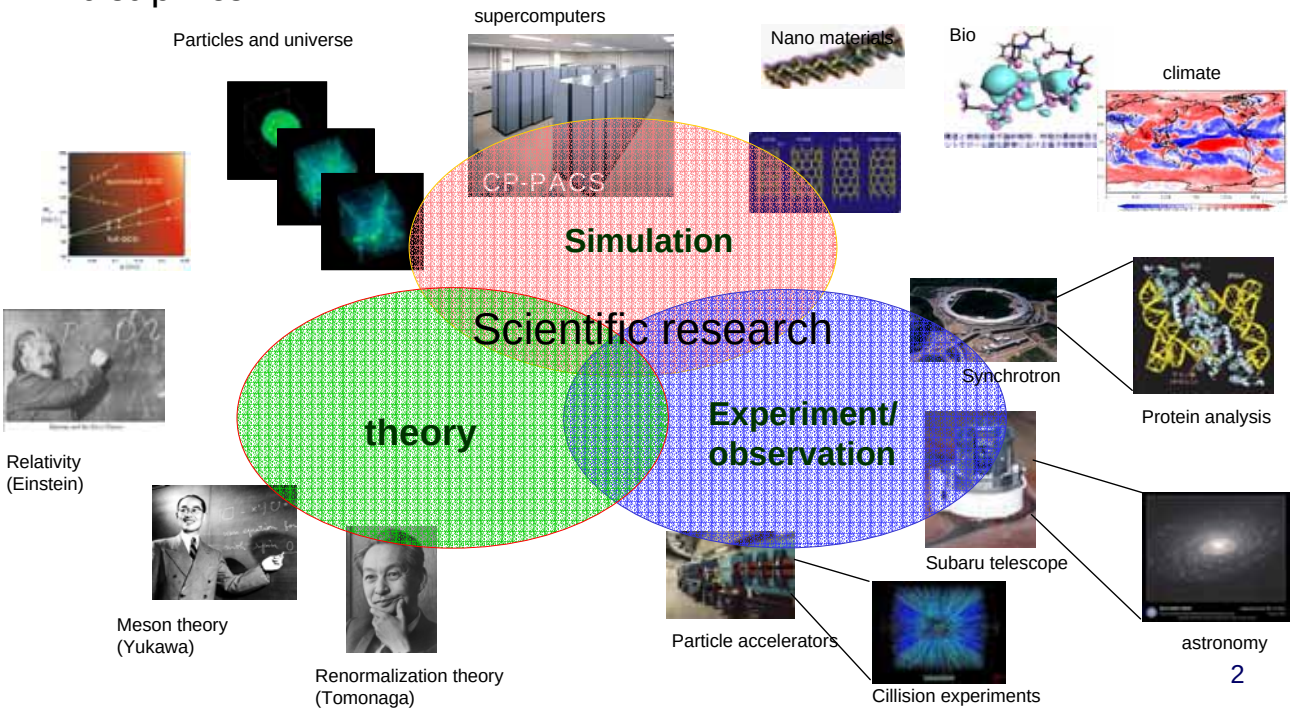
External Review on Center for computational sciences

～ Plan and Strategies of CCS ～

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

Computational science

- Large-scale simulations using supercomputers
- Critical and cutting-edge methodology in all of science and engineering disciplines



Mission of CCS

- 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 leading-edge 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.

