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

Date: Tuseday, February 4th, 2014
Venue: Sanjo Conference Hall, The University of Tokyo, Hongo Campus,
7-3-1, Hongo, Bunkyo-ku, Tokyo 113-8654, Japan
http://www.u-tokyo.ac.jp/en/about/documents/accessmap_E.pdf <- ACCESS
http://www.u-tokyo.ac.jp/en/about/documents/Hongo_CampusMap_E.pdf <- No.2 Bld.

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

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.

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Registration: http://www.cms-initiative.jp/ja/events/tcci-event/4iebr2/20140204_mppws

Program

1. International session

10:00 - 10:05	TUT	Prof. Hideo Sekino	Opening remarks
10:05 - 10:10	Univ. of Tokyo	Prof. Shinji Tsuneyuki	Welcome speach
10:10 - 10:55	Stony Brook Univ.	Dr. Robert Harrison	(TBA)
10:55 - 11:40	Univ. of Florida	Dr. Beverly Sanders	Massively parallel programming techniques in electronic structure theory
11:40 - 12:25	CEA/INAC	Dr. Laura Ratcliff	Linear Scaling Density Functional Theory with Daubechies Wavelets for Massively Parallel Architectures
12:25 - 14:00	lunch break		

2. Japan session

14:00 - 14:25	NIMS	Dr. Takahiro Yamasaki	Parallel implementation and application of planewave-based first-principles MD simulator “PHASE” on K computer
14:25 - 14:50	Riken AICS	Dr. Shigetoshi Sota	Development of massively parallel density matrix renormalization group method
14:50 - 15:15	IMS	Dr. Masashi Noda	Development of massively-parallelized electron dynamics program on the K computer and its application
15:15 - 15:40	Univ. of Tsukuba	Dr. Hiroaki Umeda	Development of FMO program for recent HPC systems: K-computer and GPGPU cluster
15:40 - 16:05	Waseda Univ.	Dr. Hiroaki Nishizawa	Acceleration and parallelization of DFTB aimed at large scale molecular dynamics (tentative)
16:05 - 16:25	coffee break		

3. Discussion session chaired by Prof. Hideo Sekino (TUT)

16:25 - 16:55	Free Discussion		
16:55 - 17:05	(TUT)	Prof. Hideo Sekino	Closing remarks

* This program would be changed without a notice.

Profiles of Invited Speakers:

Dr. Robert Harrison, Professor and Director, Institute for Advanced Computational Science, Stony Brook Univ. USA. Professor Harrison is a distinguished expert in high-performance computing and is the Endowed Chair and Director of the newly formed, $20M-endowed Institute for Advanced Computational Science at Stony Brook University. Through a joint appointment with Brookhaven National Laboratory (BNL), Professor Harrison has also been named Director of the Computational Science Center at BNL. Dr. Harrison comes to Stony Brook from the University of Tennessee and Oak Ridge National Laboratory, where he was Director of the Joint Institute of Computational Science, Professor of Chemistry and Corporate Fellow. He has a prolific career in high-performance computing with over one hundred publications on the subject, as well as extensive service on national advisory committees.
http://commcgi.cc.stonybrook.edu/am2/publish/General_University_News_2/Large_Private_Donation_Launches_Institute_for_Advanced_Computational_Science_at_Stony_Brook_University.shtml

Dr. Beverly Sanders is Associate Professor of Computer Science at the University of Florida, USA. She earned a PhD in Applied Mathematics at Harvard University and was previously on the faculty of the Swiss Federal Institute of Technology (ETH Zurich). For the past several years, she has collaborated with the Quantum Theory Project at the University of Florida on the ACES III software package. ACES III provides a modern, high-performance implementation of couple cluster and other methods optimized for high performance heterogeneous parallel computer systems, ranging from small clusters, all the way to high-end petascale systems.

Dr. Laura Ratcliff, postdoc researcher, Institute for Nanoscience and Cryogenics (INAC), CEA, France. After graduating from the University of York, UK in July 2008 with first class honours with distinction in Theoretical Physics (with a year in Europe), she began studying for a PhD in the department of Materials Science at Imperial College London, UK. The subject of her research was the calculation of experimental spectra in ONETEP, a linear-scaling density-functional theory code. Her thesis, which she completed in September 2011, was selected for publication in the Springer Theses series. Following a further three months at Imperial College, she began work as a post-doctoral researcher in the laboratory for atomistic and molecular simulation at CEA Grenoble, France, in February 2012. Since then, she has continued to work on linear-scaling density-functional theory methods, this time in the wavelet based BigDFT code, with a particular focus on development for massively parallel architectures. In particular, she has worked on an implementation of constrained density-functional theory and a fragment based approach for further accelerating calculations on large, realistic systems.

Dr. Takahiro Yamasaki, NIMS Special Researcher, Computational Materials Science Unit, National Institute for Materials Science, Japan. Dr. Yamasaki develops the first-principles MD simulator “PHASE” on parallel computers for various materials.

Dr. Shigetoshi Sota, Research scientist, Computational Materials Science Research Team, RIKEN Advanced Institute for Computational Science. Dr. Sota is working on the massively parallel density matrix renormalization group program for K-computer.
http://www.riken.jp/en/research/labs/aics/research/comput_mater_sci/

Dr. Masashi Noda, Project Researcher, Dept. of Theoretical and Computational Molecular Science, Institute for Molecular Science. Dr. Noda is working on the Grid-based Coupled Electron and Electromagnetic field Dynamics (GCEED) simulation program for the K computer.

Dr. Hiroaki Umeda, Researcher, Center for Computational Sciences, University of Tsukuba. Dr. Umeda is working on the parallelization of quantum chemistry programs for HPC computers.

Dr. Hiroaki Nishizawa, Research Associate, Waseda Research Institute for Science and Engineering, Waseda University. Dr. Nishizawa is developing the linear-scaling quantum chemical methods based on the tight binding technique.