Center for Computational Sciences, Univ. of Tsukuba

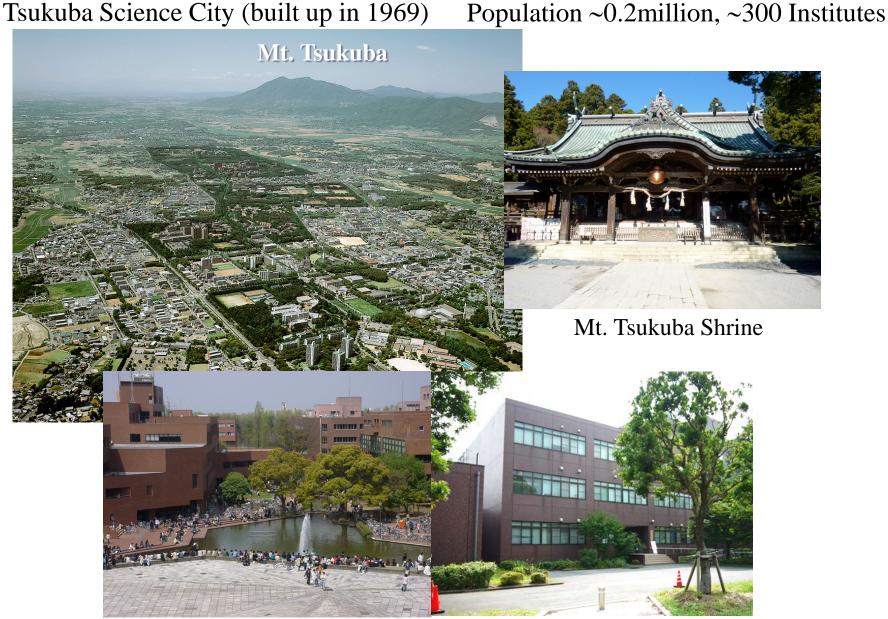


Center for Computational Sciences University of Tsukuba

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

External Review Committee:

➢ Jeffery Vetter (Chair) Professor Computer Science Computer Science and Mathematics Division, Oak Ridge National Laboratory, USA Professor Shinji Tsuneyuki (Vice Chair) Material Science \geq School of Science, The University of Tokyo, Japan Karl Jansen Professor Particle Physics John von Neumann Institut fur Computing (NIC), Germany Andreas Burkert Astrophysics Professor \geq Theoretical and Computational Astrophysics, University Observatory, Munich Germany Professor \geq James Vary Nuclear Physics International Institute of Theoretical and Applied Physics, Iowa State University, USA Joachim Burgdörfer Material Science Professor \geq Vienna University of Technology, Austria Andrew Roger **Biological Science** Professor \geq Dalhousie University, Halifax, Nova Scotia, Canada **Computational Science** Professor \geq Jack Wells National Center for Computational Science, Oak Ridge National Laboratory, USA Geoscience Professor Takemasa Miyoshi Data Assimilation Research Team, RIKEN Advanced Institute for Computational Science, Japan Hiroshi Nakashima Computer Science Professor \succ Academic Center for Computing and Media Studies, Kyoto University, Japan **Computational Informatics Professor** Xiaofang Zhou \geq University of Queensland, Australia



University of Tsukuba in 1972Center for Computational Physics in 1992from Tokyo University of Education (predecessor)Center for Computational Sciences in 2004-3-

Chronology of CCS

1992 Apri	l Ce	enter for Computational Physics (CCP) founded. CP-PACS Project begins.	
1996 Septe	ember CI	P-PACS (2048 PU) completed and installed	
Nove	ember Ra	anked as No. 1 on the Top 500 World Supercomputer List	
2004 April	CC	CP is reorganized, expanded and relaunched as the Center for	
Computational Sciences (CCS)			
2005 April	De	evelopment of Massively Parallel Cluster PACS-CS in the project begins	
2007 April	Co	osmo-Simulator FIRST completed and installed	
2008 June	OI	peration of T2K-Tsukuba begins.	
2010 April	Aj	pproved under the Advanced Interdisciplinary Computational Science	
		Collaboration Initiative (AISCI)	
	CC	CS is reorganized from five to seven divisions	
2012 Febru	uary HA	A-PACS starts operation	
2013 Marc	h Jo	int Center for Advanced HPC established in alliance with the University of	
		Tokyo	
Augus	st Aı	uthorized as one of the two prime research centers in U. Tsukuba	

Objective of External Review

• The objective of the external review is to receive the evaluation on the research activities and their outcomes in the Center in the period of FY2008 – FY2013 and recommendations for the future development of the Center.

