Center for Nanoscale Systems
Department of Chemistry and Chemical Biology
Initiative in Innovative Computing
RIKEN

Organizers:

Alan Aspuru-Guzik, Harvard University
Toshiaki Iitaka, RIKEN
Michael Stopa, Harvard University/RIKEN

SYNOPSIS: Graphical Processing Units (or GPUs) are dedicated graphics devices whose ancestors date to the 1980s and the graphical chips at the heart of Atari Game consoles and others. In order to render computer graphics, GPUs are optimized to perform various linear algebra functions, such as matrix multiplication with a high degree of parallelism. Recently it has been discovered that the highly parallel functionality of GPUs makes them potentially useful for accelerating various kinds of scientific calculation and simulation. This meeting combines scientists from RIKEN (The Institute for Physical and Chemical Research, Japan) and Harvard University who have been at the forefront of bringing GPU technology to scientific computation.

Conference Schedule (note location switches between Mallinckrodt Hall and LISE building)

- Monday: breakfast, registration and meeting (all day Monday): Division Room, Mallinckrodt Hall, Chemistry Building (12 Oxford Street)

- Monday lunch LISE Building, (11 Oxford St.) room 303

- Monday afternoon, meeting resumes in Mallinckrodt Division Room.

- Tuesday meeting (including breakfast and lunch) will be in the LISE Building, (11 Oxford St.) Room 303 (3rd floor).

Monday, March 10

7:30 - Continental Breakfast and Registration
Location: Harvard University Mallinckrodt Hall, 12 Oxford Street, Division Room (102), Chemistry and Chemical Biology - Registration in main lobby.

8:30am - Welcome Remarks and Organization
Alan Aspuru-Guzik, Harvard
Michael Stopa, Harvard
Toshi Iitaka, RIKEN

9:00am - Introduction to GPU Computing - Leslie Vogt, Alan Aspuru-Guzik Group, Harvard

9:30am - RIKEN's Next-Generation Supercomputer Project - Makoto Taiji, RIKEN

10:00am - RIKEN's Contribution to Scientific Computing with GPU - Toshi Iitaka, RIKEN

10:30am - Coffee Break

11:00am - CHARMM and GPU Computing - Martin Karplus, Harvard

11:30am - Accelerating Molecular Dynamics Simulations with a GPU and a PS3 - Tetsu Narumi, RIKEN

12:00pm - Large-Scale GPU Cluster for Many-Body Simulations - Tsuyoshi Hamada, RIKEN

12:30pm - Lunch and Discussion about Molecular Dynamics - College of Chemistry and Chemical Biology - Location: LISE Building, (11 Oxford St.) outside room 303

1:45pm - Q-Chem Software and Modern DFT Algorithms - Jing Kong, Q-Chem, Inc

2:15pm - Acclerating Correlated Quantum Chemistry Calculations Using GPGPU - Alan Aspuru-Guzik, Harvard

2:45pm - Multiscale Simulations for Complex Physical Systems - Efthmios Kaxiras, Harvard

3:15pm - Novel Linear-Algebraic Algorithm and Large-Scale Electronic Structure - Takeo Hoshi, RIKEN

4:45pm - Reception at Initiative in Innovative Computing

6:00pm - Interested people can go to dinner together in the Harvard Square area

Tuesday, March 11

8:00am - Continental Breakfast
Location: Laboratory for Integrated Science and Engineering (LISE building), 11 Oxford St., 3rd floor room 303

9:00am - The Murchison Wide-field Array - Frontiers of Radio Cosmology and Heliospheric Science - Lincoln Greenhill, Harvard

9:30am - Lab Trials of GPUs in MWA Stream Processing - Kevin Dale, Harvard

10:00am - GPUs in MWA Engineering Fieldwork Today and Full-scale Science Deployment Tomorrow – Randall Wayth, Harvard

10:30am - Coffee Break

11:00am - The Connectome Project and GPGPU - Hanspeter Pfister, Harvard

11:30am - Hardware Acceleration for Boundary Element Methods - Toru Takahashi, RIKEN

12:00pm - SETE Electronic Structure of Semiconductor Heterostructures - Michael Stopa, Harvard

12:30pm – Lunch
Location: LISE Building, (11 Oxford St.) outside room 303

2:00om - TBA - Miguel de Icaza, Novell, Inc

2:30pm - breakout groups for discussion in different areas (molecular dynamics, astronomy, biology, chemistry...)

