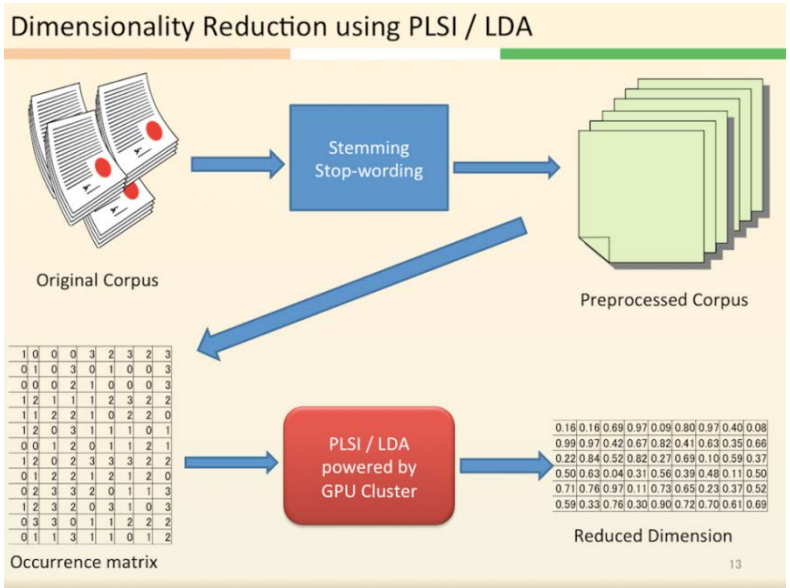


Merit of the GPU/TCA application

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.

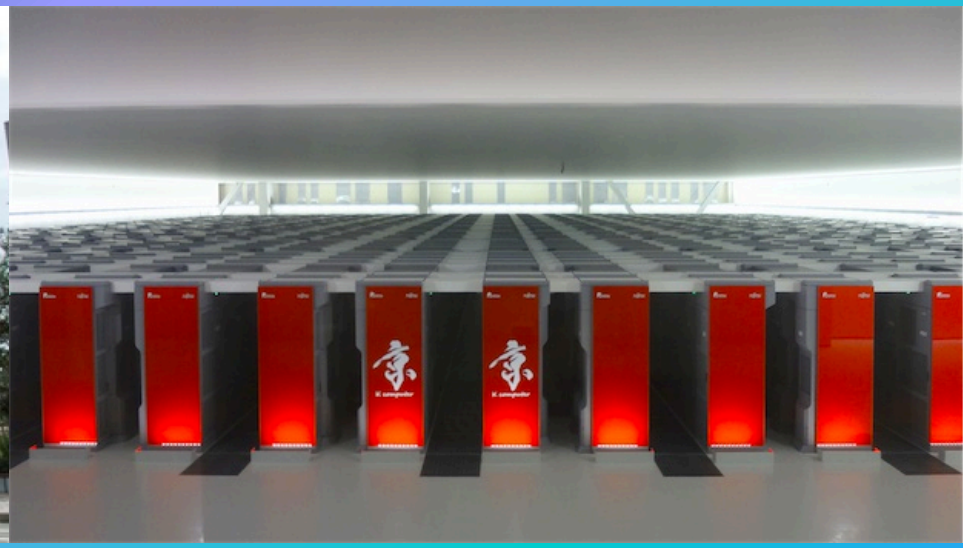
Data Mining of Big Data based on GPGPU

- 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.



京（K）computer

- SPARC64™ VIIIfx 2.0GHz octcore (128Gflops / core)
- 16 GB memory / core
- 6D torus network
- Total 82944 nodes (663552 CPU core)
- 1.3PB memory
- 10.6 Pflops peak speed



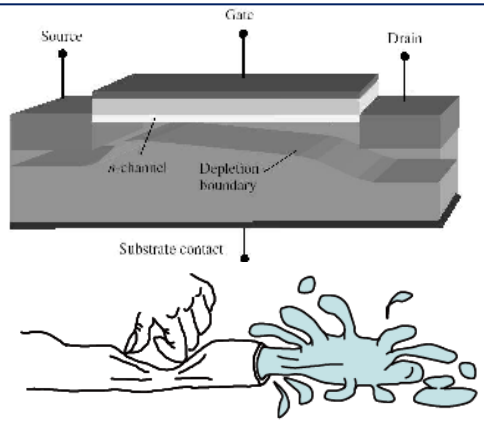
Prediction of Electron States of Si Nanowires with 100,000 atoms on K Computer