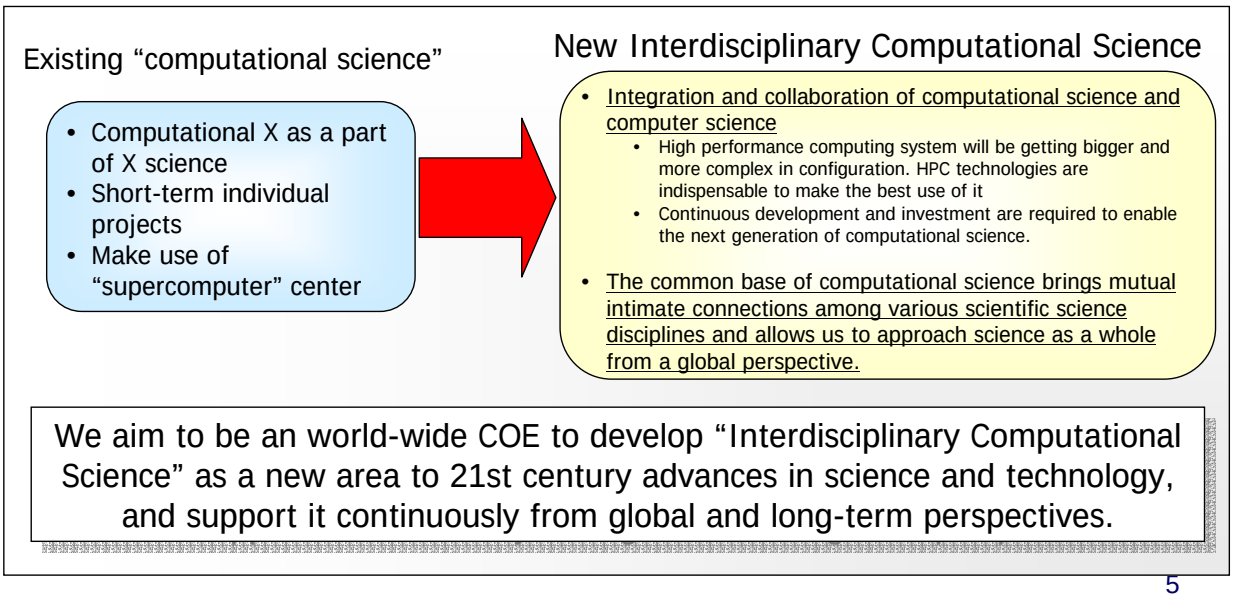
Position and Role of CCS

- From the nation-wide viewpoint of development of scientific research
  - An unique research “inter-university” organization which jointly carry out “interdisciplinary” researches on computational sciences, even including development of the leading-edge high performance computer systems
    - Computational Science in each discipline is done by university lab and institutes specific to its discipline.
    - National Institute of Informatics (NII) focuses on Information Science, neither computational science nor development of high performance computer system.
    - Supercomputer Centers in major university focus on just operation and service on computing facilities, and not researches on computational science.
- From the viewpoint of development of scientific research within our university
  - The faculty of CCS belongs to graduate schools and contribute to the education of computational science
  - Our university supports CCS as one of the most important research organizations with respect of budgets, faculty position and facilities.
  - “Academic Computing and Communications Center” (campus computer center) manages campus information infrastructures such computer systems and network systems in the university.

CCS's Vision:
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.



Strategies and Plan of CCS

- [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 inter-university 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.

Strategies and Plan of CCS (1)

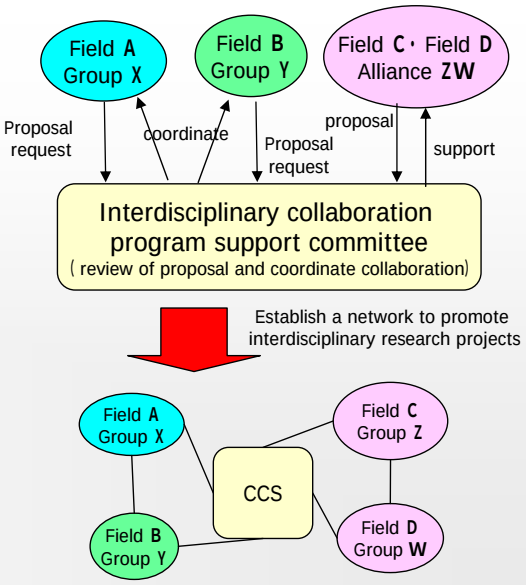
[Research & Development] Integrate the forefront of science research with that of computer science and information science, and to establish and promote new Interdisciplinary computational science

- Execute "*Interdisciplinary Computational Science Promotion Programs*" for the operation of inter-university 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

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 mach the request
    - Advice with expertise of different fields
  - Follow up the research activity produced by the interdisciplinary collaboration

