2014.Feb.18 External Review



External Review on Center for computational sciences

\sim Activities and Results 2008-2013 \sim

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

Mission of CC presented at review in 2007

- The mission of the Center of Computational Sciences is to promote scientific discovery by computational science through the application of advanced computing technologies, and to support researches of computational science in Japanese universities and institutes by operating leadingedge computing systems.
 - The center carries out R&D in high performance computing and networking systems, and applications of novel information technologies.
 - The center is an inter-university facility open to researchers throughout Japan.

CCS's Vision:

presented at review in 2007

COE of "Interdisciplinary Computational Science"

Computational Science is a cutting-edge and indispensable multidisciplinary area for the development of science and technology of the 21st century.

- Computational Science as the key to meet the grand challenges in nature and human, environments.
- Integration of science and computer/information science to realize the computational science.
- Education System to produce the next generation of scientists who carry out research from global perspectives.



We aim to be an world-wide COE to develop "Interdisciplinary Computational Science" as a new area to 21st century advances in science and technology, and support it continuously from global and long-term perspectives.

Strategies and Plan presented at review in 2007

- [Research & Development] Integrate the forefront of science research with that of computer science and information science, and to establish and promote new Interdisciplinary computational science
 - Execute "Interdisciplinary Computational Science Promotion Programs" for the operation of interuniversity facilities such as PACS-CS → Promotion and acceleration of Interdisciplinary Computational Science
 - Integrate computational science with grid/network computing, sensing technologies, data engineering and informatics → "new" concept of computational science
- [Education & Public Relations] Educate and produce the next generation of scientists who push forward new Interdisciplinary computational science from global viewpoints.
 - Dual degree (double majors) program, campus-wide courses on "computational science" for graduate students, HPC seminar series, workshops and symposium
- [Infrastructure & Service] Support researches by operating leading-edge, advanced, large-scale computing facility for inter-university computing resources, and development of advanced computing infrastructure
 - Acquire & operate the next supercomputer as a part of inter-university computing resources, making "Open supercomputer" alliance with Univ. of Tokyo and Kyoto Univ (T2K).
 - Contribution to the "national" next-generation supercomputer project, and take a leadership of national-wide computing infrastructure.
- [Collaboration & Alliance] Promote alliance and collaboration, and establish international/national networks of researches on computational science
 - Alliance with "supercomputer" centers of universities, the next-generation supercomputer center of RIKEN, and research Laboratories in Tsukuba
 - Promotion of international collaborations, and Support of Virtual Organization using Grid technologies.

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CCS Inter-University Activity: *Multidisciplinary 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.
 - <u>To promote interdisciplinary research projects of different disciplines.</u>
 - 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 mach 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



"National core-center" for the collaborative research on the Interdisciplinary Computational Science

- CCS has been approved as a "national core-center" for the collaborative research on the Interdisciplinary Computational Science from 2010 by the Ministry of Education, Culture, Sports, Science and Technology (MEXT) of Japan
 - "Advanced Interdisciplinary Computational Science Collaboration Initiative" (AISCI)
 - Funded 30M yen/year (5 years, 2010-2014)
 - Support for Multidisciplinary Computational Science Promotion Programs
 - Support for scientific meetings, hosts talented researchers from overseas, and strives to locate and retain short-term auxiliary supporters.
 - Mid-term evaluation result in 2012: "A", (Final evaluation in 2014)

Year	FY2007	FY2008	FY2009	FY2010	FY2011	FY2012
Accepted Projects	13 (Second Half)	36 (1/2:13, 2/2:23)	53 (1/2:31、2/2:22)	24 (all year)	31 (all year)	27 (all year)
System	PACS-CS From Oct.	T2K provided from the second half	FIRST was open for the program		PACS-CS Stopped at Sep	HA-PACS was provided from the second half

Accepted project in "Interdisciplinary Computational Science Promotion Programs"

"new" concept of computation of comp

"Sensing Web" project

The Computational Media Group and the Grid computing group have started projects "Sensing Web" in collaboration with Kyoto University and other university for the new integration with sensing technology and internet/grid.