Materials for the External Review

- Schedule
- Form of Review Report (tentative) (Final report by April 30)
- CCS Report
 PART I, Overview of Center for Computational Sciences
 Summary of Activities 2008-2013

 PART II, Research Activities, Results, Collaborations and Plan 2008-2013
 PART III: Strategy and Future Plans of Center for Computational Sciences
- Presentation Files on Web
- Brochures of CCS and U. Tsukuba
- Posters of CCS Researches (Lobby)
- Operating Supercomputers (Computer building)
- Display of the PACS Series of Supercomputers (Lobby)





Mission of CCS

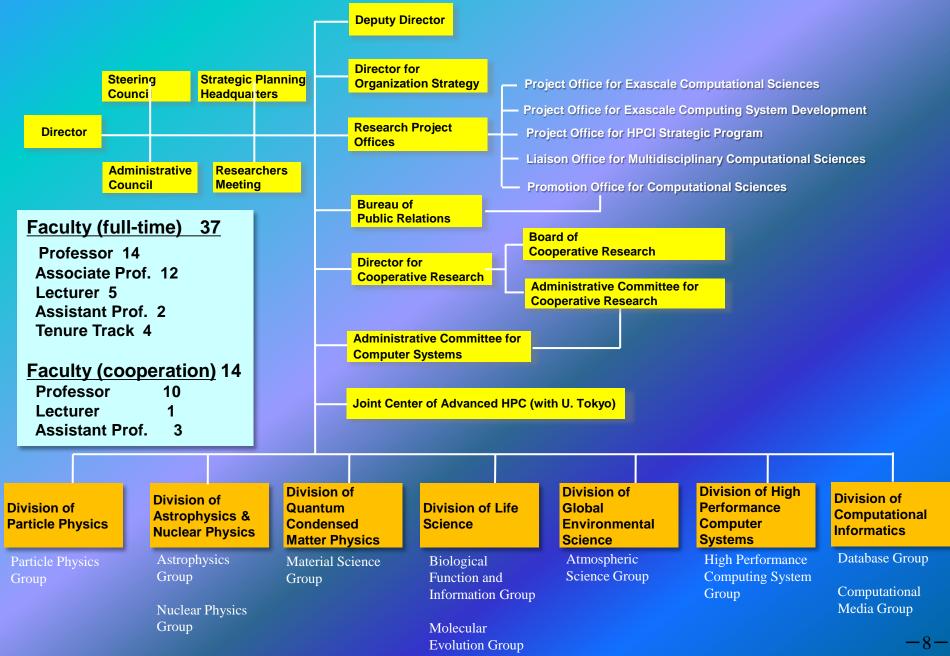
- Advance scientific researches by computational science through the application of advanced computing technologies
- Promote <u>Multidisciplinary Computational Science (MCS)</u> in Japan by the use of leading-edge advanced computing systems

Uniqueness

Collaborative researches between Computational Scientists (application) and Computer Scientists (system)

- Needs from applications and Seeds from systems
- More than 30 faculties and PDs, students: Particle Physics, Astrophysics, Nuclear Physics, Materials and Life Sciences, Global Environment and High Performance Computing System, Data base & Data Mining

Organization of CCS



8 Positions Recruited in FY2013

"Organization for the Support and Development of Strategic Initiatives"

Tenure Track*

Tenure Track*

Tenure Track*

Professor

Particle Physics Group

Astrophysics Group

Nuclear Physics Group

Condensed Matter Group

Life Science Group

Associate Prof.*

Professor Yasuteru SHIGETA

Atmospheric Science Group Tenure Track*

Astrobiology

Professor*

* new positions

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Takashi NAKATSUKASA

Research Divisions (in 2014)

- Division of Particle Physics: Particle Physics Group Leader: Yoshinobu Kuramashi Faculty 5 Postdoc 4
- Division of Astrophysics and Nuclear Physics: Astrophysics Group Leader: Masayuki Umemura / Masao Mori Faculty 5 Postdoc 4
- Division of Astrophysics and Nuclear Physics: Nuclear Physics Group Leader: Kazuhiro Yabana / Takashi Nakatsukasa Faculty 4 Postdoc 1
- Division of Quantum Condensed Matter Physics

Leader: Kazuhiro Yabana Faculty 3

 Division of Life Sciences: Biological Function and Information Group Leader: Masayuki Umemura / Yasuteru Shigeta Faculty 2 Postdoc 1

Research Divisions (cont'd)

• Division of Life Sciences: Molecular Evolution Group

Leader: Yuji Inagaki Faculty 1 Postdoc 1

Division of Global Environmental Science: Atmospheric Science Group

Leader: Hiroshi L. Tanaka Faculty 3 Postdoc 3

• Division of High Performance Computing Systems:

