External Review

on Center for Computational Sciences, University of Tsukuba

Date: October 30th, 31st, November 1st, 2007 Place: Center for Computational Sciences, University of Tsukuba (http://www.ccs.tsukuba.ac.jp)

External Review Committee:

| Chair: | Prof. Richard Kenway, The University of Edinburgh |
|-------------|--|
| Vice Chair: | Prof. Yoshio Oyanagi, Kogakuin University |
| | Prof. Michael L. Norman, University of California, San Diego |
| | Prof. Kiyoyuki Terakura, |
| | Japan Advanced Institute of Science and Technology |
| | 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 |
| | |

Schedule:

| * 30th October (Tuesday) * | | |
|----------------------------|---|--|
| 9:30-10:00 | Welcome (Sato, Director of CCS) | |
| | Objective and schedule of the external review | |
| 10:00-10:30 | Overview and current status of CCS (Sato) | |
| 10:30-11:00 | Activities and results 2004 – 2007 (Ukawa) | |
| 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 | |
| | | |
| 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

Track 1 (Reviewers: Oyanagi, Simon and Kitsuregawa) : <u>Workshop room</u>

Division of High Performance Computing Systems

16:30-16:35 Group introduction (T. Boku)

16:35-16:50 Low-power and high-performance cluster network (T. Boku)

16:50-17:15 Gfarm distributed file system (O. Tatebe)

17:15-17:40 FFT-E and math-library (D. Takahashi)

17:40-17:50 Student presentation (1) (Y. Nakajima)

17:50-18:00 Student presentation (2) (Y. Hotta)

Track 2 (Reviewers: Kenway and Norman): Meeting room A

Division of Particle Physics and Astrophysics

- 16:30-17:00 Dynamical Wilson quark simulations towards the physical point (Y. Kuramashi)
- 17:00-17:15 Nuclear force from lattice QCD (N. Ishii)
- 17:15-17:30 Warm-Hot Intergalactic Medium / SIMD Acceleration of Astrophysical Simulations (Kohji Yoshikawa)
- 17:30-17:45 High Resolution Simulation of First Generation Star Formation(Tamon Suwa)
- 17:45-18:00 Formation and Dynamical Evolution of Globular Cluster(Kenji Hasegawa)

Track 3 (Reviewers: Sumi and Philippe): Meeting room B

Division of Global Environment and Biological Science

- 16:30-16:50 Can we include EF2 in multigene phylogenetic analyses? (Inagaki)
- 16:50-17:10 Centrohelida is still searching for a phylogenetic home: Analyses of 7 Raphidiophrys contractilis genes (Sakaguchi)
- 17:10-17:20 Prediction of water resource variation in winter under the global warming: Case studies in Japan and Turkey (Kimura, F.)
- 17:20-17:30 Prediction of urbern climate using the WRF regional model (Kusaka, H)
- 17:30-17:40 Spectral energetics analysis of the general circulation of the atmosphere in the vertical wavenumber domain (Terasaki, K)
- 17:40-17:50 Evaluation of the accuracy of the ensemble Kalman filtern (Kondo, K.)
- 17:50-18:00 Artic Oscillation as a dynamical singular eigenmode of the atmosphere (Tanaka, H)
- 18:00-18:30 (Committee meeting)

19:00- (Committee meeting with dinner)

| * 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 |
| 5 | 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 |
| 11:40-12:05 | Sciences: Quantum Many-Body Systems Group (Yabana) Activities and Collaborations 9: Division of Global Environment and |
| 11:40-12:05 | Biological Sciences: Biological Science Group (Hashimoto) |
| 11:05-12:30 | Activities and Collaborations 10: Division of Particle Physics and |
| 11.00 12.00 | 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 |
| 16:00-18:00 | Parallel Tracks |
| Track 1 (Revie | ewers: Oyanagi, Simon and Kitsuregawa) : <u>Workshop room</u> |
| Division | n of Computational Informatics |
| 16:00-1 | 6:45 1) Research Activities in Computational Intelligence Group |
| | oyuki Kitagawa, Toshiyuki Amagasa, Hideyuki Kawashima, |
| Yous | suke Watanabe, Jianwei Zhang |
| 16:45-1 | 7:30 2) Research Activities in Computational Media Group |
| | ni Ohta, Yoshinari Kameda, Itaru Kitahara |
| | |
| 17:30-1 | 8:00 3) Free Discussion with Young Researchers |
| Track 2 (Revie | ewers: Kenway and Norman): <u>Meeting room A</u> |
| Divisio | n of Particle Physics and Astrophysics |
| 16:00-1 | 16:20 \$¥eta\$' meson mass from lattice QCD (T. Yoshie) |
| 16:20-1 | 16:40 Lattice QCD calculation of the \$\Frac{\Frac}\}}}}}\!}}}}}}}}}}}}}}}}}}}}}}}}}}}}}} |
| 16:40-1 | 17:00 Non-perturbative renormalization of four-quark operators and |
| | \$B_K\$ with SF scheme in quenched domain-wall QCD |

(Y. Taniguchi)

- 17:00-17:15 Radiative Magnetohydrodynamic Accretion Flows and Jets (Yoshiaki Kato)
- 17:15-17:30 High-Redshift Metal Enrichment Traced by Extinction Curves (Hiroyuki Hirashita)
- 17:30-17:45 Study of Two Temperature and Non-Equilibrium Ionization States of Plasma in Merging Galaxy Clusters (Takuya Akahori)
- 17:45-18:00 Novel Picture for Lyman Alpha Emitters (Ikkoh Shimizu)
- Track 3 (Reviewers: Terakura, Sumi and Philippe): Meeting room B
 - Division of Materials and Life Sciences
 - (Material Science Group)
 - 16:00 16:05 Overview (Atsushi Oshiyama)
 - 16:05 16:25 Prediction of New Properties in Carbon Nano-Materials (Susumu Okada)
 - 16:25 16:40 Developments and Applications of Real-Space Density Functional Theory (RSDFT) (Jun-ichi Iwata)
 - (Life Science Group)
 - 16:40 16:50 Towards Construction of Quantum Structural Biology Coupled with Structural Bioinformatics (Masaru Tateno)
 - 16:50-17:05 Development of Computational Methods for Analyses of Enzymatic Reaction Mechanism and Protein Folding Problem (Yosuke Hagiwara)
 - 17:05-17:20 Dynamical Information Flow Mechanisms Revealed by Computer Simulations of Cellular Signaling Reaction Network Systems in a Cell (Tatsunori Nishimura)

(Quantum Many-Body Systems Group)

- 17:20-17:40 Quantum Dynamics in Few-Body System (Xiao-Min Tong)
- 17:40-17:50 Materials with strong electron correlation and strong electron-phonon interaction (Hiroyasu Koizumi)
- 17:50-18:00 Microscopic Theory of Nuclear Three-dimensional Rotational Motion (Yukio Hashimoto)
- 18:00-18:30 (Committee meeting)
- 19:00- (Committee meeting with dinner)

| * 1 st November (Thursday) * | |
|---|--|
|---|--|

9:00-10:00 (Committee meeting)

- 10:00-11:00 Discussion, Q & A
- 11:00-12:30 (Committee meeting)
- 12:30-13:30 Lunch