Projects for "exascale" computing

HA-PACS project

 "Advanced research and education on computational sciences driven by exascale computing technology", 3 years (FY2010-FY2013) \$4.5M total funded by MEXT

HPCI-FS project

- "Feasibility Study" project for Japanese exascale system.
- "Study on exascale heterogeneous systems with accelerators", 2 years(FY2012-FY2013), \$2M total funded by MEXT

HA-PACS project

- HA-PACS (Highly Accelerated Parallel Advanced system for Computational Sciences)
- Apr. 2011 Mar. 2014, 3-year project (the system will be maintain until Mar. 2016), lead by Prof. M. Sato

"Advanced research and education on computational sciences driven by exascale computing technology", \$4.5M funded by MEXT

- 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)
- Two systems
 - HA-PACS *base cluster*.
 - HA-PACS/*TCA*: (TCA = Tightly Coupled Accelerators)









True GPU-direct With cooperation of NVIDA

Study on exascale heterogeneous systems with accelerators (U Tsukuba proposal)

- Two keys for exascale computing
 - Power and strong-scaling
- We study "exascale" heterogeneous systems with accelerators of manycores
 - Architecture of accelerators, core and memory architecture
 - Special-purpose functions
 - Direct connection between accelerators in a group
 - Power estimation and evaluation
 - Programming model and computational science applications
 - Requirement for general-purpose system

• etc ...



Accelerator Chip (example)

Core

Strategies and Plan presented at review in 2007



Execute "Interdisciplinary Computational Science Promotion Programs" for the operation of interuniversity facilities such as PACS-CS → Promotion and acceleration of Interdisciplinary Computational Science



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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

<u>Computational Science Dual Degree</u> (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 Interdisciplinary computational science from global viewpoints
- Started in 2009 (Physics in Doctor course and Computer sciences in Master course)
- 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











MEXT Educational Project for Establishing Core Universities for Internationalization (Global 30)

- The Ministry of Education, Culture, Sports, Science and Technology (MEXT) has launched the Global 30 Project for Establishing Core Universities for Internationalization.
- In 2009, thirteen universities were selected to lead Japan's internationalization.

Selected Universities

National	Private
Tohoku University	Keio University
University of Tsukuba	Sophia University
The University of Tokyo	Meiji University
Nagoya University	Waseda University
Kyoto University	Doshisha University
Osaka University	Ritsumeikan University
Kyushu University	

SC DD program and G30

- From 2009 Computational Science Dual Degree Program for Ph.D. course
 - Ph.D. Course: Graduate School of Pure and Applied Sciences, Physics & Frontier Science Graduate School of Life and Environmental Sciences (Geoenvironmental Sciences)
 - Master's Course: Graduate School of Systems and Information Engineering, Computer Science
- From 2011 Global 30 English Program for international students
- Exchange students: dual degree, internship, fieldwork, credits, etc.
- Promote international collaborations



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Infrastructure & Service

- From "T2K" Open Supercomputer Alliance to JCAHPC
 - Design, acquire & operate the next supercomputer as a part of interuniversity computing resources, making <u>"Open supercomputer" alliance</u> with Univ. of Tokyo and Kyoto Univ (T2K).
 - T2K activity is extended to "Joint Center for Advanced HPC"(JCAHPC) with the University of Tokyo
 - The objective of the JCAHPC mission is to design and develop of a largescale HPC system worthy of becoming the hub of Japan's computational sciences, and to design an advanced system that exploits many-core technology, which is expected to be the key to the coming HPC systems.
 - This system is scheduled to be installed for operation and management in 2015. We expect the system to be installed will have more than 20PF in theoretical peak performance.
 - COMA: a pilot manycore system for JCAHPC sub-exa system in 2014.

