



**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 - Accelerating Correlated Quantum Chemistry Calculations Using GPGPU - Alan Aspuru-Guzik, Harvard

2:45pm - Multiscale Simulations for Complex Physical Systems - Efthymios 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

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

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

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.

On Monday 17, Monday

Schedule for Dr. Toshikazy Takeda, Dr. Makoto Taiji, Dr. Shigeho Noda

(host: Akira Tsuda, 617-432-0127 (office); 508-335-6790 (cell); atsuda@hsph.harvard.edu)

- Before 10:30 Breakfast meeting with DEAS people (Cambridge)
- 11:00 -11:30 Jeff Fredberg (HSPH)
- 11:30 -12:00 Xavier will show them around Jeff's lab
- 12:00 -1:00 Akira's office & lunch with Jim Butler's Japanese visitors (HSPH R^M1302)
- 1:00 - 1:50 Sam Patz (BWH) MRI imaging
- 2:00 - 2:30 Mentzer's lab (BWH) Microcirculation
- 2:30 - John Frangioni (BIDMC) NIR molecular imaging
- 3:30 - Their presentations and discussion with Akira, Jim, & Frank (HSPH R^M1302)

Dr. Takada is interested in chlorophyll and quantum chemistry.

<http://www.iop.org/EJ/abstract/1742-6596/78/1/012073>

Dr. Taiji is a computational biologist. He studies, among other things, large proteins. His home page

<http://www.yokohama.riken.jp/eng/scientist/06/index.html>.

Dr. Noda specializes in blood flow simulation, aneurysms, etc.

<http://sciencelinks.jp/j-east/article/200613/000020061306A0402298.php>.

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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-GRAPES, 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-GRAPES, I learned a lot from them and realized, around 2004, GPU's similarity to MD-GRAPES, and its possibility of taking place of MD-GRAPES. 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://accr.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-1 library, 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 'ELSESES' (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. Fujiwara Phys. 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. Fujiwara Phys. 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/>

HARVARD-RIKEN
Overall Agenda
March 9th – March 20th, 2008

Sunday, March 9	Visitors for GPU meeting arrive, check in to DoubleTree Guest Suites
Monday, March 10	HaRiken GPU Meeting, Mallinckrodt Hall (12 Oxford St.) 7:30 am breakfast/ registration.
Tuesday, March 11	GPU Meeting continues in LISE building, (11 Oxford St.).
Wednesday, March 12	Iitaka-san and hoshi-san continue visit at Harvard (Kaxiras and Aspuru-Guzik groups
Saturday, March 15	Second phase of Riken visitors arrive
Sunday, March 16	Walking tour of Harvard with Stopa and dining out together in Harvard Square
Monday, March 17	Guest assembly, LISE Building (11 Oxford St.). Guests go to hosts laboratories
Tuesday, March 18	visit with hosts continues
Wednesday March 19	guests and hosts meet to plan fall Riken-Harvard workshop. Felice Frankel presentation.
Thursday, March 20	visit ends. Farewell.



HARVARD BIOS

GPU PARTICIPANTS

Alan Aspuru-Guzik, Harvard University, Chemistry

Alan Aspuru-Guzik researches electronic structure methods. In particular, he develops methods for emulating quantum systems such as molecules on quantum computers. He is also working on the development of novel density functional theories and the study of renewable energy materials.

Aspuru-Guzik was a postdoctoral researcher at the Head-Gordon group at UC Berkeley from January 2005 to May 2006. He received his Ph.D. in physical chemistry from University of California, Berkeley in December of 2004. He worked in the Lester group on quantum Monte Carlo (QMC) methods for the solution of the Schrödinger equation.

Amongst other projects, he developed a sparse linear-scaling QMC method for the study of large chemical systems. As an undergraduate, he was selected as the top student of Chemistry at the Universidad Nacional Autónoma de México. In 1994, he represented México at the International Chemistry Olympiad, held in Oslo, Norway. Aspuru-Guzik was also the lead-developer of the Zori electronic structure program.

Kevin Dale, Harvard University, SEAS, graduate student with Hanspeter Pfister

Kevin Dale is a graduate student in computer science at Harvard under Professor Hanspeter Pfister. His research interests are in computer graphics, particularly data-driven techniques, computational photography, and graphics hardware. He completed his Master's at the University of Virginia under David Luebke and received his B.S. in Computer Science from the University of North Carolina. He interned at HP Labs during the summer of 2006 and at IBM from 2003-2004.

