文部科学省 「革新的ハイパフォーマンス・コンピューティング・インフラ（HPCI）の構築」
ＨＰＣＩ戦略分野２「新物質・エネルギー創成」
計算物質科学イニシアティブ（ＣＭＳＩ）
第２回超並列化技術国際ワークショップ
英文名称："International Workshop on Massively Parallel Programming Now in Molecular Science"

主催：計算物質科学イニシアティブ(CMSI)/計算分子科学研究拠点(TCCI)
後援：早稲田大学高等研究所
日時：2013 年 1 月 28 日（月）10:20～16:10
場所：早稲田大学西早稲田キャンパス 55 号館 N 棟 1 階 大会議室
169-8555　新宿区大久保 3-4-1
ＪＲ　山手線 高田馬場駅から徒歩 15 分
西武鉄道 西武新宿線 高田馬場駅から徒歩 15 分
地下鉄東京メトロ副都心線 西早稲田駅に直結
東西線　早稲田駅から徒歩 22 分
バス　新宿駅西口 - 早稲田、都立身体障害者センター前バス停下車
高田馬場駅 - 九段下、都立身体障害者センター前バス停下車
http://www.waseda.jp/jp/campus/nishiwaseda.html
参加費：無料
参加登録：1 月 18 日（金）までに、以下の web ページよりお願い致します。
http://www.cms-initiative.jp/ja/events/2011events_TCCI/130128IWMPPNMS

このワークショップでは、米国 ANL 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皆様にご講演頂きます。

オーガナイザーである関野先生の狙いは、「分子科学の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. Jeff Hammond, Assistant Computational Scientist, ANL Dr. Dmitri G. Fedorov, 産総研ナノシステム研究部門主任研究員
小林正人博士、早稲田大学高等研究所助教
稲富雄一博士、九州大学情報基盤研究開発センター学術研究員(特任准教授)
安藤嘉倫博士、名古屋大学大学院工学研究科研究員

貴重な機会ですので、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 Massively Parallel Programming Now in Molecular Science

Date: Monday, January 28th, 2013
Venue: Main Conference Room, Ground Floor, 55N Bldg., Nishi-Waseda Campus, Waseda University, Tokyo.

3-4-1, Okubo, Shinjuku-ku, Tokyo 169-8555, Japan http://www.waseda.jp/eng/campus/map03.html <- ACCESS

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.
Backed by Waseda Institute for Advanced Study.

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.

Contact: Hiedo Sekino, sekino@tut.jp, Kazuya Ishimura,
ishimura@ims.ac.jp

Program
1. International session chaired by Dr. Kazuya Ishimura, IMS
10:20－10:25 (TUT) Prof. Hideo Sekino Opening remarks
10:25－10:30 (Univ. of Tokyo/IMS) Prof. Kazuo Takatsuka Opening remarks
10:30－11:30 (ANL) Dr. Jeff Hammond "Algorithms and Software for Quantum Chemistry at Petascale and Beyond"
11:30－12:00 (AIST) Dr. Dmitri G. Fedorov "Parallel implementationof the fragment molecular orbital method in GAMESS"
12:00－13:30 lunch break

2. Japan session chaired by Dr. Takehiro Yonehara, Univ. of Tokyo
13:30－14:00 (Waseda Univ.) Dr. Masato Kobayashi "Divide-and-conquer quantum chemistry program in GAMESS:Implementation and application"
14:00－14:30 (Kyushu Univ.) Dr. Yuichi Inadomi "Performance improvement
of FMO program for effective massively parallel execution on K-computer"
14:30－15:00 (Nagoya Univ.) Dr. Yoshimichi Ando "Development of
massively parallel molecular dynamics simulation software including long-range Coulomb force calculation on K computer"

15:00－15:20 coffee break

3. Discussion session chaired by Prof. Hideo Sekino (TUT)
15:20－16:00 Free Discussion
16:00－16:10 (TUT) Prof. Hideo Sekino　Closing remarks

* This program would be changed without a notice.

Profiles of Invited Speakers:
Dr. Jeff Hammond, Assistant Computational Scientist, Leadership Computing Facility, Argonne National Laboratory. Dr. Hammond develops novel algorithms and software for quantum chemistry applications and statistical sampling (of molecular ensembles). He developed the coupled-cluster response property module in NWChem (www.nwchem-sw.org) and has contributed to many other software projects, including MADNESS and Global Arrays. His current research involves programming models and application porting for Blue Gene/Q, one-sided communication on supercomputers, and optimizing NWChem for heterogeneous architectures.
　See https://wiki.alcf.anl.gov/parts/index.php/User:Jhammond for more information.

Dr. Dmitri G. Fedorov (senior research scientist, NRI, AIST, Japan) develops the FMO method for quantum-mechanical calculations of large molecular systems on massively parallel computers.

Dr. Masato Kobayashi, Assistant Professor, Waseda Institute for Advanced Study, Waseda University: Dr. Kobayashi is developing the linear-scaling qunatum chemical methods based on the divide-and-conquer method.
　See https://sites.google.com/site/chemistmasatokobayashi/ for more information.

Dr. Yuichi Inadomi, Post-doctoral Fellow, Research Institute for Information Technology, Kyushu University. Dr. Inadomi is working on
OpenFMO quantum chemistry program for K-computer.

Dr. Yoshimichi Andoh: Research Associate, Dept. of Applied Chemistry, Nagoya University. Dr. Andoh is working on the highly parallelized molecular dynamics simulation program optimized for the K computer.

"Algorithms and Software for Quantum Chemistry at Petascale and Beyond"
by Dr. Jeff Hammond

Abstract: Quantum chemistry faces many challenges on petascale supercomputers due to a changing landscape of processing architecture and the enormous scale of these systems. Over the past 10 years, systems have grown in size by a factor of a thousand in some cases and within a node there is significantly more parallelism. This talk will start by considering the NWChem software package and it's coupled-cluster (CC) codes, which are scalable to 100,000 cores on Cray supercomputers

and have rich scientific capability. From here, we consider three research projects to develop new coupled-cluster algorithms for modern supercomputers. The first of these is the development of CC for GPUs, where we observe approximately an order-of-magnitude speedup with respect to existing codes for CCSD at workstation scale. The second project is a complete redesign of tensor contraction algorithms using novel techniques from dense linear algebra. This completely eliminates load-imbalance and allows for topology-aware mapping on systems with torus interconnects (e.g. Blue Gene and ""K""). Finally, we demonstrate how inspector-executor techniques can be used to eliminate dynamic task scheduling in NWChem CC codes, which can lead to a substantial reduction in time-to-solution.

This work has been done in collaboration with Eugene DePrince (Georgia Tech), Edgar Solomonik (Berkeley), Devin Matthews (Texas), David Ozog (Oregon), Pavan Balaji (Argonne) and Jim Dinan (Argonne).