Leader: Taisuke Boku Faculty 7 Postdoc 4

• Division of Computational Informatics: Database Group

Leader: Hiroyuki Kitagawa

Faculty 2

 Division of Computational Informatics: Computational Media Group Leader: Yuichi Ohta Faculty 3

Director

Prof. Yoichi Iwasaki (particle physicist): April 1992 to March 1998,
Prof. Akira Ukawa (particle physicist): April 1998 to March 2007
Prof. Mitsuhisa Sato (computer scientist): April 2007 to March 2013.
Prof. Masayuki Umemura (astrophysicist): April 2013 -

Steering Council

The council is held twice a year, and the chair is selected from outside of U. Tsukuba. The council reviews the research activities in each field and the collaborations based on the multidisciplinary joint-use program, and discusses the direction of research of the Center and matters related to joint-use of the Center facilities.

Administrative Council

The Director of the Center chairs the council, which holds a meeting every month. The committee discusses significant issues for operating the Center, which include matters related to the organization of the Center, selection of faculty members, budget planning, and confirmation of expenditures.

Strategic Planning Headquarters

The headquarters is planning the requests for budgetary appropriations and faculty members for the enhancement of research activities as well as international collaborations.

Researchers Meeting

This meeting consists of the entire Center faculty and the Associated Research Fellows. This meeting is chaired by the Director of the Center and is held every month. At the meeting, all aspects of research are discussed, such as the status of ongoing projects, procurement of equipment and operation of the Center computer system.

<u>Research Project Offices</u>

These offices propel the missions regarding the challenge to novel computer technology, the multidisciplinary collaborations, and the nationwide/worldwide promotion of computational science. The following offices are set up:

- Project Office for Exascale Computational Sciences
- Project Office for Exascale Computing System Development
- Project Office for HPCI (High performance Computing Infrastructure) Strategic Program
- Liaison Office for Multidisciplinary Computational Sciences (MCS)
- Promotion Office for Computational Sciences

Administrative Committee for Cooperative Research

The CCS is calling for applications twice a year for the joint-use program of computer facilities. Since 2007, these activities have been reinforced by enhanced links with computer sciences through the promotion of the Multidisciplinary Cooperative Research Program (MCRP). Since 2010, the Center has been recognized as a national core-center under the Advanced Interdisciplinary Computational Science Collaboration Initiative (AISCI) by the MEXT. The administrative committee manages this joint-use program.

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Budget in FY2013

Total

JP¥ 2,631 MM (US\$ 26 MM)

Supercomputers (D&O)	JP¥	539 MM
Electricity	JP¥	182 MM
Personnel Expenses	JP¥	292 MM
Operating Expenses	JP¥	179 MM
Grant-in Aid (MEXT etc)	JP¥ 1	,350 MM
Grant-in Aid (JSPS)	JP¥	87 MM

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



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

Computing resources in CCS

PACS-CS (2006~2011)



- #node 2560 node (Intel Xeon 2.8GHz, single core /node)
- peak performance 14.34 TF
- memory 5 TB
- network 250MB/s/link x 3 (3D-HXB by GbE)

FIRST (2007~2012) Grant in aid by JSPS





Blade-GRAPE

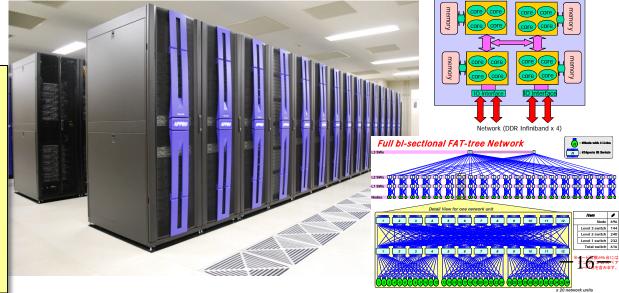
- A Special-purpose system to Astrophysics simulation by hybrid computation of radiation and N-body.
- Each node is equipped by GRAPE-6, which is an accelerator specialized for N-body Gravity calculation.
- 256 nodes
- performance: cluster 3.5TFLOPS + Grape-6 35TFLOPS

T2K-tsukuba(2008~2014)

Designed by T2K Open Supercomputer Alliance (U. Tokyo and Kyoto U)

