



2007.Oct.30-Nov.1
External Review

External Review on Center for computational sciences

~Objective and Schedule of the external review ~

Center for Computational Science
University of Tsukuba

External Review Committee

- Prof. Richard Kenway, The University of Edinburgh (Chair)
- Prof. Yoshio Oyanagi, Kogakuin University (Vice Chair)
- Prof. Michael L. Norman, UCSD
- Prof. Kiyoyuki Terakura, JAIST
- Prof. Akimasa Sumi, The University of Tokyo
- Prof. Herve Philippe, University of Montréal
- Dr. Horst Simon, Lawrence Berkeley National Laboratory
- Prof. Masaru Kitsuregawa, The University of Tokyo

Materials for the External Review

- Agenda and Schedule
- Member List of External Review Committee
- Review Form (tentative)
 - “Points to be evaluated”
- CCS Report
 - PART I: Overview of Center for Computational Sciences
Summary of Activities 2004 – 2007
 - PART II: Research Activities, Results, Collaborations and Plan 2004 – 2007
 - Research Activities and outcome in each group
 - PART III: Vision and Strategies of Center for Computational Sciences
- Pamphlet of CCS
- Posters of CCS Researches (Lobby and back-side in workshop rooms)
 - Some of Posters will be presented in SC07.

Objective of External Review (1)

- The objective of the review is to receive an outside examination on the research activities and their outcomes of the Center in view of the founding objectives, and to incorporate the recommendations from the review for future developments of the Center.
- Timeframe to be evaluated: 2004 – 2007 (present)
 - In 2004, the center was re-organized from “center for computational physics” to “center for computational sciences”
 - On April 2004, the Japanese National University system underwent a major transition. Their legal status was changed to that of independent institutes.
 - We have made 6-years plan (FY2004-FY2009). We need a mid-term evaluation at this moment to make a plan for the next.

Objective of External Review (2)

- Evaluation of research activities in the timeframe 2004-2007
 - CCS projects
 - PACS-CS project
 - FIRST project
 - ILDG/JLDG project
 - Research Activities in each group
 - Points
 - Scientific goals and achievements
 - Interdisciplinary collaborations between different groups to advance the computational science discipline, in view of CCS founding objectives
 - We want this evaluation for
- Recommendations on the future vision and strategies of CCS
 - Timeframe 2007-2010

Agenda

- Sessions “CCS projects”: Morning in 30th
 - Presentation of CCS major projects
- Sessions “Activities and Collaborations”: Afternoon in 30th, Morning in 31st
 - Presentation about overview and collaborations of each research groups
- Parallel Tracks (3 tracks): Afternoon in 30th, Afternoon in 31st
 - Presentation of detail research topics of each division and group
- “Future plan of CCS” : Afternoon in 31st
 - will be presented by Director
- Committee Meetings
 - Evening in 30th, Evening in 31st (with director and deputy directors), Morning in 1st

Agenda and Schedule

■ 30th October (Tuesday)

- 9:30-10:00 Objective and schedule of the external review (Sato, Director of CCS)
- 10:00-10:30 Overview and current status of CCS (Sato)
- 10:30-11:00 Activities and results 2004 – 2007 (Ukawa) **Former director**
- 11:00-11:30 CCS project **1**: PACS-CS project (Boku)
- 11:30-12:00 CCS project **2**: FIRST project (Umemura)
- 12:00-12:30 Tour to PACS-CS and FIRST
- 12:30-14:00 Lunch (**served at Meeting room C**) **After lunch, some paper works**
- 14:00-14:25 CCS project **3**: ILDG/JLDG project (Sato)
- 14:25-14:50 Activities and Collaborations **1**: Division of Particle Physics and Astrophysics: Computational Particle Physics Group (Aoki)
- 14:50-15:15 Activities and Collaborations **2**: Division of Global Environment and Biological Sciences: Global Environmental Science Group (Tanaka)
- 15:15-15:40 Activities and Collaborations **3**: Division of Computational Informatics: Computational Intelligence Group (Kitagawa)
- 15:40-16:05 Activities and Collaborations **4**: Division of Computational Informatics: Computational Media Group (Ohta)
- 16:05-16:30 Coffee break
- 16:30 -18:00 Parallel Tracks (**presentation by each groups**)
- 18:00-18:30 (Committee meeting) **if you need**
Start from CCS at 18:30
- 19:00- (Committee meeting with dinner) **at restaurant in Epochal.**

