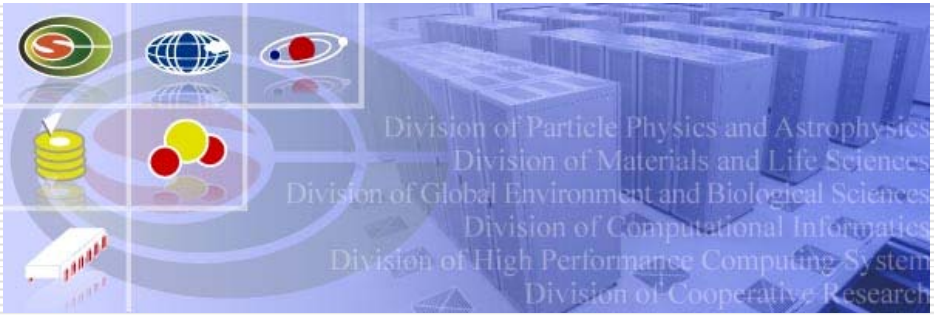
Activities and Results

2004～2007



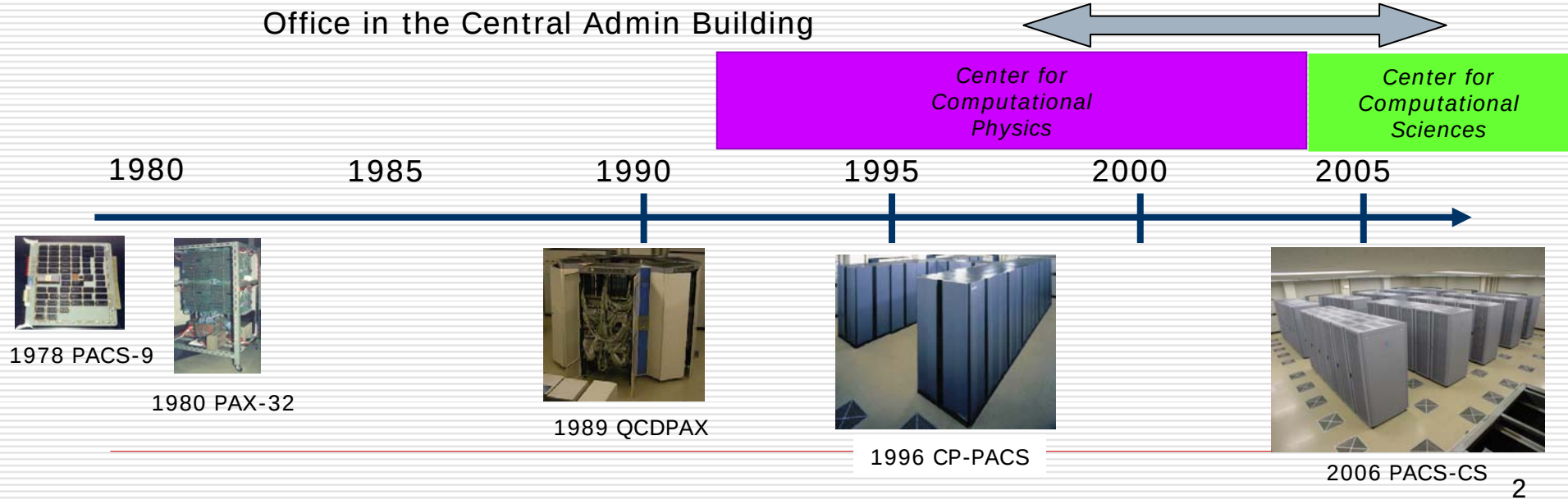
Akira Ukawa

Center for Computational Sciences
Executive Advisor to the President
(Research and Information)

- *Personal note*
- *From computational physics to computational science in 2004*
- *Major Projects since 2004*
- *Toward petascale computational science*

Personal note

- Particle physics, in particular lattice QCD
  (my 1st paper in 1980, 1st simulation paper in 1982)
- Involved in R&D of parallel computers since 1991
  - CP-PACS Project FY1992-1996 (Leader Y. Iwasaki)
  - Research for the Future Project FY1996-2000
  - PACS-CS Project FY2004-2006
- Director
  CCP April 1998-March 2003
  CCS April 2004-March 2007
- Executive Advisor to the President since April 2007
  Office in the Central Admin Building



Focus of this presentation

The current Review concerns the period 2004-2007,i.e., since Center for Computational Sciences (CCS) was founded.