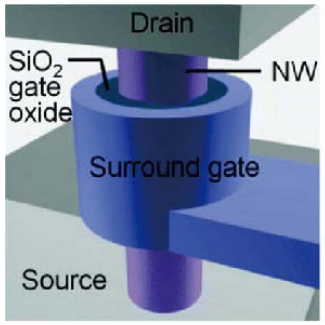
Gordon Bell Prize 2011

Si Nanowire, a booster
in the next-generation semiconductor technology

More Moore → More than Moore

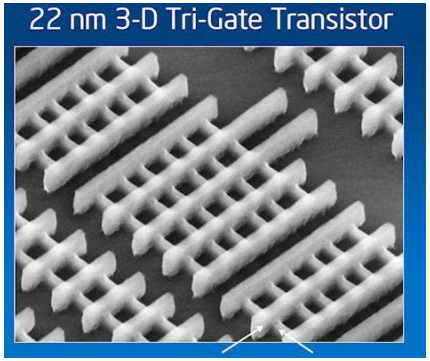
planar transistor





Surrounding gate transistor

Gate Controllability
→ Suppress short-channel effects
Suppress leaks at off state
→ save energy



Actually tri-gate by Intel in 2011

Number of atoms in SiNW channels
→ 10,000 - 100,000 atoms !

Collaborators

- Yukihiro Hasegawa (RIKEN)
- Jun-Ichi Iwata (The University of Tokyo)
- Miwako Tsuji (University of Tsukuba)
- Daisuke Takahashi (University of Tsukuba)
- Atsushi Oshiyama (The University of Tokyo)
- Kazuo Minami (RIKEN)
- Taisuke Boku (University of Tsukuba)
- Fumiyoshi Shoji (RIKEN)
- Atsuya Uno (RIKEN)
- Motoyoshi Kurokawa (RIKEN)
- Hikaru Inoue (Fujitsu Limited)
- Ikuo Miyoshi (Fujitsu Limited)
- Mitsuo Yokokawa (RIKEN)

Trillion-body Simulations of Dark Matter Universe

on K-Computer

Ishiyama (Tsukuba), Makino (TiTech), Nitadori (AICS, Riken)

Gordon Bell Prize 2012

Visualization by Takeda (CfCA, NAO)

Dynamic domain decomposition

△ Space filling curve

○ multi section

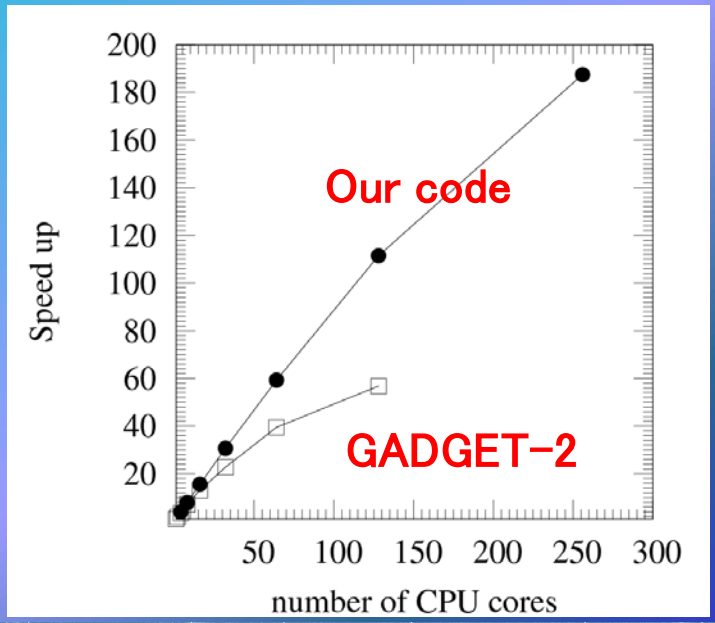
Allows each node to know easily
where to perform short communications