Agenda and Schedule

- 31st October (Wednesday)
 - 9:30- 9:45 (Committee meeting)
 - 9:45-10:10 Activities and Collaborations 5:
Division of High Performance Computing Systems (Boku)
 - 10:10-10:35 Activities and Collaborations 6: Division of Materials and Life Sciences: Computational Condensed Matter Science Group (Oshiyama)
 - 10:35-11:00 Activities and Collaborations 7: Division of Materials and Life Sciences: Computational Life Science Group (Tateno)
 - 11:00-11:15 Coffee break
 - 11:15-11:40 Activities and Collaborations 8: Division of Materials and Life Sciences: Quantum Many-Body Systems Group (Yabana)
 - 11:40-12:05 Activities and Collaborations 9: Division of Global Environment and Biological Sciences: Biological Science Group (Hashimoto)
 - 11:05-12:30 Activities and Collaborations 10: Division of Particle Physics and Astrophysics: Computational Astrophysics Group (Umemura)
 - 12:30-14:00 Lunch
 - 14:00-15:00 Future plan of CCS (Sato)
 - 15:00-15:30 Discussion
 - 15:30-16:00 Coffee break
 - 16:30 -18:00 Parallel Tracks (presentation by each groups)
 - 18:00-18:30 (Committee meeting) if you need
Start from CCS at 18:45
 - 19:00- (Committee meeting with dinner) at restaurant in University
Director and Deputy Directors will join.

Agenda and Schedule

- 1st November (Thursday)

9:00-10:00	(Committee meeting) Open for the committee
10:00-11:00	Discussion, Q & A
11:00-12:30	(Committee meeting) Open for the committee
12:30-13:30	Lunch



2007.Oct.30-Nov.1
External Review

External Review on Center for computational sciences

~ Overview of CCS ~

Mitsuhisa Sato, Director & Professor
Center for Computational Science
University of Tsukuba

CCS, University of Tsukuba



- Center for Computational Sciences
 - <http://www.ccs.tsukuba.ac.jp/>
- Mission of CCS is to enable scientific discovery by computational science through the application of advanced computing technologies, and support researches of computational science in Japanese universities by running (& developing) leading-edge advanced computing systems as inter-university facilities.
- Founded on 1992 as CCP (Center for Computational Physics) expanded and reorganized to CCS in 2004
 - Extended its research area from Computational Physics to Computational Sciences
- We have carried out Collaborative researches with Computational Scientists (application) and Computer Scientists (system)
 - Needs from applications
 - Seeds from systems

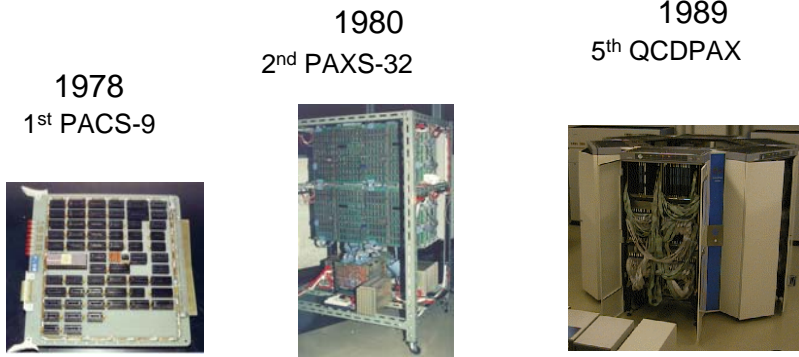
Development of Massively Parallel Computer Systems in University of Tsukuba