Lincoln Greenhill, Harvard University, Astronomy

Dr. Lincoln Greenhill, Senior Research Fellow, Faculty of Arts and Sciences
Lincoln Greenhill is a Senior Fellow in the Faculty of Arts and Sciences at Harvard University and Radio Astronomer at the Smithsonian Astrophysical Observatory. He received an S.B. degree from MIT in 1984 (physics) and a Ph.D. from Harvard in 1990 (astronomy). From 1990 to 1992, Dr. Greenhill was a Fellow with the Miller Institute for Basic Research in Science at the University of California at Berkeley, working with Charles Townes. Today, Dr. Greenhill's interests include cosmology and the early universe, super-massive black holes at the centers of galaxies, and formation processes of high-mass stars in our own galaxy. He leads the group developing a high-speed, real-

time, data processing pipeline for the international Murchison Wide-field Array (MWA). The MWA is a facility under construction in Western Australia for detection of radio emission from the Hydrogen that filled the early universe soon after the Big Bang, as well as study of the Sun and heliosphere, the Earth's ionosphere, and local space weather. The flood of data that must be processed in real-time and on-site by the MWA pipeline places this next-generation facility on frontiers of both astronomical and computing research.

Jing Kong, Q-Chem, Inc.

CEO & Chief Scientist of Q-Chem, Inc.

Dr. Jing Kong obtained his Ph.D. degree in Theoretical Chemistry from Dalhousie University in 1996. Previously, he obtained B.S. from Nanjing University, and M.S. from Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences. At Q-Chem Inc., he executes business strategies and manages daily business and technical operations under the leadership of Prof. Gill, Prof. Head-Gordon and the board.

He also leads a group of scientists on some innovative research. The main focus of Q-Chem research team is to extend the capacity of the quantum chemistry models to the research areas where the first-principle calculations are desirable but not yet practical. He has been very fortunate to work with some very talented quantum chemists. The research is generously supported by SBIR grants (Small Business Innovative Research).

Martin Karplus, Theodore William Richards Professor of Chemistry, Emeritus, Harvard University

Martin Karplus is an Austrian-born U.S. theoretical chemist is also Director of the Biophysical Chemistry Laboratory, a joint laboratory of CNRS and Universite Louis Pasteur in Strasbourg, France. He received a B.A. from Harvard University in 1950, and a Ph.D. from California Institute of Technology in 1953 while working with Linus Pauling. He was an NSF Postdoctoral Fellow at Oxford University (1953-55) where he worked with Charles Coulson.

Martin Karplus has made significant contributions to many fields in physical chemistry, including the nuclear magnetic resonance spectroscopy, chemical dynamics, quantum chemistry, and most notably, the molecular dynamics simulations of biological macromolecules. Karplus has made varied contributions to nuclear magnetic resonance spectroscopy, particularly to the understanding of nuclear spin-spin coupling and electron spin resonance spectroscopy. The Karplus equation describing the correlation between coupling constants and backbone torsional angles in protein nuclear magnetic resonance spectroscopy is named after him. With Andrew McCammon and Bruce Gelin, he published the first molecular dynamics simulation of a Bovine Pancreatic Trypsin Inhibitor BPTI.

His current research is concerned primarily with the properties of molecules of biological interest. His group originated and currently coordinates the development of the CHARMM program for molecular dynamics simulations. He is a member of the International Academy of Quantum Molecular Science. He has supervised over 200

graduate students and postdoctoral researchers in his long career (since 1955) in the University of Illinois, Columbia University, and Harvard University.

Efthimios 'Tim' Kaxiras, Harvard University, Physics

Since the 1980s, physicists have developed a theoretical framework for studying the nature and properties of solids, using a quantum mechanical description that does not rely on adjustable parameters. Advances in computational power have made it possible to use this approach for describing realistic solids, including their defects, with remarkable accuracy - even to predict properties of novel materials not yet synthesized in the laboratory. Kaxiras and his coworkers use these theoretical methods to study the properties of solids, surfaces, and interfaces. They also employ them to explain the microscopic reasons for ductile or brittle behavior. In recent work, they have applied them, in combination with other techniques, to semiconductor crystal growth and other nonequilibrium phenomena. Kaxiras has used this approach to unravel the features of complex dynamical phenomena such as surfactant-mediated hetero-epitaxial growth of semiconductors. Their analysis correctly reproduces growth instabilities, including the transition from layer-by-layer to island growth, and more detailed microscopic features, such as the fractal nature of islands and their size distribution during growth.