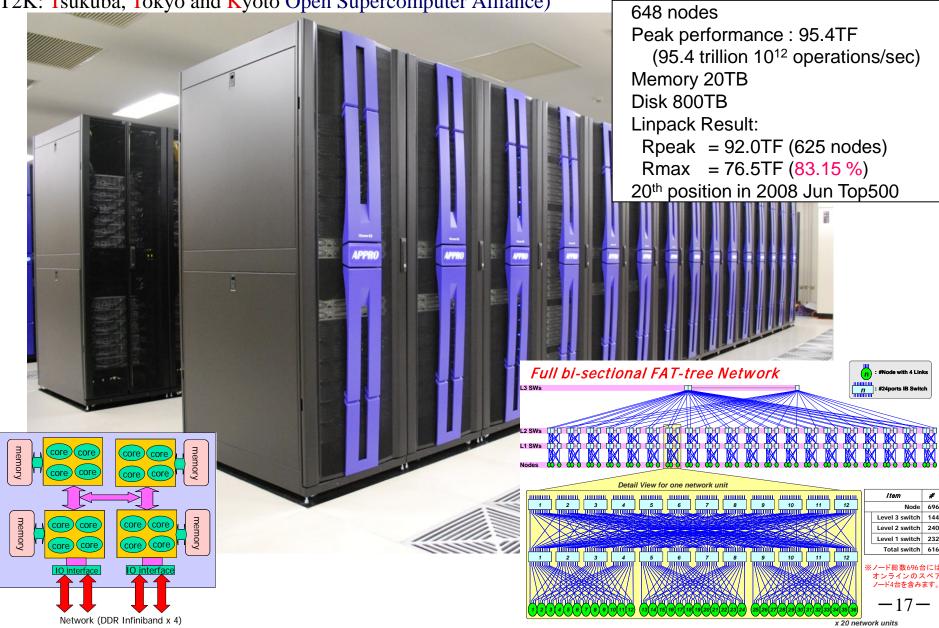
Spec;

- 648 nodes (quad Opteron, 4sockets/node)
- 10000 cores
- Peak performance 95.4TF
- total memory 20TB
- total disk capacity 800TB
- (20th in top 500, June, 2008)



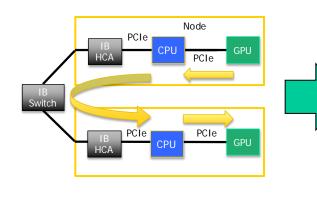
T2K Tsukuba System

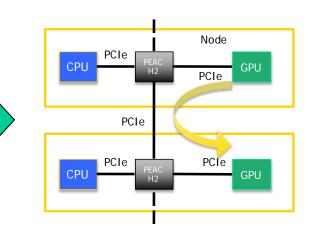
(T2K: Tsukuba, Tokyo and Kyoto Open Supercomputer Alliance)



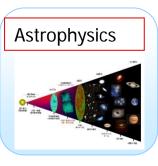
HA-PACS project

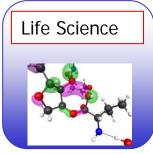
- HA-PACS (Highly Accelerated Parallel Advanced system for Computational Sciences)
- Funded by MEXT, The objective is exploiting technologies and applications for exascale computing
- Research topics
 - 1. Code development of the next-generation computational science applications for exascale (3 important area)
 - 2. Design of system architecture for exascale: Direct interconnect between GPU
 - 3. Programming environment for exascale (XcalableMP device extension)
- Project organization
 - Project Office for Exascale Computing System Development
 - Project Office for Exascale Computational Sciences











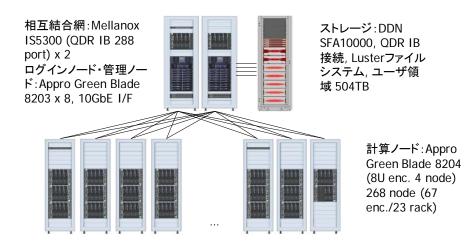
True GPU-direct With cooperation of NVIDA

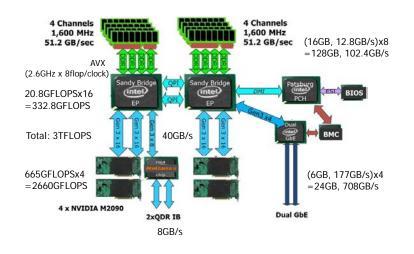
HA-PACS system



System spec.