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

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

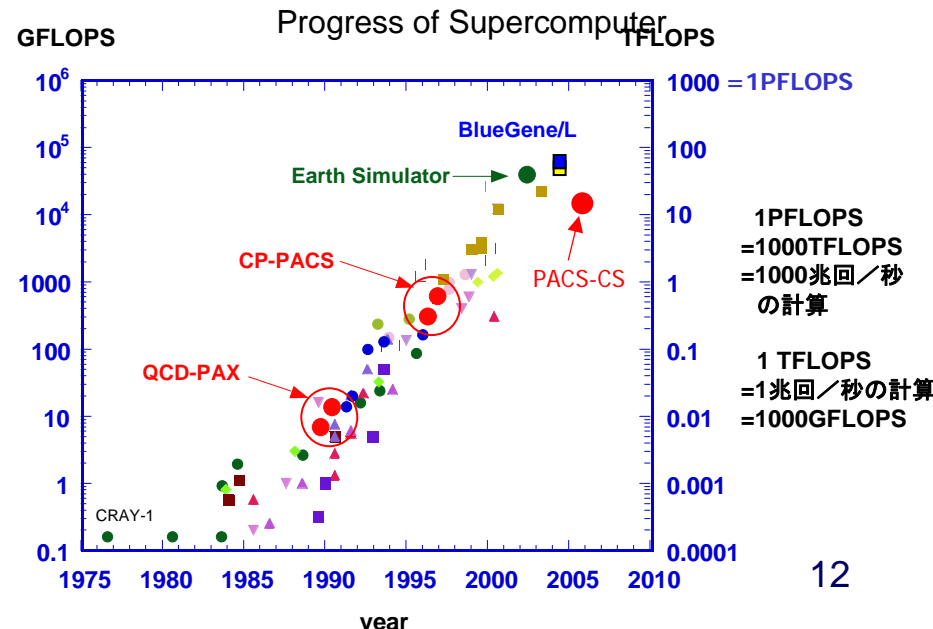
PACS-CS
Massive Parallel Clus
(2006)



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



year	system	Performance
1978	PACS-9	7 KFlops
1980	PAX-32	500 KFlops
1983	PAX-128	4 MFlops
1984	PAX-32J	3 MFlops
1989	QCDPAX	1.4 GFlops
1996	CP-PACS	614 GFlops
2006	PACS-CS	14340 GFlops



Chronology of CCS

- 1992 April Founding of Center for Computational Physics (CCP)
(10 year term / 10 faculty members and 3 visiting faculties)
development of massively parallel computer CP-PACS begins
- 1996 October Massively parallel computer CP-PACS completed
November Ranked as No. 1 in the Top 500 World Supercomputer List
- 1997 April JSPS research for the Future Project “Computational Science”
「Development of Next-Generation Massively Parallel
Computers」 begins
- 2002 April The Second 10 year term of Center for Computational
Physics begins
(11 faculty members and 3 visiting faculties)
- 2003 July-Dec. Planning on reorganization and expansion of CCP
- 2004 April Founding of Center for Computational Sciences (CCS)
(31 faculty members and 3 visiting faculties)
- 2005 April Development of Massively Parallel Cluster PACS-CS in the project
「Discovery, Synthesis and Emergence of Novel Knowledge
through Computational Sciences」 begins (3years, FY2005～FY2007)

Organization of Education and Research for Computational Science in University of Tsukuba