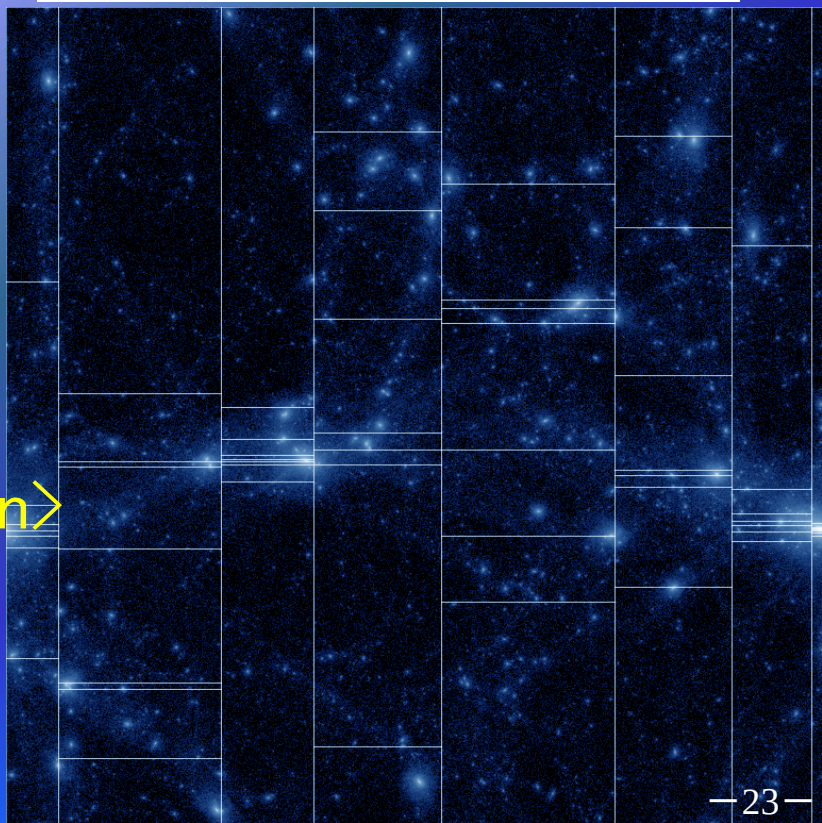
× equal #particles

△ equal #interactions

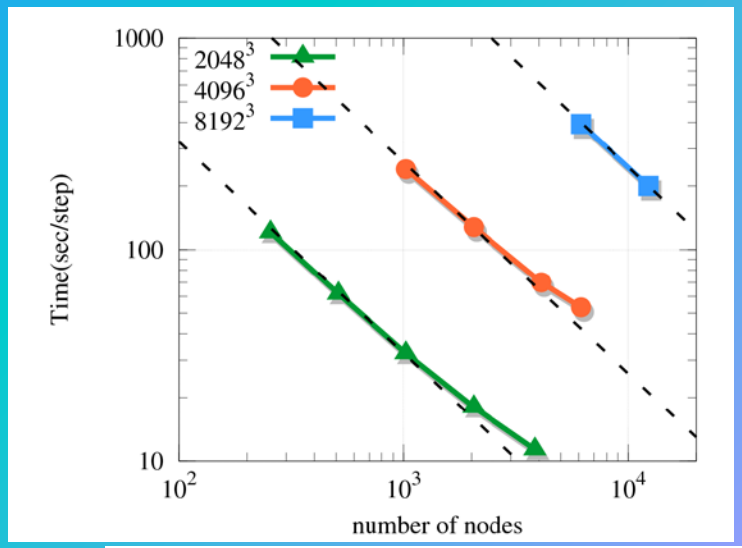
◎ equal <#interactions + correction>

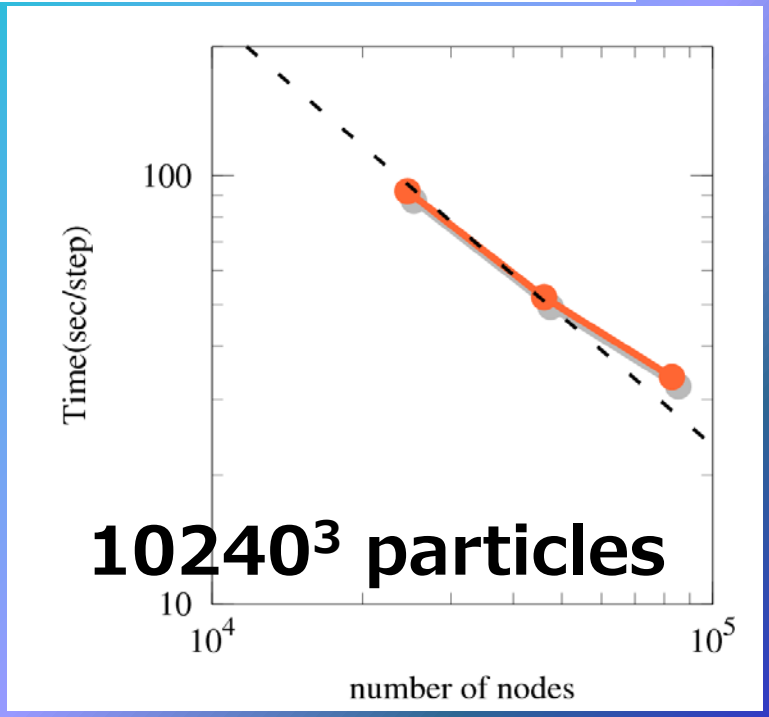
= equal calculation time





Performance results

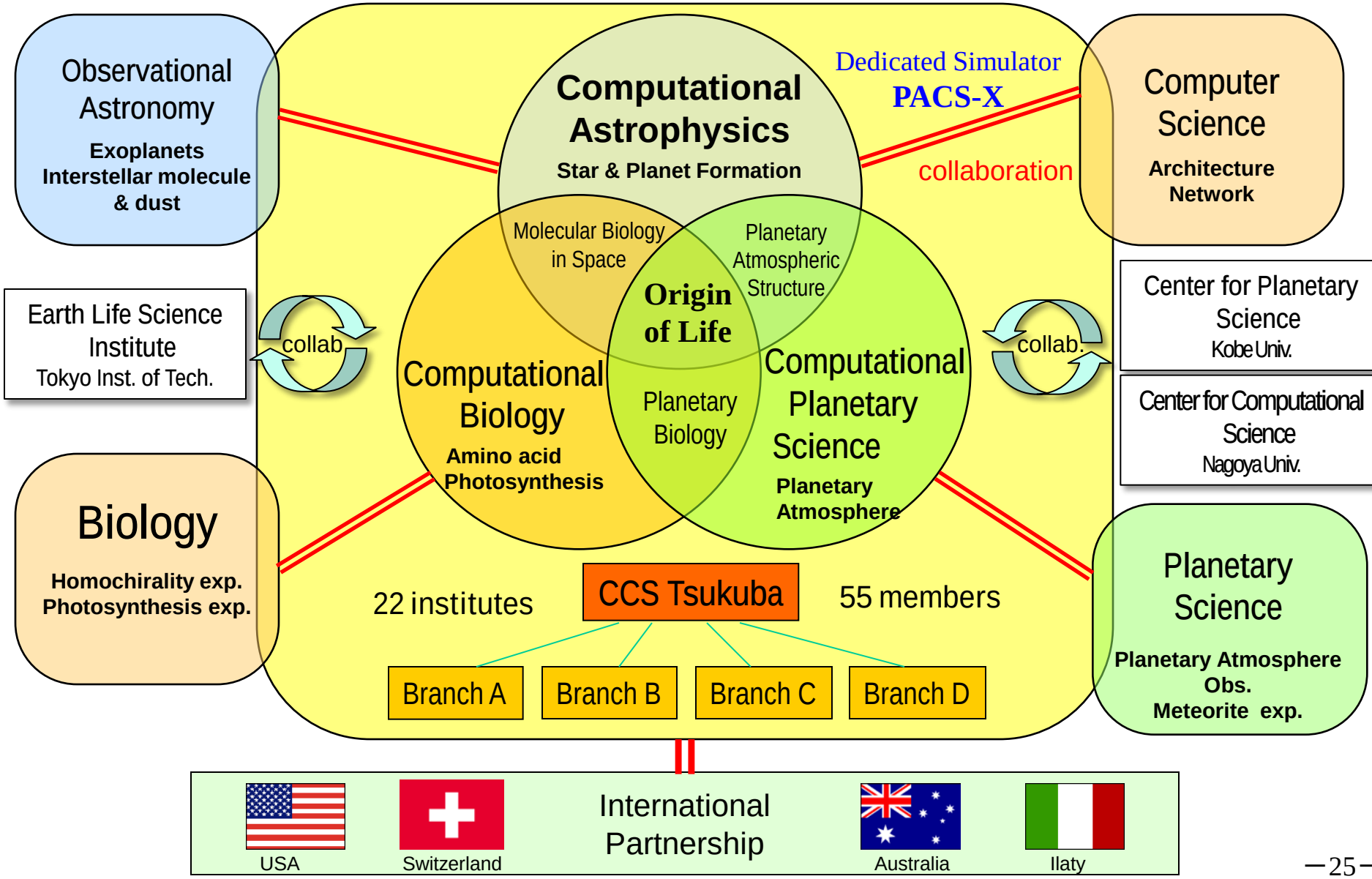




- **Scalability (2048^3 - 10240^3)**
  - Excellent strong scaling
  - 10240^3 simulation is well scaled from 24576 to 82944 (full) nodes of K computer
- **Performance (12600^3)**
  - The average performance on fullsystem is ~**5.67Pflops**, which correspond to ~**55**% of the peak speed