Miguel de Icaza, Novell, Inc.

Miguel is currently the Vice President of Developer Platforms at Novell and best known for starting projects like GNOME, Gnumeric and Mono.

Miguel is a free software programmer from Mexico, best known for spawning the GNOME and Mono projects. He started writing free software in 1992 and created the GNOME project in August 1997 with Federico Mena Quintero, to create a completely free desktop environment and component model for Linux and other Unix-like operating systems. Earlier, De Icaza had worked on the Midnight Commander file manager, as well as the Linux kernel. He was also the creator of the spreadsheet program Gnumeric.

In 1999, de Icaza co-founded Helix Code, a GNOME-oriented free software company with Nat Friedman, and employed a large number of other GNOME hackers. In 2001, Helix Code, now renamed to Ximian, announced the Mono Project, a project led by Miguel. In August 2003, Ximian was acquired by Novell. De Icaza is currently the Vice President of Developer Platforms at Novell.

Miguel de Icaza has received the Free Software Foundation 1999 Free Software Award, the MIT Technology Review Innovator of the Year Award 1999, and was named one of Time Magazine's 100 innovators for the new century in September 2000.

Hanspeter Pfister, Harvard University, Connectome Project and GPGPU

Hanspeter Pfister's research lies at the intersection of visualization, computer graphics, and computer vision. It spans a wide range of topics, including scientific visualization, computational photography, point-based graphics, appearance modeling, 3D television, and face recognition.

He received his Ph.D. in Computer Science in 1996 from the State University of New York at Stony Brook and his M.S. in Electrical Engineering from the Swiss Federal Institute of Technology (ETH) Zurich, Switzerland, in 1991.

Prior to his appointment at Harvard, Pfister worked for 11 years at Mitsubishi Electric Research Laboratories (MERL) where he was most recently Associate Director and Senior Research Scientist. He was the chief architect of VolumePro, Mitsubishi Electric's award-winning real-time volume rendering hardware for PCs. During his time at MERL he made many pioneering contributions that lead to over 40 US patents and 58 peer-reviewed publications, including 14 ACM SIGGRAPH papers, the premier forum in Computer Graphics. He is co-editor of the first textbook on Point-Based Computer Graphics, published by Elsevier in 2007, and of the 2006 NIH/NSF Visualization Research Challenges Report.

Pfister is chair of the IEEE Visualization and Graphics Technical Committee, Executive Committee Member of the IEEE Computer Society Technical Activities Board, Member of the IEEE Computer Society Conferences and Tutorials Board.

Pfister's awards include a U.S. Government Fulbright Grant, Switzerland, 1991; Swiss Academy of Technical Sciences Grant, 1992; ABB Switzerland Research Grant, 1991 and 1992; The Jack Heller Award, SUNY Stony Brook, 1994; Mitsubishi Electric Presidents Award, 2000; Distinguished Teaching Performance Award, Harvard Extension School, 2002-2004; Harvard Extension School Dean's Thesis Prize for ALM thesis supervised in 2005 and 2007.

Pfister has been teaching introductory and advanced graphics courses at the Harvard Extension School since 1999. He has taught courses and served on the papers committees of all major visualization and graphics conferences, including ACM SIGGRAPH, IEEE Visualization, Eurographics, Pacific Graphics, and many others. He served as the conference chair of IEEE Visualization in 2002, has been the co-organizer of various international symposia, and is serving on the editorial boards of various journals. He is a senior member of the IEEE Computer Society and member of ACM, ACM SIGGRAPH, and the Eurographics Association.