Infrastructure & Service

- Collaboration with RIKEN on the petaflops system
 (K computer) development and operations, applications
 - Formal agreement between U. Tsukuba and RIKEN signed in September 2006
 - Participation of several CCS faculty in the system
 - design as visiting researchers



- 2 researchers are appointed to team leader in AICS since completion of system installations.
- We carried out actual collaboration in tuning of representative petascale applications (QCD, RS-DFT and FFT)
 - Two Gordon Bell Prizes
 - Gordon Bell Prize 2011 for Peak Performance (University of Tsukuba, University of Tokyo, RIKEN) in an atomic state simulation at actual semiconductor device scale.
 - Gordon Bell Prize 2012 (University of Tsukuba, RIKEN, Tokyo Institute of Technology) for scalability and sustained performance in a world's largest scale of a dark matter simulation.
 - FFT-e, FFT in HPCC Class1 Awards (2011-2013)
 - XcalableMP, HPCC Class2 Award
- Joining HPCI: National-wide High Performance Computing Infrastructure
 - Gfram2 is used as a global file system to share data.

National-wide High Performance Computing Infrastructure Project (HPCI)

- Background:
 - After re-evaluation of the project at "government party change" in 2011, the NGS project was restarted as "Creation of the Innovative High Performance Computing Infra-structure (HPCI)".
- Building HPCI: High-Performance Computing Infrastructure
 - To establish a hierarchical organization of supercomputers linked with the K computer and other supercomputers at universities and institutes
 - To set up a large-scale storage system for the K computer and other supercomputers
- Organizing HPCI Consortium
 - To play a role as the main body to design and operate HPCI.
 - To organize computational science communities from several application fields and institutional/university supercomputer centers.
 - Including Kobe Center



AICS and Supercomputer Centers in Japanese Universities



Storage System in first phase for HPCI



Strategies and Plan presented at review in 2007



 Promotion of international collaborations, and Support of Virtual Organization using Grid technologies.

Collaboration & Alliance

- Joint Institute for Computational Fundamental Science (JICFuS) was organized by CCS U. Tsukuba and KEK, NAOJ in 2010.
- CCS (JICFus) was selected as a core organization for "Field 5: The origin of matters and the universe" in HPCI SPIRE (Strategic Programs for Innovative Research) for K computer apps.
 - Funded \$5M/year (2011-2017?)
- International Lattice Data Grid (ILDG), an international project aimed at the development of data grids for sharing lattice quantum chromodynamic (QCD) configurations worldwide since 2007.
- JLDG for national-wide global file system for particle physic community.
- International Collaborations (joint workshop, and researchers exchanges)
 - MOU with University of Edinburgh (universities MOU)
 - MOU with LBNL, US (Center's MOU)
 - International HPC school with KISTI, Korea
- Two G8 RCI projects for exascale computing (2011-2013): ECS (Enabling Climate Simulation at Extreme Scale) and NuFUSE(Nuclear Fusion Simulations at Exascale)

Five strategic areas of SPIRE

(Strategic Programs for Innovative Research) for K computer



Collaboration & Alliance

- Collaborations with Research Labs in Tsukuba
 - the High Energy Accelerator Research Organization (KEK), the Advanced Institute for Science and Technology (AIST), the National Institute for Materials Science (NIMS), the Meteorological Research Institute (MRI), and the National Institute for Environmental Studies (NIES).

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Transition of external project funds (2005-2010)



Strategies and Plan of CCS



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Final Remarks

- Two projects for post-petascale, and exascale computing
 - Post-petascale system (> 20PF) with manycore in JCAHPC.
 - HPCI-FS projects "Study on exascale heterogeneous systems with accelerators"
- As system is getting larger and more complex (acc such as GPU), it is a time to need

Our vision: "Interdisciplinary Computational Science"

Integration and collaboration of computational science and computer science

Thanks for your attention!

Question and comments ?