

External Review on Center for Computational Sciences University of Tsukuba 2013.2.18-20

Multidisciplinary Cooperative Research

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Multidisciplinary Cooperative Research Program

Computer resources open to nationwide academic researchers free of charge

PACS-CS 2006-2011 14.34TF



FIRST (GRAPE-6) 2007-2012 38.5TF



T2K-Tsukuba 2008-2014 95.4TF



HA-PACS (GPU) 2012- 802TF



COMA (Xeon-Phi) 2014-

NO IMAGE

Multidisciplinary Cooperative Research Program

Computer resources open to nationwide academic researchers free of charge

- 2002- Computer resources open to collaborative researches
- 2007- Started "Multidisciplinary Cooperative Research Program"
- 2010- CCS has been recognized as a national core-center(*) under the Advanced Interdisciplinary Computational Science Collaboration Initiative

In addition to computer resources, supports of inviting visitors, travels, short-time employment are provided.

(*)MEXT (Ministry of Education, Culture, Sports, Science and Technology) – Japan approves 90 research centers (in 41 universities) as Joint Usage/Research Center.

Call for proposal: once (or twice) a year

Research fields

- Computational sciences including particle and nuclear physics, astrophysics, material sciences, life sciences, global environmental sciences, biology
- Computer sciences including high performance computer systems, computational informatics, numerical analysis

3 types of proposals are accepted

1. Multidisciplinary pioneering program

Promotes combining different fields

-e.g. Code developing by application researcher under support of HPC researchers.

2. Priority subjects promoting program

Promote computational science subjects via large-scale computations

3. Cooperative research promoting program

Promote advancements in computational approaches to sciences and technologies through close collaboration between researchers inside and outside the Center

Number of approved projects



Approved projects in 2013

Global Computer Environment. Science Computer Science **Particle Physics Particle Physics** Life Science **Astrophysics** Global Material_ Environment Astrophysics Nuclear Science Physics Life Science Material

Science



T2K-Tsukuba (2013)



Number of projects





Processes of application and approval of projects (2013)

2013. 1. 18 Application deadline

Peer review by 3 reviews for each field (Board of Cooperative Research)

- 2013. 2. 15 Decision for projects
 - approved without hearing
 - subject to hearing
 - rejected
- 2013. 3. 1 Hearing, notice of acceptance (Administrative Committee)
- 2013. 4. 1 Start project

2013. 11. 5-6 5th Symposium on "Discovery, Fusion, Creation of New knowledge by Multidisciplinary Computational Sciences"

- Intermediate report of projects of 2013
- Progress report of projects of 2012

Organization of CCS



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It becomes more and more difficult for researchers of scientific fields to make full use of cutting-edge supercomputers

GPU, MIC, ...

Project Office for Exascale Computational Sciences Project Office for Exascale Computing System Development

Collaboration between Computational Science and Computer Science

Members from

- Particle physics
- Astrophysics
- Nuclear physics
- Condensed matter physics
- Life sciences
- Global environment science
- Computational Informatics
- Numerical algorithms

Preparation for new architecture machines

- HA-PACS (multi-GPU)

- COMA (Xeon-Phi)

Hot spot analysis and acceleration

Examples: Efforts at Project Office for Exascale Computational Sciences for HA-PACS (multi-GPU calculation)

Particle physics

- Finite temperature/density QCD (Matrix-matrix product of dense matrix)
- Nucleus from QCD (Solution of large-scale sparse linear equation)

Astrophysics

- Realization of computational astrophysics in 6-dim (Ray-tracing calculation)
- Gravitational many-body simulation of colliding system (Gravitational acceleration and its derivative)

AMO physics

- Laser-atom interaction (Real-time, real-space finite difference calculation of Schroedinger eq.)

Condensed matter physics

- Electron dynamics calculation using hybrid functional (3D FFT by cufft)

Life science

- QM/MM study of enzymatic reaction (Molecular dynamics simulation)
- Molecular dynamics simulation of biomolecules (Quantum mechanical calculations)

Global environmental sciences

- Next-generation atmospheric circulation model NICAM (3D normal-modes expansion)
- Calculation of urban climate (LES)

Computational Informatics

- Knowledge discovery from large-scale database (Association rule mining, Time series data retrieval)

Thank you!