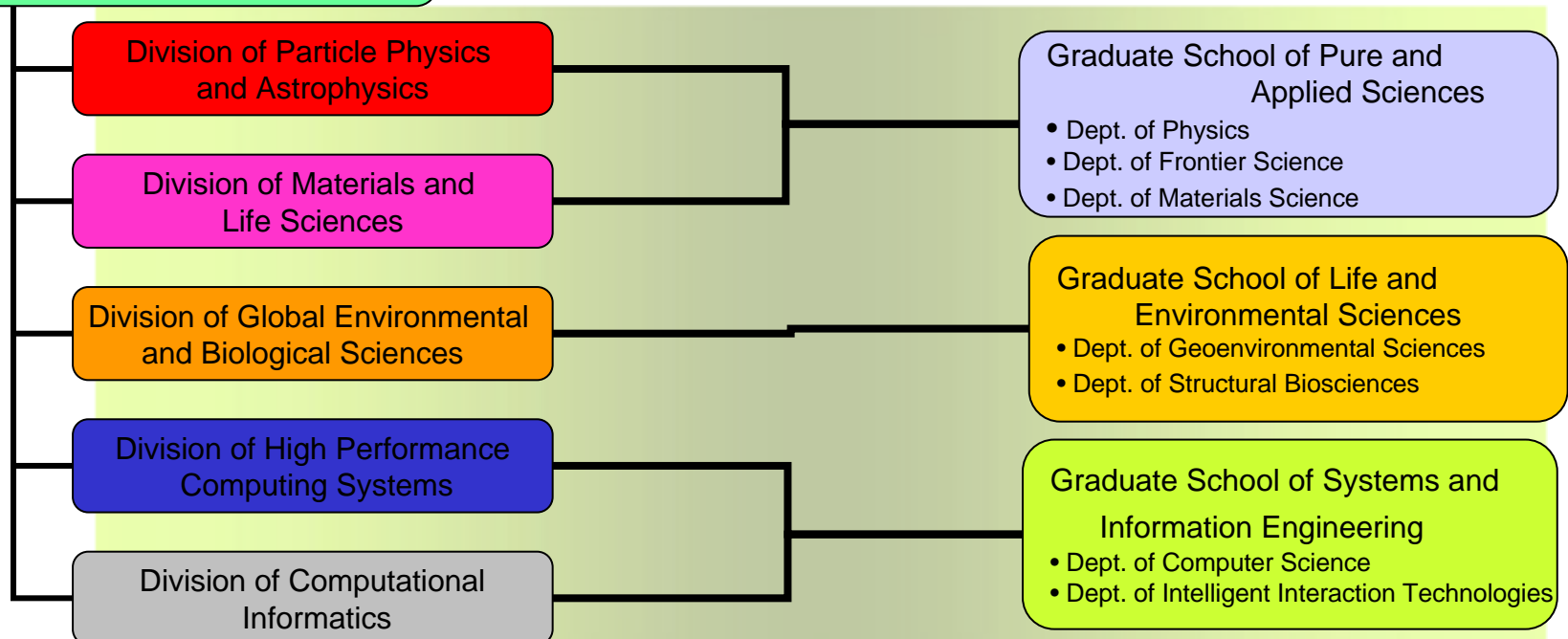


Founded in 1996, re-organized in 2004

- CCS integrates the development of supercomputing facilities and several researches of computational science.
- CCS carries out researches in major computational science fields.
- The faculty members of CCS “belong” to a Graduate School for education, and “work” for the Center for research.