Abstracts and Titles

Monday, March 10

9:00am - Introduction to GPU Computing
Leslie Vogt, Teaching Fellow in Chemistry and Chemical Biology; Research Assistant in Chemistry and Chemical Biology, Harvard University

9:30am - RIKEN's Next-Generation Supercomputer Project
Makoto Taiji, RIKEN

We are currently developing the next-generation supercomputer, which will have performance of 10 PFLOPS for general use. As its applications, we also run the next-generation integrated life science project. In the talk, I will give brief introduction of these projects, including other HPC activities - the MDGRAPE project and GPU computing in RIKEN.

10:00am - RIKEN's Contribution to Scientific Computing with GPU
Toshiaki Iitaka, RIKEN

RIKEN has a long history of developing "special purpose computer", MD-GRAPE's, which solve molecular dynamics problems much faster than the fastest supercomputers in the world. Dr. Narumi, Dr. Taiji and Dr. Ebisuzaki are the main players of these projects. In the culture of MD-GRAPE, I learned a lot from them and realized, around 2004, GPU's similarity to MD-GRAPE, and its possibility of taking place of MD-GRAPE. Since then I implemented the core parts of molecular dynamics, astronomical n-body problem (with Dr. Hamada), boundary element methods (with Dr. Takahashi), fluid dynamics [1], quantum many body problem [2] ("Heisenberg Machine") and quantum molecular dynamics [3] (with Dr.Hoshi) to GPU machines by using Cg or CUDA. In this talk, I will make emphasis on the last two problems, where multiplication of the Hamiltonian matrix on the quantum state vector plays the crucial role in computation.

[1] http://accc.RIKEN.jp/HPC/HimenoBMT/contest_e.html
[2] T.Iitaka and T.Ebisuzaki, Phys. Rev. Lett. 90, 047203 (2003). http://www.iitaka.org/
[3] T.Fujiwara, T.Hoshi and S.Yamamoto, http://arxiv.org/abs/0802.0748

11:00am - CHARMM and GPU Computing
Martin Karplus, Theodore William Richards Professor of Chemistry, Emeritus, Harvard University

11:30am - Accelerating Molecular Dynamics Simulations with a GPU and a PS3
Tetsu Narumi, RIKEN

Classical Molecular Dynamics (MD) simulations can be accelerated by special-purpose computers or game consoles, such as a GPU or a Playstation 3 (PS3). We have used an MDGRAPE-3 special-purpose computer for CHARMM and AMBER. Recently, we also used a GPU or a PS3 for simple MD simulations. These machines have high performance, performance by cost, and performance by power compared with usual general-purpose computers. Difficulties in using them include how to satisfy required accuracy with single precision operations, how to use many cores in parallel, and etc. Ideas used for the MDGRAPE-3 are useful for solving these difficulties.

12:00pm - Large-Scale GPU Cluster for Many-Body Simulations
Tsuyoshi Hamada, RIKEN

Astronomical many-body simulations have been widely used to investigate the formation and evolution of various astronomical systems, such as planetary systems, globular clusters, galaxies, clusters of galaxies, and large-scale structures of the universe. In such simulations, we treat planetesimals, stars, or galaxies as particles interacting with each other through Newtonian gravity. We numerically evaluate interactions between the particles and advance the particles according to Newton's equation of motion. In many cases, the size of a many-body simulation is limited by the available computational resources. The calculation of the interaction between particles is usually the most expensive part of the entire calculation, and limits the number of particles we can handle. Thus, accelerating the calculation of interaction is important. We have developed the CUNBODY-1 library (CUDA NBODY library), which is the earliest implementation of C library to accelerate many-body interaction using graphics card. Using CUNBODY-1library, we can achieve a measured performance of 652 Gflop/swith single graphics card for calculation of gravitational interactions. In this talk, we present our GPU cluster system which consists of 128 graphics card and discuss the problem that should be overcome.

1:45pm - Q-Chem Software and Modern DFT Algorithms
Jing Kong, Q-Chem, Inc.

2:15pm - Acceleration of Electronic Structure Codes Using GPU: Correlated Calculations.
Alan Aspuru-Guzik, Assistant Professor of Chemistry and Chemical Biology, Harvard University

The modification of a general-purpose code for quantum mechanical calculations of molecular properties (Q-Chem) to use a graphical processing unit (GPU) is reported. A 4.3x speedup of the resolution-of-the-identity second-order Mller-Plesset perturbation theory (RI-MP2) execution time is observed in single point energy calculations of linear alkanes. The code modification is accomplished using the compute unified basic linear

algebra subprograms (CUBLAS) library for an NVIDIA Quadro FX 5600 graphics card. Furthermore, speedups of other matrix algebra based electronic structure calculations are anticipated as a result of using a similar approach. We will discuss our current work on accelerating other parts of the code, including the self-consistent loop of Q-Chem. The ultimate goal is to work with Q-Chem, Inc. to develop a production-level GPU-enabled quantum chemistry code in the very near future.