Michael Stopa, Senior Research Scientist and Director of National Nanotechnology Infrastructure Network Computation Project

Dr. Michael Stopa received his Ph.D. in Physics from the University of Maryland, studying under Dr. Sankar Das Sarma. His dissertation concerned the electronic structure, optical and transport properties of lower dimensional systems, particularly semiconductor quantum wells and shallow donor impurities. Dr. Stopa's subsequent research career included two years at NTT Basic Research Laboratories in Musashino, Tokyo in a group headed by Dr. Seigo Tarucha. Following this, he spent six years as a senior theorist at Riken, The Institute of Physical and Chemical Research, in Wako-Shi, Japan. From there Dr. Stopa was recruited by the Walter Schottky Institute to head a Sonderforschungsbereich (special research initiative) on simulation of transport through lower dimensional electronic devices, such as quantum dots and quantum wires. He returned to Japan in the year 2000 to join Seigo Tarucha again in the mesoscopic



PROGRAMS

CENTER FOR NANOSCALE SYSTEMS

The Center for Nanoscale Systems (CNS) is a part of Harvard University's Faculty of Arts and Sciences (FAS), and resides in the new Laboratory for Integrated Science and Engineering (LISE).

MISSION:

The scientific focus is on how nanoscale components can be integrated into large and complex interacting systems. Studying very small structures and how their behavior differs from macroscopic objects is only part of the story.

CNS also investigates how systems emerge, how they can be built, and how they behave. CNS is a member of the National Science Foundation's National Nanotechnology Infrastructure Network (NNIN) initiative to create a national network of world-class facilities available to all researchers.

BACKGROUND:

CNS was created by FAS in 1999 to assist and support the research community of Harvard University researchers and collaborators. The inclusion of CNS in the National Nanotechnology Infrastructure Network (NNIN) in 2004 has expanded that function to include any and all other members of the larger research community both local and national, academic and non-academic who conduct research in any aspect of the large and growing field of nanoscale science.

CNS accomplishes this mission by purchasing, operating and maintaining large, centralized scientific facilities for use by users. CNS also provides training, and assistance to users to ensure that the next generation of scientists has the knowledge to answer the questions being raised by the research of today. Development of new advanced facilities for the imaging and fabrication of nanoscale structures is also a high priority for CNS.

While operating user facilities is a large component of CNS' operation, it is not the only contribution of the Center to the scientific community of Harvard and beyond. For example, CNS hosts seminars and provides seminar support to Harvard faculty members; has Seed Money and Visiting Scientist Programs to financially support faculty research efforts; provides cost-sharing support to facilitate the acquisition of new equipment facilities; hosts NSF Research Experience for Undergraduates (REU) students; and has CNS technical staff members who teach and guest lecture in Harvard classes.



PROGRAMS

THE NATIONAL NANOTECHNOLOGY INFRASTRUCTURE NETWORK

The **National Nanotechnology Infrastructure Network (NNIN)** is an integrated networked partnership of user facilities, supported by the National Science Foundation, serving the needs of nanoscale science, engineering and technology.

The mission of the **National Nanotechnology Infrastructure Network** is to enable rapid advancements in science, engineering and technology at the nano-scale by efficient access to nanotechnology infrastructure. We provide shared open, geographically diverse laboratories, each with specific areas of technical excellence, and provide fabrication, synthesis, characterization, and integration resources to build structures, devices, and systems from atomic to complex large-scales. Our users belong to diverse areas: astronomy, plant pathology, materials science, physics, chemistry, life-sciences, various branches of engineering, etc., and come from academe, national laboratories, and industry.

THE NATIONAL NANOTECHNOLOGY INFRASTRUCTURE NETWORK COMPUTATION PROJECT (NNIN/C)

NNIN/C is the computational wing of NNIN. The goals and strategies of NNIN/C are:

- Assemble and create a wide suite of *robust* software that addresses critical issues related to the physical, chemical, and biological properties of artificial and natural nanoscale structures.
 - Maintain and, where necessary, *modify* these simulations to address a broad range of research problems.
 - Provide strong technical support and thorough *instruction* on the software tools so that even novice users can rapidly develop solutions to their own unique research problems.
 - Conduct hands-on workshops and conferences to further the high performance computation literacy of the research community thereby enabling wider utility of NNIN/C's software resources.
 - Recruit computational scientists whose computer codes are potentially of use to the community beyond the researcher's own group and assist these scientists in making their codes user-friendly and broadly accessible.
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PROGRAMS

INITIATIVE IN INNOVATIVE COMPUTING

The Initiative in Innovative Computing (IIC) is an interdisciplinary research and development center at Harvard dedicated to using innovative computing tools to accelerate discovery across all of the scientific disciplines. The IIC's researchers work in close collaboration with scientists and engineers in other fields, fostering a two-way collaborative flow of ideas and inventions between basic science and computer science, academia and industry, professional staff and faculty, teachers and students. The IIC trains the next generation of creative and computationally capable scientists, and communicates with the public at large about the value of computing in science and the science it enables.