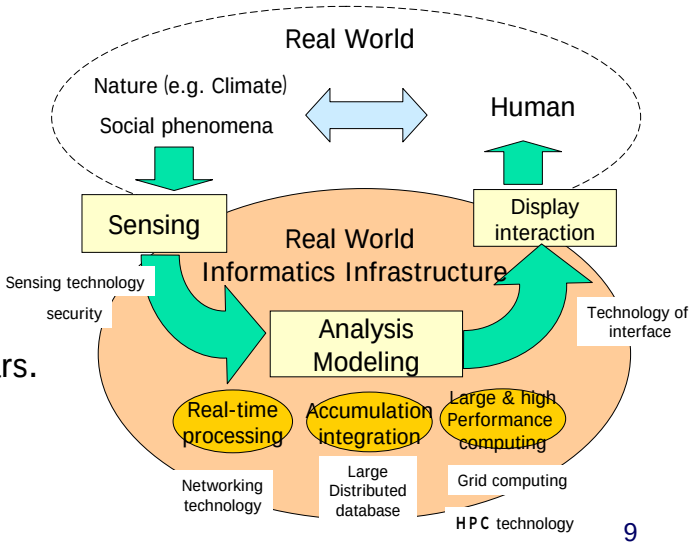


- Large-scale scientific simulation program
  - Push forward the grand challenge of several fields in computational sciences by providing the computational power of the PACS-CS.
  - Review proposals and concentrate our computational power to make new scientific discoveries
  - Follow up the scientific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

“new” concept of computational science

- “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.

- “Initiative for Real-World Computational Informatics”
  - The Computational Informatics Division and High Performance Computing System Division, Global Environment and Biological Sciences division propose the idea to integrate sensing, database and computation to capture and observe phenomena of human and nature in real world.
  - Accepted as a strategic project of the university for two years.



Strategies and Plan of CCS (2)

[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
  - A plan of “***Long-term Computational Science Workshop***” where an advanced subject encompassing multiple disciplines of science and computer science is to be chosen, and participants who stay from a few weeks to a few months are encouraged to carry out interdisciplinary research collaborations.
  - International symposium once in every year
    - there has been 10 symposia over the past 5 years

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 in July 2007(more than 80 participants)
  - 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)
  - Start 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 Interdisciplinary computational science from global viewpoints
  - Plan: will be started in 2008 (Physics in Doctor course and Computer sciences in Master course)

- Education in each graduate school
  - CCS allocates space for some of students, and create environment to enable interactions to other fields.

Strategies and Plan of CCS (3)

[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.
- Explore the next-generation high performance platform.

What's "T2K" Open Supercomputer Alliance

- Three Japanese national universities: **Tsukuba, Tokyo and Kyoto**
- We are now going to perform the procurement for next supercomputers at the same time-flame for replacement of current ones

- We agree to cooperate and make an alliance to share the main system architecture on three machines
  - Common Architecture - Node and Interconnection
  - Use of Open System/Software – based on Linux Cluster
  - Source code level compatibility – easy code porting & grid
  - Grid computing – resource sharing both on CPU and Data

⇒ T2K Open Supercomputer Alliance

Background

- Current satisfied users of PC Clusters are:
  - Scientific computation users with small to medium size system
  - Embarrassingly Parallel Application users
    - Such as Monte-Carlo simulation, no communication is required

- Many unsatisfied users still exist:
  - Lower performance than estimated
    - Poor performance of interconnection network … and memory bandwidth

- Explore new application fields of PC Cluster
  - Large scale genomic informatics
  - Large scale archive search (database & data-mining)

We will find the way for large scale systems and new app

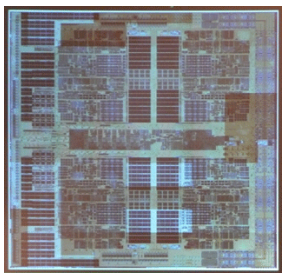
Concept of “Open Supercomputer”

- Openness of basic architecture
  - Use High-performance commodity processor
    - Market leading processor enables the high-performance, high-density and low-power computing facility in the supercomputer center
- Openness of system software
  - Use Open source based operating system and libraries
    - Seamless environment both on multi-scale and multi-site provides users to develop various fields and size of application
- Openness of user’s needs
  - Support much wider area of users than traditional supercomputer centers
    - To explore new application fields