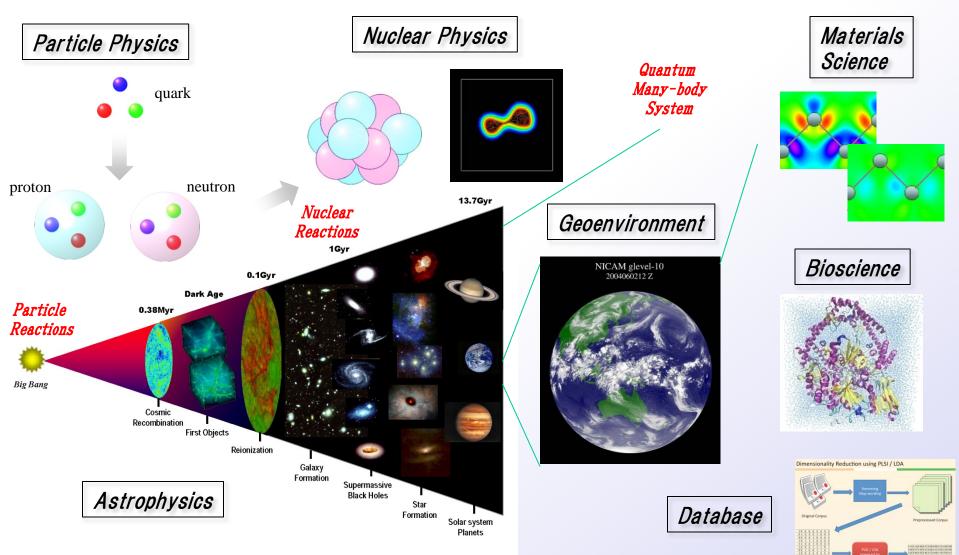
- 268 nodes
- CPU 89TFLOPS + GPU
 713TFLOPS = total 802TFLOPS
- Memory 34TByte, memory bandwidth 26TByte/sec
- Bi-section bandwidth 2.1TByte/s
- Storage 504TByte
- Power 408kW
- 26 ranks, Installed on Jan, 2012
- Operation started from Feb, 2012





Center for Computational Sciences, Univ. of Tsukuba

Computational Sciences by HA-PACS



Hydrodynamics, Radiation, Chemical Reactions

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Promotion of Multidisciplinary Computational Science (MCS) 🥯

- Collaboration between Computational Science and Computer Science
- Collaboration among Computational Sciences

Project Office for Exascale Computational Sciences

Computational Science

- **Division of Particle Physics**
 - Particle physics Lattice QCD
- Division of Astrophysics and Nuclear Physics
 - Astrophysical Radiation Hydrodynamics
 - Quantum many-body systems, DFT
- Division of Quantum Condensed Matter Physics
 - Materials science, Nano-science, DFT
- Division of Life Sciences
 - Quantum mechanics, Molecular dynamics
 - Phylogenetic analyses
- Division of Global Environment Science
 - Global environment, Urban climate

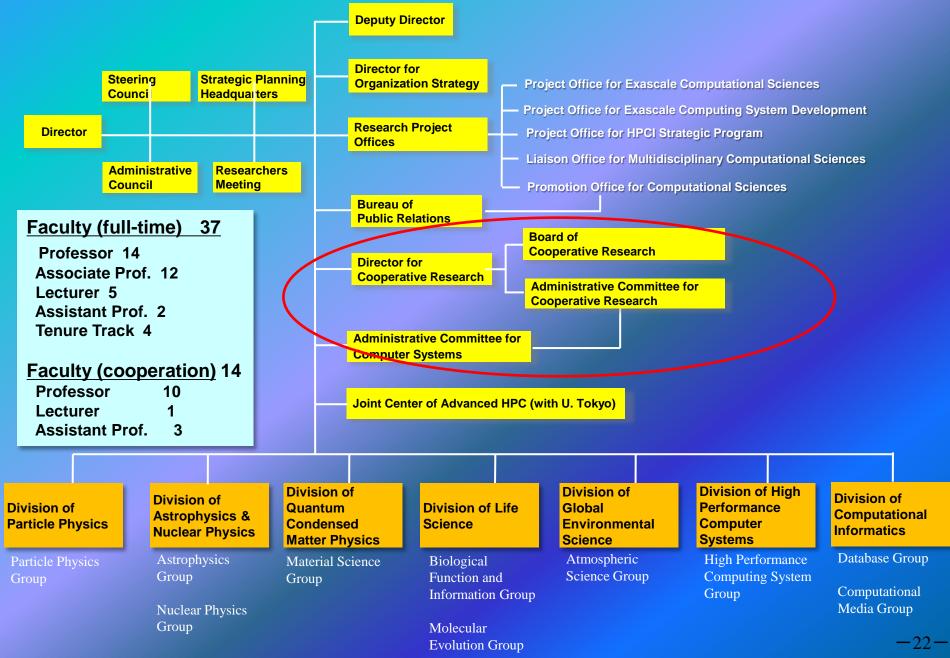
Project Office for Exascale Computing System Development

Center for Computational Sciences, Univ. of Tsukuba

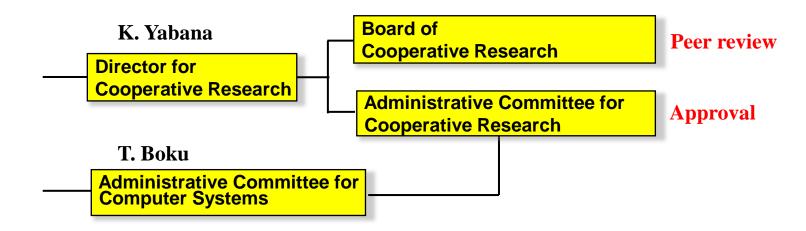
Computer Science

- Division of High Performance Computing Systems
 - System architecture
 - Grid computing
- Division of Computational Informatics
 - Computational Intelligence Data Mining & Knowledge Discovery, Large scale database
 - Computational Media Visualization, Computer graphics