The IIC enables science that would not be possible today without the innovative use of computational technology. The IIC takes a project-focused approach, addressing problems that are insoluble in the near term without direct collaboration between researchers in computation and researchers in domain science disciplines. IIC projects address challenges raised by the need to handle and understand data sets that are literally billions of times larger than scientists are used to now, and by the need to run computer simulations of processes as complex as blood flow in the human body or the formation and evolution of structure in the Universe.

Many of the challenges faced by the scientists participating in IIC projects are nearly identical between fields. For example, the IIC's Astronomical Medicine collaboration involves researchers from both the extensive medical imaging community associated with Harvard Medical School and the Harvard-Smithsonian Center for Astrophysics, working together to create new solutions for viewing, analyzing, and sharing large three-dimensional images, whether CT scans, MRIs, or maps of star-forming regions or the infant Universe. The team's results are being shared in scientific journals, and the software produced is made freely available by the IIC. The software will be used by the worldwide medical imaging and astronomical imaging communities as well as by researchers in other related fields, such as geology and geo-spatial demography.



PROGRAMS

HARVARD UNIVERSITY DEPARTMENT OF CHEMISTRY

The Department of Chemistry and Chemical Biology offers a program leading to the degree of Doctor of Philosophy in Chemistry, with research and training opportunities in organic, inorganic, and physical chemistry, and in chemical biology. An interdepartmental Ph.D. program in Chemical Physics is also available.

Thesis research becomes the student's chief concern following an initial period of course work, teaching, and sampling research opportunities through our laboratory rotation system. Students' own interests and those of their faculty supervisor(s) guide the direction of the doctoral studies. The department's interactive and supportive social structure is a key element for promoting a high quality-of-life while achieving a high level of success.

Science in the 21st century is rich with opportunity and challenge. Our pillars for success in this complex world are all tied to interactions -- between people, and between disciplines. By building both strong interpersonal connections between our students and faculty, and effective bridges between disciplines, the entering graduate student at Harvard can thrive at the frontiers of research in the chemical and life sciences.

RESEARCH FACILITIES

The Chemical Laboratories of Harvard University are the major part of the Cabot Sciences Complex. The 278,000 sq. ft. of modern research laboratories offered by the Department are housed in four buildings, Edward Mallinckrodt Chemical Laboratory, James Bryant Conant Laboratory, Converse Memorial Laboratory, and the new Naito Laboratory. These buildings are conveniently located in a group with the Fairchild Laboratory of Biochemistry and Molecular Biology and with the Hoffman Geological Laboratories. Undergraduate instruction for Harvard College is conducted in the adjacent Cabot Science Center. Nearby are the Biological Laboratories, the Division of Engineering and Applied Sciences, and the Physics Laboratories.

Participant Pairings
 Harvard-RIKEN Visit
 March 10-21, 2008

GPU Meeting Participants	Marcus, Yacoby, Westervelt Group Visitors	Kaxiras, Aspuru-Guzik Group Visitors	Tsuda Group Visitors
Tetsu NARUMI	Keiji ONO	Toshiaki IITAKA	Toshikazu TAKADA
Tsuyoshi HAMADA	Yuiko KAWANO	Takeo HOSHI	Makoto TAJI
Toru TAKAHASHI	Takahiro MORIMOTO	Seiji YUNOKI	Shigeho NODA
Toshiaki IITAKA	Taro YAMADA		
Takeo HOSHI			
Makoto TAJI			



CONTACTS

HARVARD CONTACTS:

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Cell: 617-699-9258

Alan Aspuru-Guzik

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April Edrington

Office: 617-496-8740

Cell: 617-692-0730

TAXIS:

Cambridge Checker Cab 617-497-1500

Ambassador Brattle Cab 617-492-1100

Cambridge Cab 617-497-6100

Hello Taxi 617-734-1111

Star Taxi of Cambridge 617-876-8888

HOTEL:

DoubleTree Hotel 617-783-0090

DoubleTree Hotel Shuttle 617-562-4104**

**The shuttle service is complimentary for guests, but reservations must be made in advance for pick up and drop off. Please contact guest services (number listed above) to arrange for transportation.