So, rather than actual research results, try to provide background on:

- The reorganization and expansion from
  Center for Computational Physics (CCP) to
  Center for Computational Sciences (CCS) in 2004
- Roles of the major research projects since 2004 for developing and establishing CCS
- The Japanese Petaflops Project (2006-2012) and future of CCS

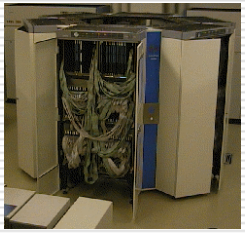
Three decades of R&D of massively parallel PAX/PACS systems at U. of Tsukuba

- 1977 research begins (Hoshino, Kawai)
- 1978 1st system
- 1996 6th system CP-PACS(top of Top500)
- 2006 7th system PACS-CS

1978
1st gen. PACS-9

1980
2nd gen. PAXS-32

1989
5th gen. QCDPAX



1996
6th gen. CP-PACS

2006
7th gen. PACS-CS

year	name	speed
1978	PACS-9	7 kflops
1980	PAX-32	0.5 Mflops
1983	PAX-128	4 Mflops
1984	PAX-32J	3 Mflops
1989	QCDPAX	14 Gflops
1996	CP-PACS	614 Gflops
2006	PACS-CS	14.3 Tflops

- Application-driven R&D of MPP through collaboration of
  - Scientists
  - Computer scientists
  - Industry
- Concentrated use of computer power on fundamental science problems

- PAX Parallel Array Experiment
- PACS Parallel Array Continuum Simulation

  Parallel Array Computer System

Several boards on display in the Hall

Our stance

- *We have a long history of interdisciplinary research in computational science, including HPC systems development, by a tight collaboration between science and computer science*
- *We believe that this approach is a key to bring out breakthroughs in the field of computational science*
- *Research activities and organizational actions at CCP/CCS have been set up toward advancing computational science along this approach*

Chronology of CCS (from M. Sato's slide)

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)
2002	***Government decides to change the National University System in 2004***
2002 July-2003Dec.	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)