Faculty	31
Professor	11
Associate Prof.	12
Assistant Prof.	8

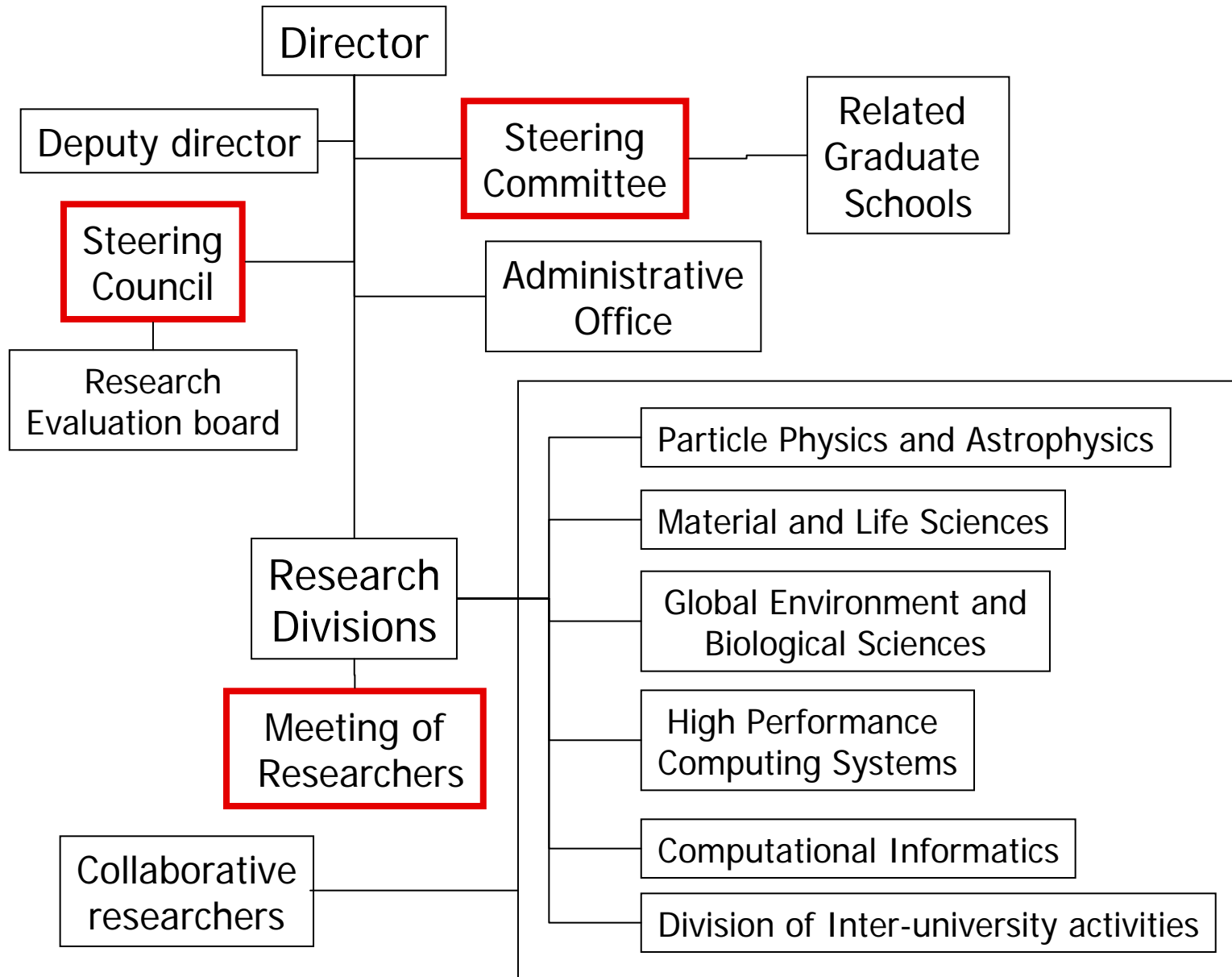
Center for Computational Sciences



CCS Research divisions and Expertise

- More than 30 faculties (31) and PostDocs, students (see Appendix A)
- Research organization of computational sciences, not supercomputer “service” center
- 5 Research Division and 11 Groups
- Computational Science
 - Division of Particle Physics and Astrophysics
 - Particle physics – Lattice QCD
 - Astrophysics – Formation of early cosmic objects and galaxies
 - Division of Material and Life Sciences
 - Material science – nano-science, DFT
 - Life sciences – Molecular dynamics, CPMD
 - Quantum Many-Body Systems
 - Division of Global Environment and Biological Sciences
 - Global environment – Meteorological science, global climate simulation
 - Biological science – molecular phylogenetic analyses
- Computer Science
 - Division of High Performance Computing Systems
 - System architecture
 - Grid computing
 - Computational Informatics
 - Computational Intelligence - Data Mining & Knowledge Discovery, Large scale database
 - Computational Media - Visualization, Computer graphics

Organization of the Center for Computational Sciences



Organization of the Center for Computational Sciences

■ Director

- Yoichi Iwasaki (physics) from April 1992 to March 1998, Akira Ukawa (physics) from April 1998 to March 2007.
- The current director is Mitsuhsa Sato (computer science) since April 2007.

■ Meeting of Researchers

- This meeting consists of the entire Center faculty and the Associated Research Fellows who are collaborators of other universities and research institutes.
- It 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 equipments and operation of the Center computer system.

■ Steering Committee

- The Director of the Center chairs the Committee, which is held every month.
- The Committee discusses important issues for running of the Center, which includes matters related to the organization of the Center, selection of faculty members, budget planning and confirmation of expenditure.

■ Steering Council

- The Council is held once a year, and is chaired by the director of the Center.
- The Council hears annual reports of the Center research activities, and discusses the direction of research of the Center, and matters related to inter-university use of the Center facility.
- Under the Steering Council, Research Evaluation Board is organized to evaluate the research activities annually.

Inter-university Activities

- ① Acquire (and development) and operate leading-edge advanced computing systems as inter-university facilities for large-scale computational science

Operation of Large Cluster PACS-CS

- ② Symposium, workshop and colloquium organized by CCS
- ③ Operation and support of scientific database and data Grid
- ④ Education, Outreach, Public Relations