Organization of CCS



Multidisciplinary Cooperative Research - Joint-use Program of Supercomputers -



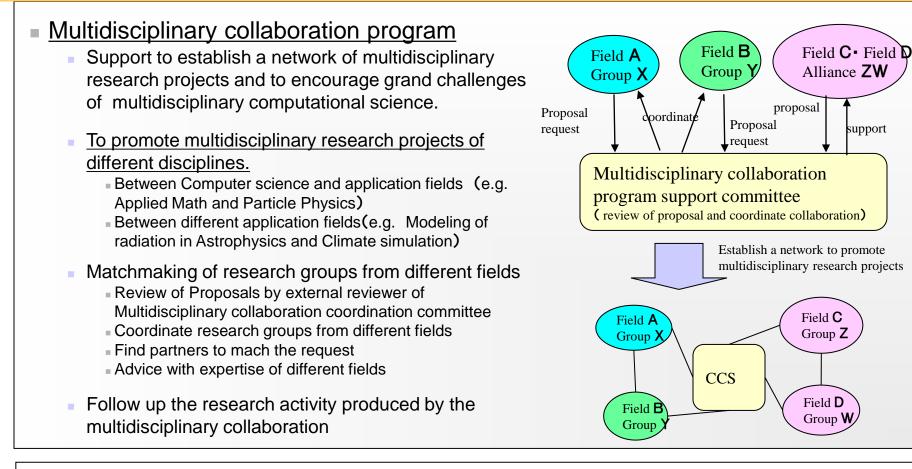
Since 2010, the CCS has been approved as a "national core-center" under the Advanced Interdisciplinary Computational Science Collaboration Initiative (**AISCI**) launched by the Ministry of Education, Culture, Sports, Science and Technology (MEXT) of Japan, and has provided the use of its computational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

FYear	2008	2009	2010	2011	2012	2013
Number of Projects	36	53	24	31	27(T2K) 21(ha-pacs)	26(t2k) 33(ha-pacs)
System	PACS-CS T2K	PACS-CS T2K, FIRST	PACS-CS T2K, FIRST	PACS-CS T2K, FIRST	T2K HA-PACS	T2K HA-PACS

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CCS Inter-University Activity

Multidisciplinary Computational Science Promotion Programs

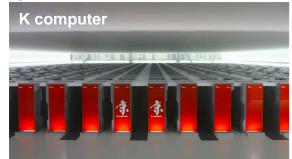


- Large-scale scientific simulation program
 - Push forward the grand challenge of several fields in computational sciences by providing the computational facilities in CCS.
 - Review proposals and concentrate our computational power to make new scientific discoveries
 - Follow up the scientific results

HPCI (High performance Computing Infrastructure)

Nation-wide computational science and next-generation supercomputing

- CCS was recognized as a national core-center for the collaborative research on the Multidisciplinary Computational Science from 2010
 - Advanced Interdisciplinary Computational Science Collaboration Initiative (AISCI)
- Collaboration with RIKEN on the next-generation system development
 - Formal agreement between U. Tsukuba and RIKEN signed in September 2006
 - Participation of several CCS faculty in the system design as a concurrent researchers
- Involvement to the national high performance computing infrastructure HPCI and the petascale system "K computer"
 K computer
 - CCS was selected as a core organization for
 "Field 5: The origin of matters and the universe" in HPCI Strategic programs for K computer apps.
 - CCS is one of sites in the national HPCI



- In 2012, MEXT initiated the "Feasibility Study on Future HPC Infrastructure" projects to study the architecture of post-petascale systems following the K computer
 - As four projects have been accepted including CCS, we have been conducting the project "Study on exascale heterogeneous systems with accelerators

 $(\rightarrow 20^{th} \text{ by M. Sato})$

Highlights of Researches in CCS

- CP-PACS Project(1992 1996): Developed the CP-PACS parallel computer (ranked as No. 1 in the Top 500 List of November 1996), which has produced ground-breaking results in computational particle physics, astrophysics and condensed matter physics.
- Research for the Future Project "Development of Next-Generation Massively Parallel Computers" (1997-2001): Heterogeneous Multi-Computer System (HMCS) to integrate different type of computers
 - The project was extended into FIRST Project (2004 2012) for pioneering large-scale astrophysical radiation hydrodynamic hydro-dynamics calculation.
- PACS-CS Project (2005 2007): Developed a massively parallel cluster PACS-CS with a peak performance of 14.3 Tflops.
- HA-PACS Project (2012): Developed a accelerator (GPU)-embedded massively parallel cluster HA-PACS with a peak performance of 802 Tflops.
- Gordon Bell Prize 2011 (K-computer) Peak Performance