Change in 2004

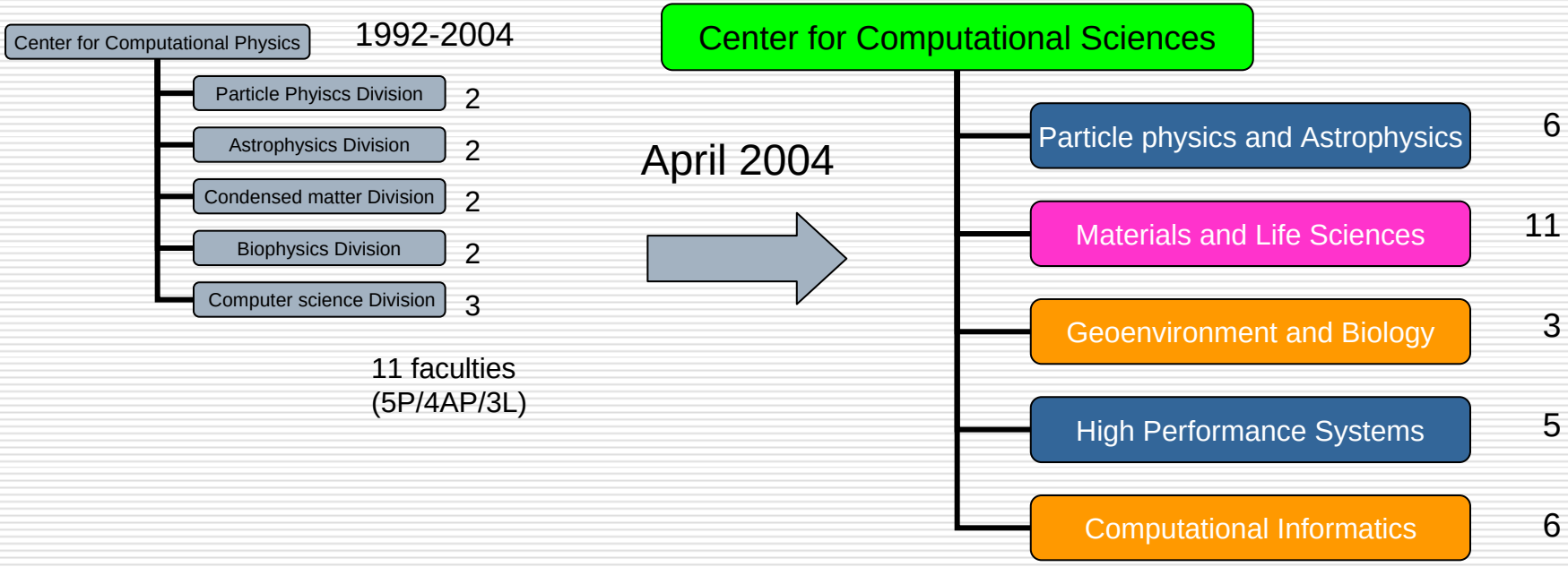
- Prior to JFY2004
  - National universities were a part of the Government strictly controlled by the Ministry of Education, Culture, Sports, Science and Technology (MEXT)

- Since JFY2004
  - The status of the national universities was changed to that of “independent institutions”
    - Pressure toward a reformation of the Government itself
    - Pressure toward a more effective university system in the era of global competition
  - Budget still provided by the Government, but universities are granted much wider freedom of action on their own
  - 6 year cycle of PDCA;need midterm evaluation of the present cycle JFU2004-2009

Strategy of CCP

- CCP viewed the transition as a welcome opportunity to reconsider its future plan
  - A 20 year history of R&D of high performance computers, and forefront computational physics research with them
  - A unique interdisciplinary research environment with a tight collaboration between physicists and computer scientists
- Not only physics but a wider area of science would benefit from the interdisciplinary approach pursued by CCP, so reorganize and expand
  - In terms of science area covered
  - In terms of faculty
- University Executive Office welcomed the CCP proposal to expand CCP, and provided strong support within the University and during the negotiations with MEXT (winter 2002-summer of 2003)