Drop off/Pick up Times and Locations.

Doubletree Guest Suites can provide transportation to the following destinations:

Copley Square: On the corner of Stuart and Dartmouth Street. (By Wainwright Bank across from Star Bucks coffee.) - **Copley Station-Green Line Back Bay-Orange Line/AMTRAK**

Boston Common/Theater District: On the corner of Boylston and Charles Streets near the "Trolley Stop" - **Boylston Station-Green Line**

Quincy Market/Faneuil Hall (Weekends only): Corner of Commercial and State Street in front of the "Black Rose Pub" - **Aquarium Station-Blue Line**

Aquarium: Milk Street in front of the Aquarium - **Aquarium Station-Blue Line**

Harvard Square: 14 JFK Street in front of Z SQUARE restaurant - **Harvard Square Station-Red Line**

RESERVATIONS ARE REQUIRED FOR PICK-UPS AND DROP-OFFS

Leaves	Arrival/Pick-up Times					
	Doubletree Guest Suites	Copley Square	Boston Common	N.E Aquarium	Quincy Market	
Monday Through Friday	9:00am	9:10am	9:15am	9:25am	N/A	
	10:00am	10:10am	10:15am	10:25am	N/A	
	11:00am	11:10am	11:15am	11:25am	N/A	
	3:00pm	3:10pm	3:15pm	3:25pm	N/A	
	4:00pm	4:10pm	4:15pm	4:25pm	N/A	
	5:00pm	5:10pm	N/A	N/A	N/A	
	6:00pm	6:10pm	6:15pm	6:25pm	N/A	
	7:00pm	7:10pm	7:15pm	7:25pm	N/A	
	8:00pm	8:10pm	8:15pm	8:25pm	N/A	
	9:00pm	9:10pm	9:15pm	9:25pm	N/A	
Leaves	Arrival/Pick-up Times					
Saturday	9:00am	9:10am	9:15am	9:25am	9:30am	
	10:00am	10:10am	10:15am	10:25am	10:30am	
	11:00am	11:10am	11:15am	11:25am	11:30am	
	12:00pm	12:10pm	12:15am	12:25pm	12:30pm	
	2:00pm	2:10pm	2:15pm	2:25pm	2:30pm	
	3:00pm	3:10pm	3:15pm	3:25pm	3:30pm	
	4:00pm	4:10pm	4:15pm	4:25pm	4:30pm	
	5:00pm	5:10pm	5:15pm	5:25pm	5:30pm	
	6:00pm	6:10pm	6:15pm	6:25pm	6:30pm	
	7:00pm	7:10pm	7:15pm	7:25pm	7:30pm	
8:00pm	8:10pm	8:15pm	8:25pm	8:30pm		
9:00pm	9:10pm	9:15pm	9:25pm	9:30pm		
Leaves	Arrival/Pick-up Times					
Sunday	9:00am	9:10am	9:15am	9:25am	9:30am	
	10:00am	10:10am	10:15am	10:25am	10:30am	
	11:00am	11:10am	11:15am	11:25am	11:30am	
	12:00pm	12:10pm	12:15pm	12:25pm	12:30pm	
	2:00pm	2:10pm	2:15pm	2:25pm	2:30pm	
	3:00pm	3:10pm	3:15pm	3:25pm	3:30pm	
	4:00pm	4:10pm	4:15pm	4:25pm	4:30pm	
	Leaves	Arrival/Pickup Times				
	Harvard Square (Monday - Saturday)	9:45am	7:45pm	9:50am	7:50pm	8:45am
		10:45am	8:45pm	10:50am	8:50pm	9:45am
11:45am		9:45pm	11:50am	9:50pm	10:45am	
(12:45pm Sat only)			(12:50pm Sat only)		11:45am	
2:45pm			2:50pm		12:45pm	
(4:45pm Sat only)			(4:50pm Sat only)		2:45pm	
(5:45pm Sat only)			(5:50pm Sat only)		3:45pm	
6:45pm			6:50pm		4:45pm	
Leaves		Arrival/Pickup Times				
9:45am		7:45pm	9:50am	7:50pm	8:45am	
10:45am	8:45pm	10:50am	8:50pm	9:45am		
11:45am	9:45pm	11:50am	9:50pm	10:45am		
(12:45pm Sat only)		(12:50pm Sat only)		11:45am		
2:45pm		2:50pm		12:45pm		
(4:45pm Sat only)		(4:50pm Sat only)		2:45pm		
(5:45pm Sat only)		(5:50pm Sat only)		3:45pm		
6:45pm		6:50pm		4:45pm		



