関係各位

いつも大変お世話になっております。分子研の石谷です。
CMSI/TCCI では、以下のように量子化学超並列プログラミング国際ワークショップを開催致します。

英文名称：″International Workshop on Quantum Chemistry Massively Parallel Programming Now in Supercomputers″
日時：2012 年 2 月 28 日（火）10:00～
場所：東大駒場 ファカルティハウス　セミナー室
　　東京都目黒区駒場 3-8-1
http://www.komed.c.u-tokyo.ac.jp/ilovekomaba/house.htm

参加費：無料
参加登録：以下の web ページよりお願い致します。
http://www.cms-initiative.jp/ja/events/CMSI_events/120228IWQCMPPNS

このワークショップでは、米国より、量子化学分野で超並列プログラミングで活躍されている２名の研究者をお招きし、また、CMSI からは、現在、京で高度化に従事されている研究者の方々にご発表を頂きます。

オーガナイザーである関野先生の狙いは、「量子化学超並列プログラム構築にあたってのノウハウを、実際にプログラム開発に携わっている内外の第一線で活躍している研究者をお招きしてガンガン学ぶ」です。

招待講演者：
Dr. Edward Valeev, Associate Professor, Virginia Tech.
Dr. Edoardo Aprà, Pacific Northwest National Laboratory
石村和也博士、神戸大学大学院システム情報学研究科計算科学専攻助教
岩田潤一博士、東京大学大学院工学系研究科物理工学専攻特任講師
渡辺宙志博士、東京大学物性研究所物質設計評価施設助教
濱田信次博士、豊橋技術科学大学情報知能工学系研究員

貴重な機会ですので、量子化学分野の超並列プログラミングに興味のある方は是非ご出席をお願い致します。

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
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
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
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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