(University of Tsukuba, University of Tokyo, RIKEN)

Gordon Bell Prize 2012 (K-computer) Scalability and Sustained Performance (University of Tsukuba, RIKEN, Tokyo Institute of Technology)

京(K) computer

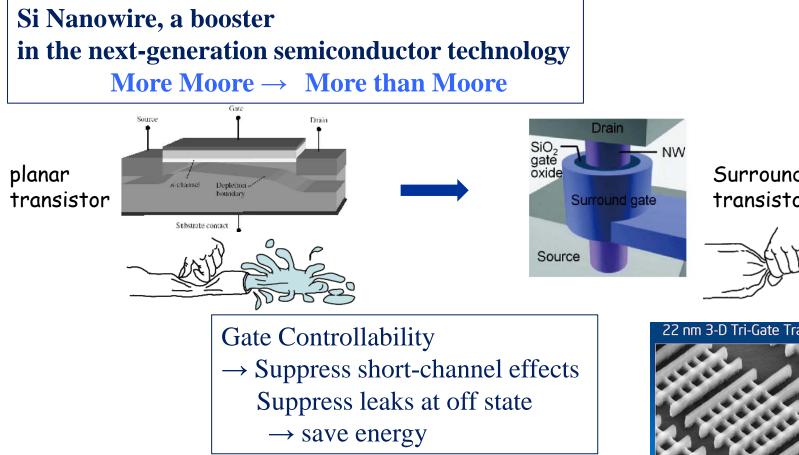
- SPARC64TM VIIIfx 2.0GHz octcore (128Gflops / core)
- 16 GB memory / core
- 6D torus network

- 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



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

Surrounding gate transistor



2 nm 3-D Tri-Gate Transistor

Actually tri-gate by Intel in 2011 -28-

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)

Promotion Office for Computational Sciences

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 since July 2007
- 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)
 - Started from 2008

Computational Science Dual Degree (double major) Program

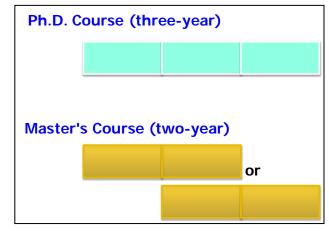
- Enables a graduate student in a doctoral program to simultaneously belong to a masters program of a different Graduate School, and receive both a doctoral degree in science and a masters degree in computer science, or *vice versa*, upon graduation.
- Design of curriculum and courses for advanced computational science
- Educate researchers who can push forward new multidisciplinary computational science from global viewpoints
- Started in 2009 (Physics in Doctor course and Computer sciences in Master course)
- To be expanded to "Environmental Science and Biological Science"
- Computational Science Courses in English in "Global 30 Program"
 - To accept International Students.

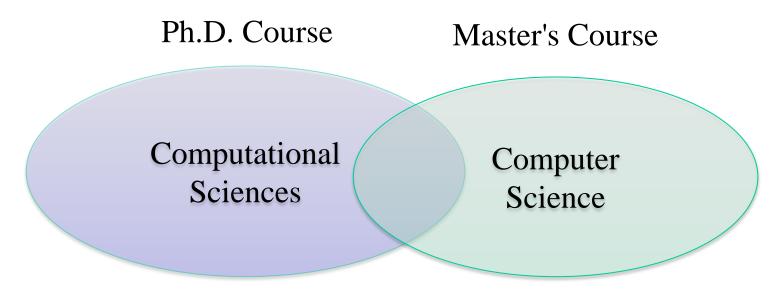
Computational Science Dual Degree Program

Computational Science Dual Degree Program

fosters qualified researchers in multidisciplinary computational science with research ability in both computational and computer sciences.

- So far, 8 students have taken this course.