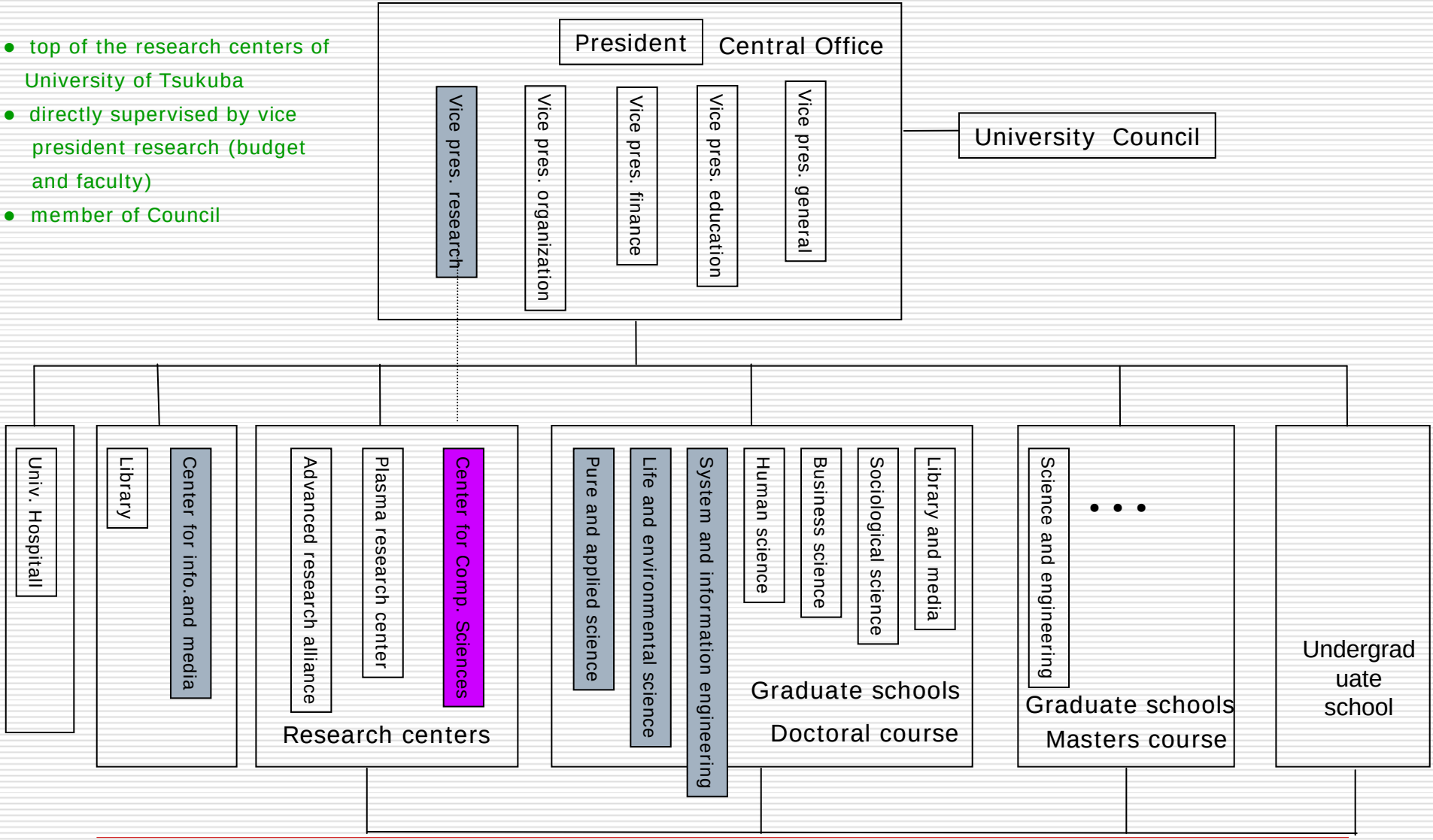
Expansion to Center for Computational Sciences



- An expansion (11→31 fuculty) keeping the unique feature of collaboration between computer science and applications
  - Materials and Life Science Division sizably expanded (2→11)
  - 2 new divisions added (Geo-environment and Biology, Computational Informatics)
- Of the 20 members added, 14 are faculty members who moved from the Graduate School; 6 new positions were provided by the University and filled by new recruitments

CCS within University of Tsukuba

- top of the research centers of University of Tsukuba
- directly supervised by vice president research (budget and faculty)
- member of Council



institutes

Major projects of CCS

- 「PACS-CS」Project (2005-2007)
  - Computational science as a whole, in particular particle physics and materials/life science and computer science
  - PACS-CS = Successor to CP-PACS

- 「FIRST」Project (2004-2007)

  「1st generation cosmic objects through heterogeneous multicompter system」
  - Astrophysics and computer science
  - FIRST = special purpose cluster with GRAPE-6 embedded nodes

- ILDG/JLDG Project（2002-）

  International/Japanese Lattice Data Grid
  - Grid project for lattice QCD (particle physics)
  - Particle physics and computer science

- Other projects pursued by each areas/divisions

PACS-CS Project

Parallel Array Computer System for Computational Sciences

- Official Project title: “Discovery, Synthesis, and Emergence of Novel Knowledge through Computational Science”
- Funding: Special Fund for Education and Research of National University Institutions (Buildup of Centers)
- Amount and Period: 2.3 billion Yen over JFP 2005～2007 (3 years)
- Project goal: to serve as a kickoff project of CCS, in particular
  - Expand the interdisciplinary approach of a collaboration of science and computer science from particle physics/astrophysics areas, where CCP has established itself, to materials/life sciences and Geo-environmental/biological sciences, thereby advancing the forefront of computational science
  - Develop a massively parallel cluster PACS-CS as a successor to CP-PACS to provide a computational engine to meet the computing needs of the applications