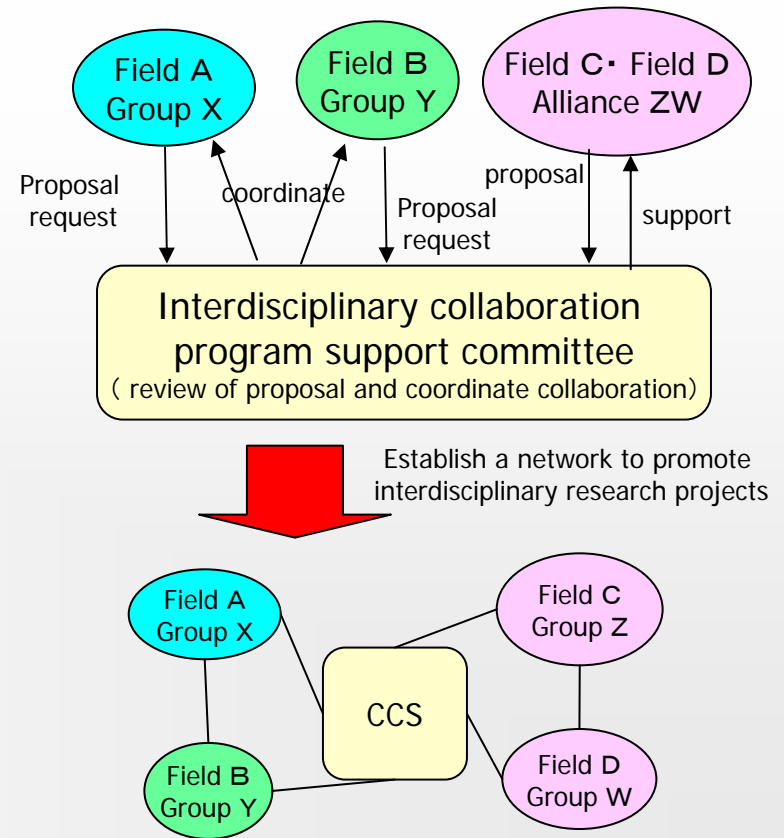
Inter-university Activities (1)

- ① Acquire (and development) and operate leading-edge advanced computing systems as inter-university facilities for large-scale computational science
 - Since 1998 to September 2005, we have conducted “Large-scale simulation project”. In this project, we 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. We accepted proposals and allocated computing resources according to review result by review committee including external reviewers.
 - **From October 2007**, we execute “Interdisciplinary Computational Science Promotion Programs” to make the best use of PACS-CS.
 - The *Interdisciplinary collaboration program* is to promote interdisciplinary research activities of different disciplines.
 - The *Large-scale scientific simulation program* is to push forward the grand challenge of several fields in computational sciences by providing the computational power of the PACS-CS.
 - No charge. A amount of computing resource may be allocated for large-scale simulation.

CCS Inter-University Activity: *Interdisciplinary Computational Science Promotion Programs*