Liaison Office for Multidisciplinary Computational Sciences

Cooperation among Different Fields

Gordon Bell Prize 2011 RIKEN The University of Tokyo University of Tsukuba Fujitsu Limited

International Collaborations

EPCC, University of Edinburgh, UK

Lawrence Berkeley National Laboratory, US

KISTI Supercomputing Center, Korea

Inter-university Activities

- Acquire (and development) and operate leading-edge advanced computing systems as inter-university facilities for large-scale computational science
- 2 Symposium, workshop and colloquium organized by CCS
- **③** Operation and support of scientific database and data Grid (e.g. ILDG/JLDG)
- (4) Education, Outreach, and Public Relations

Agenda of External Review

18th February (Tuesday)

Morning

Overview of CCS (Workshop Room)

Afternoon

Activities & Collaborations of Divisions (Workshop Room)

19th February (Wednesday)

Morning

Activities & Collaborations of Divisions (cont'd) (Workshop Room) Afternoon

Parallel Tracks for Divisions

Night

Committee Meeting with Dinner (Banquet)

20th February (Thursday)

Morning

Future Plans (Workshop Room)

Afternoon

Committee Meeting & Q & A to draft the report (Workshop Room)

Final Review Report

April 30, 2014

<u>Schedule</u> 18th February (Tuesday)

Overview of CCS (Workshop Room)

9:00-10:00 Welcome & Overview of CCS (M. Umemura, Director of CCS)
10:00-10:30 Activities and Results 2008-2013 (M. Sato, ex-Director of CCS)
10:30-10:45 Coffee Break
10:45-11:45 T2K-Tsukuba & HA-PACS Projects (T. Boku, Deputy Director of CCS)
11:45-12:10 Tour to HA-PACS
12:10-13:10 Lunch
13:10-13:30 ILDG/JLDG Project (T. Yoshie)

Activities & Collaborations of Divisions (Workshop Room)

13:30-14:00 Division of Particle Physics: Particle Physics Group (Y. Kuramashi)
14:00-14:30 Division of Global Environmental Science: Atmospheric Science Group (H. Tanaka)
14:30-14:45 Coffee Break
14:45-15:15 Division of Astrophysics and Nuclear Physics: Nuclear Physics Group (K. Yabana, T. Nakatsukasa)
15:15-15:45 Division of Astrophysics and Nuclear Physics: Astrophysics Group (M. Mori)
15:45-16:15 Division of Quantum Condensed Matter Physics (K. Yabana)
16:15-16:30 Coffee Break
16:30-17:00 Multidisciplinary Cooperative Research (K. Yabana)
17:00-17:30 Bureau of Public Relations (T. Yoshito)

<u>Schedule</u>

19th February (Wednesday)

Activities & Collaborations of Divisions (cont'd) (Workshop Room)

9:00-9:30 Division of High Performance Computing Systems: High Performance Computing Systems Group (T. Boku)
9:30-10:00 Division of Computational Informatics: Database Group (H. Kitagawa)
10:00-10:30 Division of Computational Informatics: Computational Media Group (Y. Kameda)
10:30-10:45 Coffee Break
10:45-11:15 Division of Life Sciences: Molecular Evolution Group (T. Hashimoto)
11:15-11:45 Division of Life Sciences: Biological Function and Information Group (K. Shiraishi, Y. Shigeta)
11:45-13:00 Lunch

12:45 Meeting Photo @Workshop Room

Parallel Tracks for Divisions

13:00-17:30	
Division of Particle Physics	
Reviewer: Karl Jansen	Room:D410,D411 (Physics)
Division of Astrophysics and Nuclear Physics: Astrophysics Group	
Reviewer: Andreas Burkert	Room: room A (CCS)
Division of Astrophysics and Nuclear Physics: Nuclear Physics Group	
Reviewer: James Vary	Room: D412 (Physics)
Division of Quantum Condensed Matter Physics	
Reviewer: Joachim Burgdörfer, Shinji Tsuneyuki	Room: D201 (Physics)
Division of Life Sciences	
Reviewer: Andrew Roger	Room: room B (CCS)
Division of Global Environmental Science	
Reviewer: Jack Wells, Takemasa Miyoshi	Room: room C (CCS)
Division of High Performance Computing Systems	
Reviewer: Jeffery Vetter, Hiroshi Nakashima	Room: SB911-1 (SysInfo)
Division of Computational Informatics	
Reviewer: Xiaofang Zhou	Room: SB911-2 (SysInfo)
18:00- Committee Meeting with Dinner (A bus departs from CCS.)	

<u>Schedule</u> 20th February (Thursday)

Future Plans (Workshop Room)

9:00-9:30 The Strategy of CCS (M. Umemura)
9:30-10:00 COMA (PACS IX) Project (T. Boku)
10:00-10:30 JCAHPC Project (M. Sato)
10:30-10:45 Coffee Break
10:45-11:15 Feasibility Study toward Exa-scale Computing (M. Sato)
11:15-11:35 Joint Institute for Computational Fundamental Science (JICFuS) (Y. Kuramashi)
11:35-11:55 Organization for Collaborative Research on Computational Astrobiology (CAB) (M. Umemura)

11:55-13:00 Lunch

<u>Committee Meeting</u> (Workshop Room)

13:00-14:00 Committee Meeting 14:00-15:00 Discussion, Q & A 15:00-16:00 Committee Meeting