Brief chronology

2003	June-August	initial blueprint of the PACS-CS Project discussed
	December	Government budget for JFY2004 includes the founding of CCS
2004	January	1st negotiation with MEXT toward budget application of the PACS-CS Project in JFY2005
	April	Formal founding of CCS
	June	Formal application procedure within University of Tsukuba
	June-August	Negotiation with MEXT
	August	MEXT request to Ministry of Finance for JFY2005 budget includes the PACS-CS Project
	September	Evaluation by CSTP (Committee for Science and Technology Policy of the Japanese Government)
	October	Announcement of results by CSTP (ranked “A” of the SABC scale)
	December	Government budget for JFY2005 includes the PACS-CS Project
2005	April	PACS-CS Project formally starts

PACS-CS Project time chart

2004 Summer	setup *working groups* in each science target area with computational science and started collaborative research : *pacs-cs (particle physics), comas-dft (materials/life sciences)、gpv-jma(geo-environment)、mol-evol(biological science)*
2005 April	official start of the PACS-CS Project
July	official contract with Hitachi Ltd. for systems development
August	official contract with Fujitsu Ltd. for network driver develoment
	Set up *Systems Working Group* and *Network Working Group* (members from CCS and vendor engineers) to discuss technological issues in R&D of PACS-CS at 2 to 4 weeks intervals
2005 Fall ～2006 Spring	System Planning/Verification/Manufacturing
2006 June	full system test at Hitachi Factory/ranked 34th in the June 2006 Top 500 list (ranked 2nd after Earth Simulator among Japanese systems)
2006 July 1	full system installation at CCS/start of operation for user applications
2007 September 3	Official commissioning of PACS-CS
2007 October	start of *Interdisciplinary Computational Science Promotion Program*