[1] J. Phys. Chem. A, ASAP Article 10.1021/jp0776762 Web Release Date: January 30, 2008

2:45pm - Multiscale Simulations for Complex Physical Systems
Efthimios Kaxiras, Gordon McKay Professor of Applied Physics and Professor of Physics, Harvard University

3:15pm - Novel Linear-Algebraic Algorithm and Large-Scale Electronic Structure Calculation
Takeo Hoshi, RIKEN

We have developed a set of theories and program code for large-scale electronic structure theory and nanomaterial process. [1]-[9] See Ref. [9] for review. As a crucial point, large-scale calculation can be realized with novel linear-algebraic algorithms, in which the one-body density matrix or the Green's function are calculated, instead of one-electron eigenstates. Moreover, the algorithms are mathematical ones and were applied also to a many-body wave function theory [8]. The calculations were carried out with up to 107 atoms and/or bases. Now the code is being reorganized as a simulation package, called 'ELSES' (Extra Large Scale Electronic Structure calculation) [10]. My talk is devoted to an overview of our project and the possibility of further improvement in performance.

[1] Full reference list, MD results (movies);http://fujimac.t.utokyo.ac.jp/lses/index_e.html
[2] T.Hoshi and T. Fujiwara, J. Phys. Soc. Jpn, vol. 69, No.12, pp3773-3776 (2000)T.Hoshi and T. Fujiwara, J. Phys. Soc. Jpn, vol. 72, No.10, pp.2429-2432(2003)
[3] R. Takayama, T. Hoshi, T. Fujiwara, J. Phys. Soc. Jpn, vol. 73,No.6, pp.1519-1524 (2004)
[4] T. Hoshi, Y. Iguchi, and T. Fujiwara, Phys. Rev. B72, 075323 (2005)
[5] R. Takayama, T. Hoshi, T. Sogabe, S.-L. Zhang, and T. FujiwaraPhys. Rev. B 73, 165108, pp.1-9 (2006)
[6] T. Hoshi, T. Fujiwara, J. Phys.: Condens. Matter 18 10787-10802 (2006)
[7] Y. Iguchi, T. Hoshi, T. FujiwaraPhys. Rev. Lett. 99, 125507, pp1-4 (2007)
[8] S. Yamamoto, T. Fujiwara and Y. Hatsugai, Phys. Rev. B 76, 165114（2007);S. Yamamoto, T. Sogabe, T. Hoshi, S-L. Zhang, T. Fujiwara, http://arxiv.org/abs/0802.2790
[9] T. Fujiwara, T. Hoshi and S. Yamamoto, http://arxiv.org/abs/0802.0748
[10]http://www.elses.jp/

Tuesday, March 11

9:00am - Towards a GPU Cluster for the MWA
Kevin Dale, Graduate Student, School of Engineering and Applied Science, Harvard University

9:30am - TBA
Lincoln Greenhill, Research Fellow, Senior; Lecturer on Astronomy; Associate of the Harvard College Observatory, Harvard University

10:00am - The Connectome Project and GPGPU
Hanspeter Pfister, Gordon McKay Professor of the Practice of Computer Science; Director of Visual Computing in the Initiative in Innovative Computing

1:00am - TBA
Randall Wayth, Associate of the Harvard College Observatory, Harvard

11:30am - Hardware Acceleration for Boundary Element Methods
Toru Takahashi, RIKEN

Since the Boundary Element Method (BEM) is highly time-consuming, it is not a practical method to solve large-scale boundary value problems without using fast algorithms and/or high-performance computing techniques. As such a technique, I have investigated how to run a BEM code on the special-purpose computer MDGRAPE-2 and commercially available graphic devices (GPU). This will be reviewed in my talk. In addition, I will talk about an ongoing study on the CUDA-based GPGPU for BEM.

12:00pm - SETE Electronic Structure of Semiconductor Heterostructures
Michael Stopa, Researcher, Phys/Med/Basic Science, Harvard University

Electronic structure problems solved on real space meshes frequently make use of sparse matrix manipulations for the solution, for example, of Poisson's Equation. Linear algebra operations of GPUs that are highly parallelized are, conversely, often best optimized for dense matrix operations. I will review the current state of the art of GPU programming for sparse problems and discuss the SETE electronic structure code in this context

2:00pm – TBA - Miguel de Icaza, Novell, Inc.