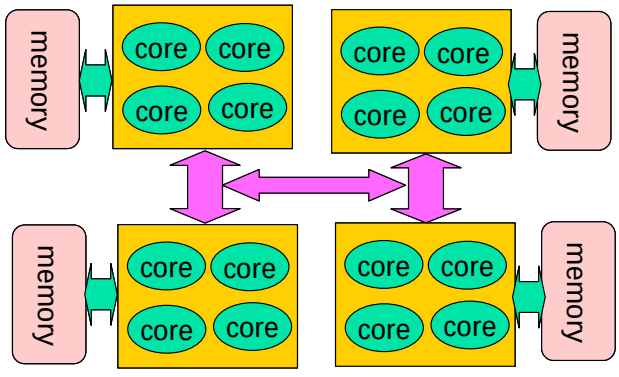
Architecture to cover from laboratories to SC centers

Design: node architecture and choice of processor

- The next generation processor is a Quad-core, 2xFPU, with over 2GHz
  - Peak performance > 32 GFlops/socket
  - Eg. Barcelona/AMD, Intel Tigerton and Kentsfield
  - Memory bandwidth becomes more serious problem.

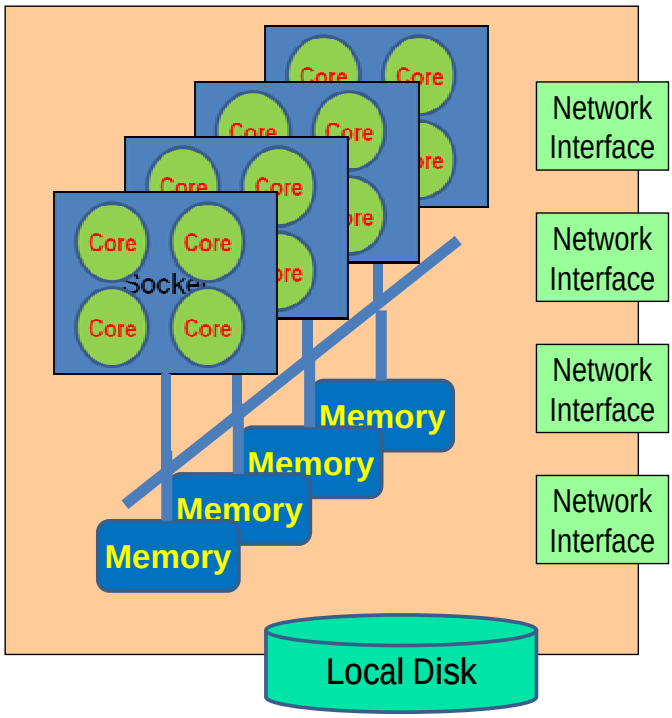


- NUMA architecture
  - Each processor should have its own memory
  - When memory affinity fits, it can exploit good memory bandwidth.
  - Eg. AMD HyperTransport



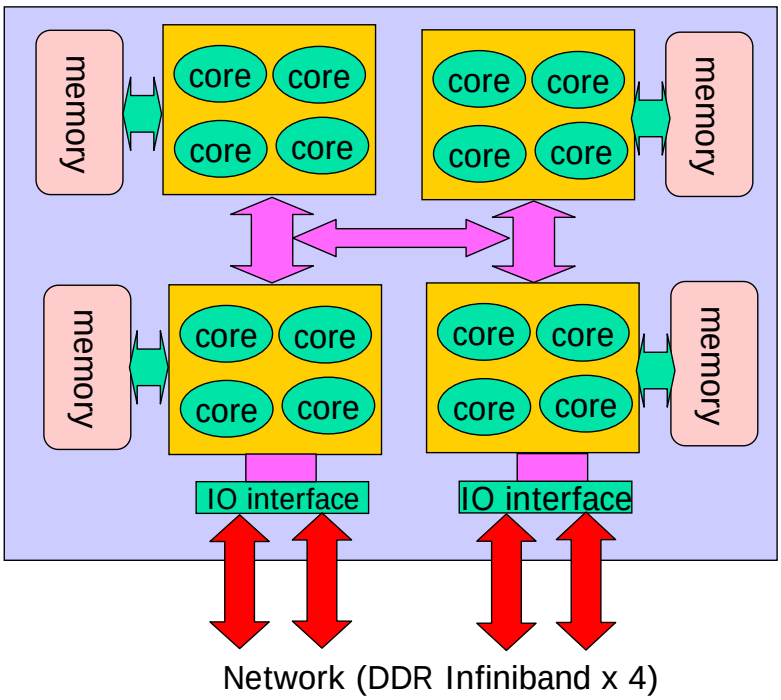
Expected basic configuration (As of March, 2007)