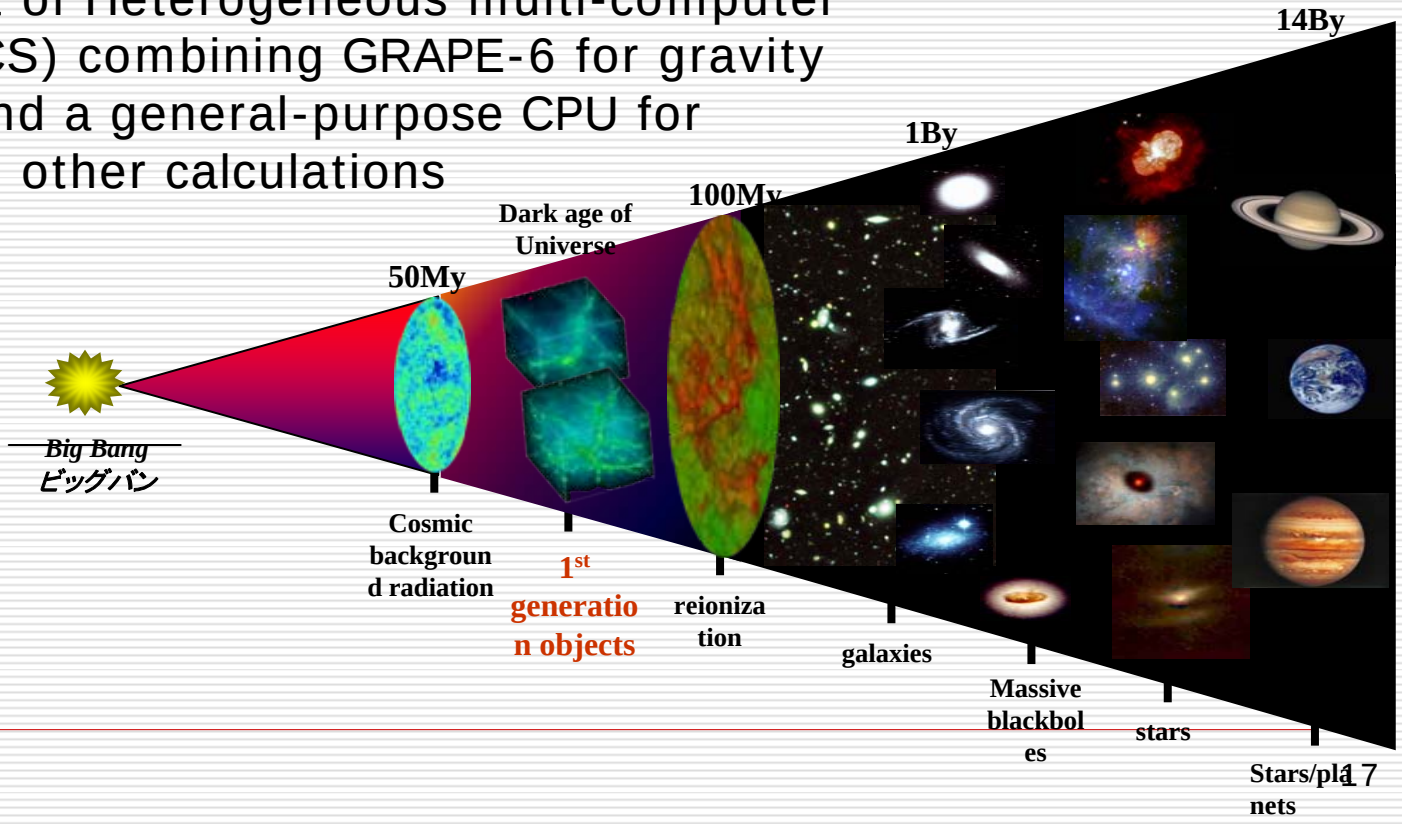
PACS-CS Project organization

- Project leader — CCS director
  - Akira Ukawa (2005-2006)
  - Mitsuhisa Sato (2008)
- Systems development leader — Taisuke Boku
- Collaborative research WGs
  - Pacs-cs (particle physics) — A. Ukawa et al (7+5)
  - Comas-dft(materials/life) — A. Oshiyama et al (7+3)
  - Gpv-jma (geo-environment) — H. Tanaka et al (2+5)
  - Mol-evol(biology) — Y. Inagaki et al (2+1)

(science, computer science)

FIRST Project (I)

- Research on 1st generation celestial objects in the Universe
- Astrophysical simulation including gravity/radiation/hydrodynamics of matter needed
- Development of Heterogeneous multi-computer system (HMCS) combining GRAPE-6 for gravity calculation and a general-purpose CPU for radiation and other calculations



FIRST Project (II)