Gordon Bell Prize 2012

Organization for Collaborative Research on Computational Astrobiology (CAB)



Computational Astrobiology

Astrophysics

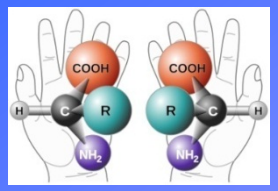
Biophysics

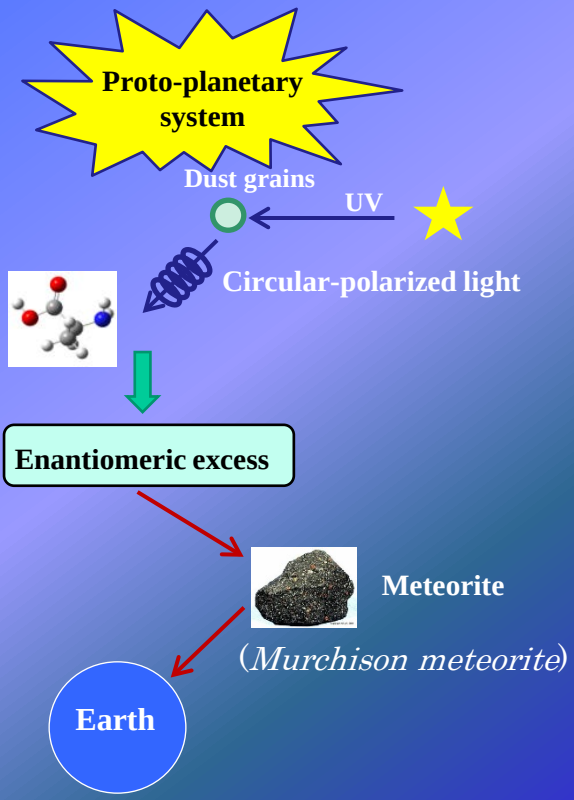
Planetary Science

Collaboration of Astrophysics, Biophysics, and Planetary Science

Cosmic origin of L-amino acid

Enantiomeric excess of Amino Acid by interstellar circular-polarized light



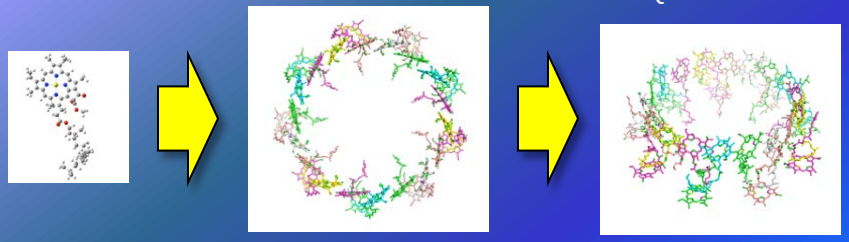


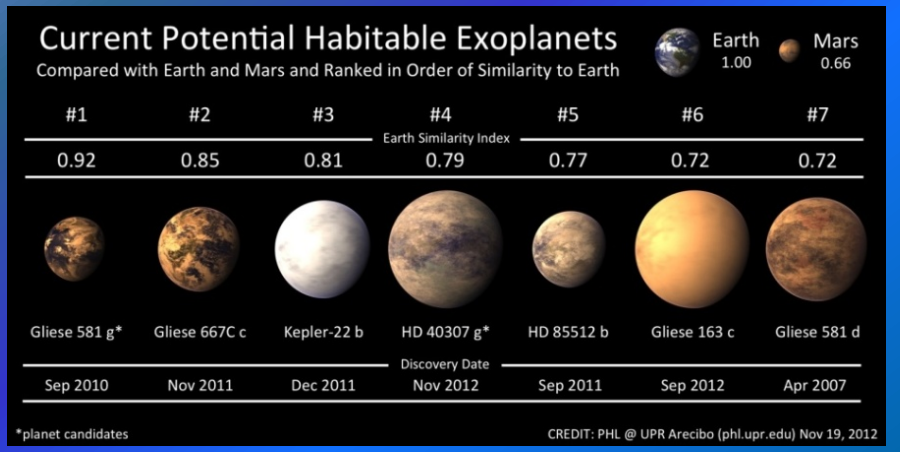
Photosynthesis on extra-solar planets

Red edge as a biomerker

TDDFT calculations of chlorophylls

Chlorophyll dynamics QM/MM





Thank you