- Node architecture
  - 64-bit IA32 architecture
  - > 16 cores / node
  - > 32 Gbyte memory/node, > 40 Gbyte/sec memory bandwidth
  - > 128 Gbyte local hard disk
- Interconnection network
  - Physical performance
    - > 5 Gbyte/sec
  - MPI performance
    - > 4Gbyte/sec



A possible configuration

- AMD Barcelona (Quad Core)
  4 socket/node
  2.3 GHz
- Memory:
  8 Gbytes memory/socket
  10GB/s DDR2
  NUMA by HyperTransport
- DDR infiniband x 4 or Mrinet10G x 4



T2K schedule and expected performance

- Three universities share the same time-line on the procurement schedule.
- The final specification will be published on early October.
  - Biding will be on December.
- Operation is expected to get started on June 2008

- Expected performance of each university
  - Univ. of Tokyo > 150 TFLOPS
  - Univ. of Tsukuba > 80 TFLOPS (> 500 nodes)
  - Kyoto Univ. > 70 TFLOPS
- We expect more than 300 TFLOPS in total!

Toward Petascale computing

- "Element technology for next-generation supercomputer" Project
  - Collaboration with Hitachi Ltd. on low-power on-chip memory architecture 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 visiting researchers
  - Agreement of actual collaboration in tuning of representative petascale applications (QCD, RS-DFT and FFT)

- As a leading research organization, it is very important issue for us to take a leadership concerning to operation of the petascale system in national-wide computing infrastructure.

R&D of Next-generation HPC platform

- The next generation high-performance computing platforms may be:
  - arithmetic accelerators such as GRAPE-DR, Clear-speed, GPU
  - many-core architectures which integrate many functions on one chip.

- These architectures are promising for some special-purpose applications.
  - This approach is possible just in our center.
    - The FIRST project is very good example we have achieved so far in this approach.

Is it still possible to take an approach
to develop large machine by our own?

"Commitment" to design of high performance system
is really important !!

Strategies and Plan of CCS (4)

[Collaboration & Alliance] Promote alliance and collaboration, and establish international/national networks of researches on computational science

- Develop (futher!) alliance with:
  - "Supercomputer" centers of universities (also T2K)
  - The next-generation supercomputer center of RIKEN
  - … and research Laboratories in Tsukuba

- Promotion of international collaborations
  - A plan of "***Computational Science Researchers Invitation Program***" to invite researchers who are leading the forefront of research in science and computational science.
  - Based on pear-to-pear personal/group relationship

- Support of Virtual Organization using Grid technologies.
  - Collaboration with NII CSI project

International collaborations

- ***International Lattice Data Grid*** in particle physics (Edinburgh University (UK), DESY(Germany), Univ. di Roma(Italy), FNAL/BNL/JLAB(USA))
- ***Astronomical Radiation Hydrodynamics Research*** (National Astronomical Observatory(Japan), SISSA(Italy))
- ***Nano-Bio Science Collaboration*** (ETH(Switzerland), Princeton University/Vanderbilt University(USA), Advanced Institute for Science and Technology(AIST), National Institute for Materials Science (NIMS)),
- ***Quantum Structural Biological Science Collaboration*** (AIST, Hyogo Prefectural University(Japan), ETH/IBM Zurich(Switzerland)
- ***Quantum Dynamics Collaboration*** (RIKEN(Japan), Washington University (USA))
- ***Warming of Arctic Research*** (IARC of Alaska University/Hawai University(USA), Pusan University(Korea), Academia Sinica(China))
- ***France-Japan Grid Computing*** (National Institute of Informatics(Japan), INRIA(France), Pennsylvania State University(USA))
- ***Information integration/Knowledge discovery Research*** (Carnegie-Mellon University/Georgia Institute of Technology(USA), Hong-Kong Chubun University).

Finally, …

CCS's vision: 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.

- What is "Interdisciplinary Computational Science"?
  - Computational X exists!
  - Interaction between computational X and computer science
  - Interaction between computational X and computational Y with respect to modeling and methodologies.
  - What's is "more"?
    - US NSF's "cyberinfrastructure" vision
- It must help to accomplish our mission
  - Promotion of scientific discovery
  - Support for researches of computational science as inter-university activity.

Thanks for your attention!

Question and comments
And Discussion!