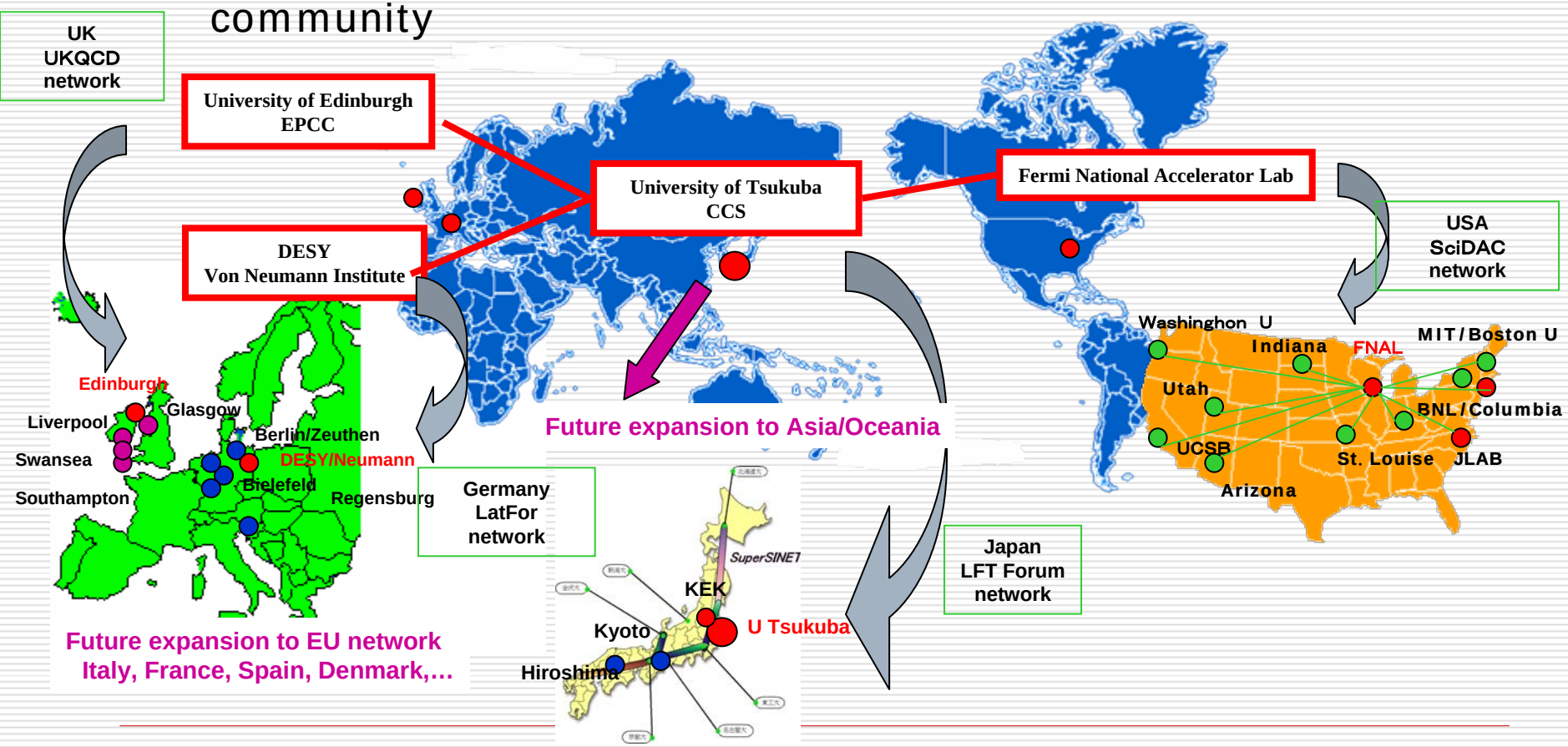
- Project leader: M. Umemura
- Members: 4 astrophysicists and 4 computer scientists, post docs, students
- Funding: Specially Promoted Research in Grants-in-Aid for Scientific Research, 0.33 billion Yen over 2004-2007
- FIRST system
  - Total system 256nodes general purpose 3.5TFLOPS+gravity 35TFLOPS
  - System started operation in October 2006

Blade-GRAPE board
(136.8GFLOPS)

Front view of FIRST

ILDG/JLDG Project

- R& D of International Lattice Data Grid(ILDG) and Japanese Lattice Data Grid (JLDG) to share configuration data in the world lattice QCD community and within the Japanese lattice QCD community



Funding and members

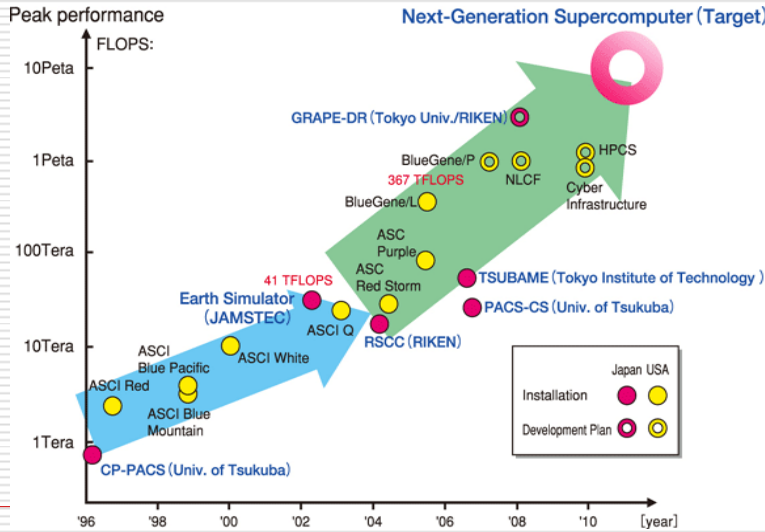
- Various funding over the years
  - JSPS core-to-core program (ILFTNet Project)
    - 40 million Yen over 2004-2005
  - NII(National Institute of Informatics) Cyber Infrastructure Project
    - About 40 million Yen over 2005-2007