■ Interdisciplinary collaboration program

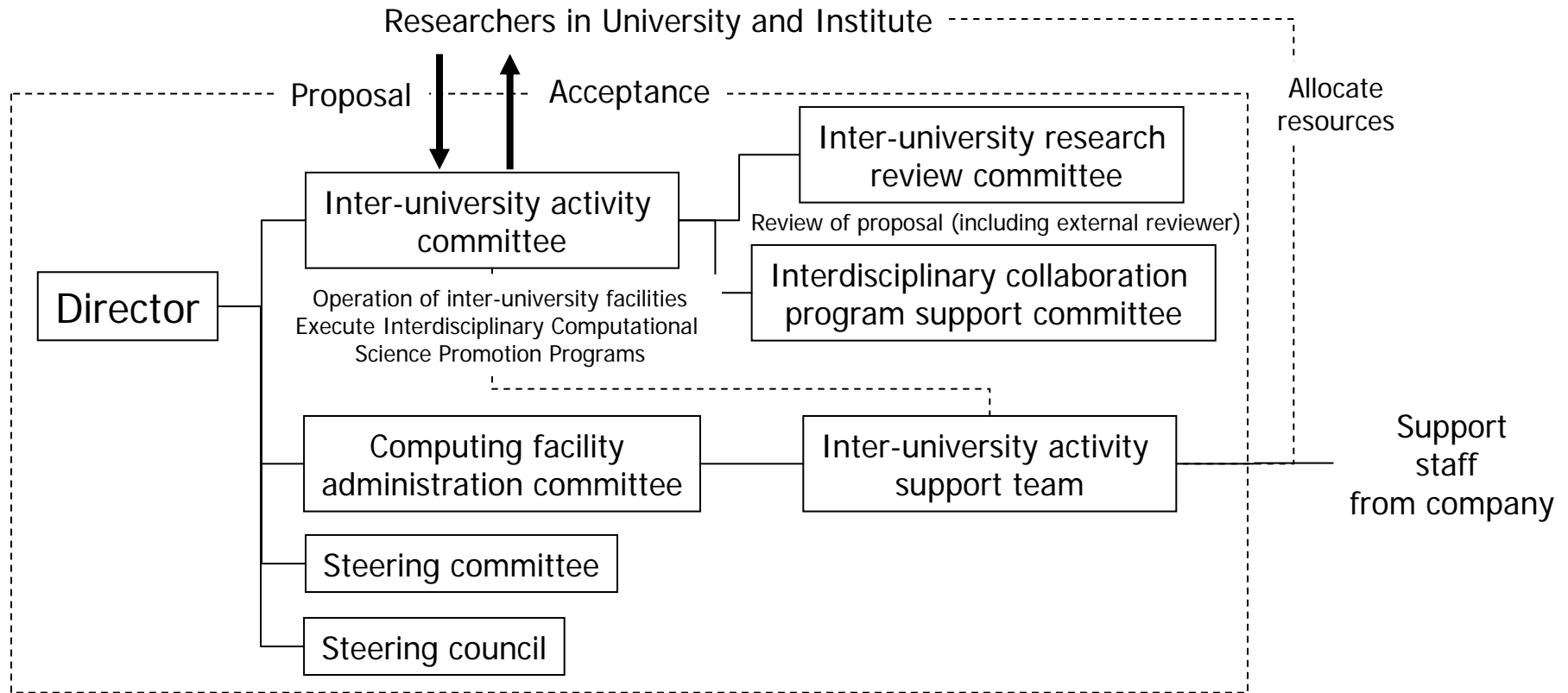
- Support to establish a network of interdisciplinary research projects and to encourage grand challenges of interdisciplinary computational science.
- To promote interdisciplinary research projects of different disciplines.
 - Between Computer science and application fields (e.g. Applied Math and Particle Physics)
 - Between different application fields (e.g. Modeling of radiation in Astrophysics and Climate simulation)
- Matchmaking of research groups from different fields
 - Review of Proposals by external reviewer of Interdisciplinary collaboration coordination committee
 - Coordinate research groups from different fields
 - Find partners to match the request
 - Advice with expertise of different fields
- Follow up the research activity produced by the interdisciplinary collaboration



■ Large-scale scientific simulation program

- Push forward the grand challenge of several fields in computational sciences by providing the computational power of the PACS-CS.
- Review proposals and concentrate our computational power to make new scientific discoveries
- Follow up the scientific results

Organization for Inter-university Facilities Operation



- In order to execute “Interdisciplinary Computational Science Promotion Programs”, we organize Inter-university research review committee, including external members, to evaluate the proposal.
- We also organize “Interdisciplinary collaboration program support committee” to review the proposals and coordinate collaborations between different fields.
- We report the policy, results and status of inter-university activities in Steering council held annually.

Inter-university Activities (2)

- ② Symposium, workshop and colloquium organized by CCS
 - Organize an annual symposium on computational science, which covers all fields related computational science. The Center also organizes international symposia, and invites visitors from abroad in order to promote international exchange and collaboration of scholars in computational sciences
 - Workshops on each field and colloquium are held occasionally.

- ③ Operation and support of scientific database and data Grid
 - We support and open scientific database for Particle Physics research and Climate research
 - Lattice QCD Archive, Particle Physics (open since Feb 2004), extended to International Lattice Data Grid ILDG (2007)
 - GPV/JMA archive, Climate research (open since Jan 2005)

Inter-university Activities (3)

④ Education, Outreach, Public Relations

- Seminar and lecture for HPC technology: Educate the community to increase participation in advanced computing technology careers
- Accept many visitors and public guests from High-school, etc : Inform society about value of advanced computing technologies.

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)**: Carried out basic research for high performance processor and, developed the concept of ***Heterogeneous Multi-Computer System (HMCS)*** to integrate different type of computers
 - The project was extended into **FIRST Project (2004 – 2007)**, which developed a special-purpose simulator ***FIRST*** for pioneering large-scale astrophysical astronomical 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. The system started operation in July 2006, and calculations are actively pursued to carry out several projects including nano- and bio-sciences and lattice QCD simulation, and climate simulation.
- International Collaboration for global infrastructure on computational science to connect major research sites such as ILDG (International Lattice Data Grid) for sharing Lattice data world-wide.

Besides the above researches, researchers in CCS win several funds (Grand-in-Aid for scientific research by MEXT, JST-CREST) and conduct research projects actively.

Thanks for your attention!

Questions and comments?