The Strategic Programs for Innovative Research (SPIRE), MEXT Japan
The Computational Materials Science Initiative (CMSI)
"International Workshop on Quantum Chemistry Massively Parallel Programming Now in Supercomputers"

Date: Tuesday, February 28th, 2012
Venue: The seminar room of Komaba Faculty House, the University of Tokyo
3-8-1 Komaba, Meguro-ku, Tokyo 153-8902, Japan
http://dir.u-tokyo.ac.jp/en/usefulinfo/housing/shukusha/komabafaculty
http://www.komed.c.u-tokyo.ac.jp/ilovekomaba/house.htm (in Japanese)

Organized by Prof. Hideo Sekino, Computer Science and Engineering, Toyohashi University of Technology (TUT)

Supported by the Computational Materials Science Initiative (CMSI), and the Strategic Programs for Innovative Research (SPIRE), MEXT Japan.

Focus: Several researchers who are engaged in massively parallel program developments in quantum chemistry, are invited from overseas and domestic. You can learn the programming techniques and know-how here extensively.

Registration Fee: free

Registration through the following web page:
http://www.cms-initiative.jp/ja/events/CMSI_events/120228IWQCMPPNS

Registration Deadline: Tuesday, February 21th, 2012

Contact: Hiedo Sekino, sekino@tut.jp

Program

1. US session chaired by

10:00	-	10:05	(TUT)	Prof. Hideo Sekino	Opening remarks
10:05	-	11:05	(Virginia Tech.)	Dr. Edward Valeev	Domain-Specific Languages for Quantum Chemistry: High Productivity and Performance
11:05	-	11:20	coffee break		
11:20	-	12:20	(PNNL)	Dr. Edoardo Aprà	Recent Developments of Molecular Electronic Structure Methods at Large Scale
12:20	-	13:40	lunch break		

2. Japan session chaired by

13:40	-	14:10	(Kobe Univ.)	Dr. Kazuya Ishimura	Parallelization and Acceleration for Large-Scale Quantum Chemistry Calculations
14:10	-	14:40	(Univ. Tokyo)	Dr. Junichi Iwata	Real-Space Density-Functional Theory program -Development and Application-
14:40	-	14:55	coffee break		

14:55	-	15:25	(Univ. Tokyo)	Dr. Hiroshi Watanabe	Massively Parallel Molecular Dynamics Simulations: Implementations and Applications
15:25	-	15:55	(TUT)	Dr. Shinji Hamada	Analysis tools and their application to NWChem.
15:55	-	16:10	coffee break		

3. Discussion session chaired by

16:10	-	17:10	Free Discussion		
17:10	-	17:20	(TUT)	Prof. Hideo Sekino	Closing remarks

* This program would be changed without a notice.

Profile of Invited Speakers

Dr. Edward Valeev, Associate Professor, Department of Chemistry, Virginia Tech. Dr. Valeev's group is developing the Massively Parallel Quantum Chemistry program (www.mpqc.org). His scientific interests include.domain-specific languages for tensor computation in science, finite-element representations for electron correlation, and explicitly-correlated electronic structure methods. http://www.valeyev.net/

Dr. Edoardo Aprà, Molecular Science Computing Performance Software group, Environmental Molecular Sciences Laboratory at the Pacific Northwest National Laboratory (PNNL). A team led by Dr. Aprà obtained a performance of 1.39 petaflops with the NWChem software in 2009. http://www.hpcwire.com/specialfeatures/people_to_watch_2011/Dr-Edoardo-Apra-113294114.html

Dr. Kazuya Ishimura, Assistant Professor, Graduate School of System Informatics, Kobe University. Dr. Ishimura is working on GELLAN quantum chemistry program for K-computer. http://www.gellan.cs.kobe-u.ac.jp/group/en/profiles/ishimura-e.html

Dr. Junichi Iwata, CMSI Lecturer, Graduate School of Applied Physics, the University of Tokyo. Dr. Iwata is working on the real-space DFT program for K computer. http://oshiyama.t.u-tokyo.ac.jp/eng/members/index.html

Dr. Hiroshi Watanabe, Research Associate, Institute for Solid State Physics, the University of Tokyo. Dr. Watanabe is developing his own MD program for supercomputers, and is also supporting CMSI members with his expertise of supercomputers, to work on K-computer. http://apollon.issp.u-tokyo.ac.jp/~watanabe/

Dr. Shinji Hamada, Research Associate, Computer Science and Engineering, Toyohashi University of Technology. Dr. Hamada developed his own simple wavelet based electron dynamics simulator, and is currently working on code analysis and evaluation of NWChem, to work on K-computer.

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