RESTAURANTS AND BOOKSTORES

HARVARD SQUARE RESTAURANT INFORMATION:

Cambridge 1

27 Church Street Cambridge , MA 02138
617-576-1111

Hours of Operation:

open 7 days 11:30 am until 1:00 am (food until midnight)

Charcoal grilled pizza, fresh salads, cold beer, great wine selection, BSA award winning design, 42" plasmas, take out available, from the owners of Miracle of Science and Audubon Circle.

Daedalus

45.5 Mt. Auburn Street Cambridge, MA 02138
www.daedalusharvardsquare.com
617-349-0071

Hours of Operation:

Lunch: 11:00 am to 4:00 pm

Dinner: 4:00 pm to 10:30 pm

Sunday Brunch: 10:00 am to 3:00 pm

Housed in a converted greenhouse, Daedalus makes good use of its two-story digs, with a separate bar and dining area on the first floor and a dark lounge area upstairs where there is another bar, couches, and tables situated under the glass roof. Sample appetizers such as crispy, tangy panseared crab cakes with chipotle aioli served over tossed greens. The menu changes seasonally, highlighting traditional dishes with interesting twists.

Henrietta's Table

The Charles Hotel, Harvard Square
One Bennett Street Cambridge, MA 02138
www.henriettastable.com
617-661-5005

Hours of Operation:

Breakfast: Mon-Fri 6:30am-11:00am; Sat. 7:00am-11:00am; Sun. 7:00am-10:30am

Lunch: Mon-Fri Noon-3:00pm, Supper: Mon-Sun 5:30pm-10:00pm
Sat. and Sun. Brunch (Reservations Recommended): Noon-3:00pm

Situated in the Charles Hotel, Henrietta's Table celebrates classic New England cooking with no-nonsense taste. That means full, robust flavors with the freshest of ingredients. Working with local organic farmers and fisherman, Executive Chef Peter Davis brings you the best of each season's offerings. "If its not in season, then its not on the menu," asserts Chef Peter Davis.

The menu offers daily and weekly specials, using the best of open market fare. Chef Davis uses organic and native ingredients from local producers throughout and beyond Massachusetts, creating an original and simple approach to classic regional cuisine. The 138-seat restaurant, whose menu includes breakfast, lunch, supper and Saturday and Sunday brunch, includes hearty favorites like Creamed Chipped Beef on Buttermilk Biscuits, Homemade Granola served with fresh berries, Cod Fish Cakes, Corned Beef on Rye, Yankee Pot Roast, Grilled Smoked Pork Rib chops with Macintosh Apple Sauce, and of course, Chocolate Bread Pudding.

Legal Sea Foods

20 University Road Cambridge , MA 02138
www.legalseafoods.com
617-491-9400

Hours of Operation:

Mon-Thu 11:00 am - 10:00 pm
Fri-Sat 11:00 am - 11:00 pm
Sunday - Noon - 10:00 pm
Sat & Sunday Brunch 10-2:30pm

For over 50 years, Legal Sea Foods has set the standard for quality and freshness in the restaurant business. We've dedicated ourselves to serving absolutely the freshest fish in the seafood industry. This means we source our own fish, handle it ourselves, prepare it and serve it, so you can enjoy the finest seafood available. Our quality assurance team oversees this process from the pier to your plate. The difference? You get the highest quality seafood, a cut above the rest. Taste the Legal Difference! The evolution of our reputation is full of interesting highlights and surprises. From lobsters to clambakes to clam chowder, we wrote the book. Read more about our heritage in the restaurant business on our web site www.legalseafoods.com

Le's

36 JFK Street Cambridge, MA 02138
617-864-4100

Le's is a regional chain of unique restaurants that specialize in Pho – the traditional fragrant noodle soup of Vietnam. The restaurant takes its name after a former Pho

restaurant in Saigon on Avenue Pasteur: reflective of the fact that Vietnam has a strong restaurant culture with a long standing historical French influence.

Affordable prices, abundance of vegetables and diet conscious society have contributed to the run away success of the Vietnamese food in general and to Pho Pasteur cuisine in particular; the timing could not have been more propitious.