- Collaborations
  - within CCS: particle physics (2+1 PDF) + computer science (3)
  - National: Tsukuba, KEK, Osaka(RCNP), Hiroshima

Next-generation supercomputer Project (Japanese Petaflops Project)

http://www.nsc.riken.jp/index-eng.html

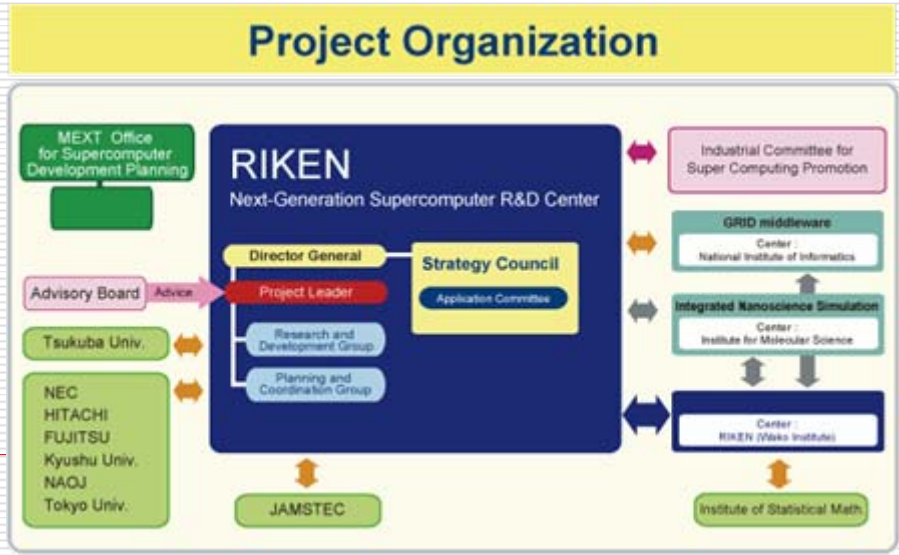
- Development of a general-purpose 10-petaflops class system by 2012
- Shared use of the system by researchers in various fields of computational science
- Buildup of a center for research and education in computational science around the petascale system in Kobe
- Continual R&D of supercomputers (i.e., next, next-next, ...) as a key national technology envisaged



Involvement of CCS

- "Element technology for next-generation supercomputer" Project
  - National project funded by MEXT through JST
  - Collaboration with Hitachi Ltd. on low-power on-chip memory archtecture for next-generation systems

- Collaboration with RIKEN on the petaflops system development
  - Formal agreement between U. Tsukuba and RIKEN signed in September 2006
  - Participation of several CCS faculty in the system design as RIKEN Visiting Researchers
  - Collaboration in tuning of representative petascale applications (QCD and RS-DFT)
  - Members in various committees



Once more, Our stance, and ...

- *We have a long history of interdisciplinary research in computational science, including HPC systems development, by a close collaboration between science and computer science*
- *We believe that this approach is a key to bring out breakthroughs in the field of computational science*
- *Research activities and organizational actions at CCP/CCS have been set up toward advancing computational science along this approach*
- *We wish to have your assessment and advice on how well we have been doing in this approach since 2004, and how best we can continue to do well and continue to be a key organization nationally and internationally in computational science in the coming era of petascale computing*