OM

57 JFK Street, Entrance on Winthrop Cambridge, MA 02138

www.omrestaurant.com

617.576.2800

Hours of Operation:

Open 5pm to 1am everyday.

The perfect haven for après-work, après-university, pre-theatre or late night - The Lounge at OM - with all its transforming elements - takes Harvard Square Nightlife to new heights. While the upstairs dining room promises a calming, museum-like journey through the Far East, the swanky lower lounge kicks up the vibe with edgy design, sexy food and an eclectic scene of vibrant professionals, students and fashionistas. Sink into sumptuous leather sofas through a veil of steel mesh draperies. Gaze thoughtlessly at the mesmerizing video art or ponder more deeply the meaning of the Buddhist art. Commune with friends and colleagues over Momos & Martinis or hideaway in the Mandala Room sipping aromatherapy cocktails.

OM's cuisine is created by rising star and native New Yorker Rachel Klein, whose range and wildy creative style have made her stand out in a sea of chefs.

Small Plates

56 JFK Street Cambridge, MA 02138

www.smallplatesrestaurant.com

617-441-0056

Hours of Operation:

Sun&Mon: only Dinner 5pm - 10pm

Tue - Sat Lunch & Dinner 11am - 10pm

Reservations are recommended but not required.

Located down the sidewalk alley at 56 JFK Street, this cozy hidden bistro serves an eclectic variety of New American Tapas, Entrees & Desserts, along with distinctly paired wines, finely crafted beers & unique "cocktails". Our beautifully renovated dining room & bar will set the mood for a casual yet sophisticated dining experience.

The culinary team at Small Plates Restaurant, Tapas & Wine Bar loves introducing new & exciting tapas. We use as much sustainable, local & seasonal ingredients as possible.

Along with participating in the Northeast Family Farms Program which supports growers of organic & sustainable meats & makers of New England Cheeses, we are passionate about incorporating these ingredients & agriculture in our preparations.

Takemura Japanese Restaurant
18 Eliot Street (basement) Cambridge, MA 02138
takemurasushi@hotmail.com
617-492-6700

Hours of Operation:
Monday-Saturday -Lunch 11:30am-2:30pm
Dinner 5:00pm-11:00pm
Sunday-12:30pm-10:00pm

Takemura, meaning Bamboo Village, is a traditional Japanese restaurant offering a complete menu of sushi, sashimi, maki and your favorite Japanese entrees including agemono, teriyaki, tempura, and nabemono. We also offer traditional Korean barbeque grilled to perfection.

Z Square Cambridge
14 JFK St Cambridge, MA 02138
www.z-square.com
617-576-0101

Located steps away from the Harvard Square MBTA stop, Z Square IS Harvard Square: centrally located, hopping with energy, open day and night, smart and delicious. Whether you choose a quick meal or snack in our upper level café, or the more relaxed environment of our lower level dining room, three things are guaranteed at Z Square ...great value, creative American cuisine, and friendly service.

HARVARD SQUARE BOOKSTORES AND GIFT SHOPS:

Harvard COOP

1400 Massachusetts Avenue
Cambridge, MA 02138
617-499-2000
www.thecoop.com

Hours of Operation:
Book Building- Monday - Saturday 9
AM-10 PM
Sunday 10 AM-9 PM

Brattle/Palmer Street COOP

Monday - Saturday 9 AM-9 PM
Sunday 12 PM-7 PM

Harvard Book Store

1256 Massachusetts Avenue
Cambridge, MA 02138
617.661.1515
www.harvard.com

Hours of Operation:
Monday - Thursday 9am - 11pm
Friday - Saturday 9 am- 12am
Sunday 10am - 10pm

The Globe Corner Bookstore

90 Mount Auburn Street
Cambridge, MA 02138
617-497-6277
www.globecorner.com

Hours of Operation:
Mon - Sat 9:30 am - 9:00 pm
Sun 11:00 am - 6:00 pm

The Harvard Shop

52 J.F.K. Street
Cambridge, MA 02138
(617) 864-3000
www.theharvardshop.com

Hours of Operation:
Mon - Fri 10am - 6pm
Sat 10am - 5pm
Sun closed

Hidden Sweets

25 Brattle Street
Cambridge, MA 02138
617-497-2600
www.hiddensweets.com

Hours of Operation:
Mon - Fri 9:30am - 7pm